Competing orders and inter-layer tunnelling in cuprate superconductors: A finite temperature Landau theory

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We propose a finite temperature Landau theory that describes competing orders and interlayer tunnelling in cuprate superconductors as an important extension to a corresponding theory at zero temperature [Nature 428, 53 (2004)], where the superconducting transition temperature $T_c$ is defined in three possible ways as a function of the zero temperature order parameter. For given parameters, our theory determines $T_c$ without any ambiguity. In mono- and double-layer systems we discuss the relation between zero temperature order parameter and the associated transition temperature in the presence of competing orders, and draw a connection to the puzzling experimental fact that the pseudo-gap temperature is much higher than the corresponding energy scale near optimum doping. Applying the theory to multi-layer systems, we calculate the layer-number dependence of $T_c$. In a reasonable parameter space the result turns out to be in agreement with experiments.

The essential phenomenology of high-$T_c$ superconductors are the dome-shaped superconducting phase diagram as a function of doping $x$, and the existence of a pseudo-gap normal state. The mechanism of the novel superconductivity remains to be a challenge to researchers. The fact that superconductivity follows from doping antiferromagnetic Mott insulators and that the transition temperature depends on doping non-monotonically suggest the importance of the effects of strong correlation among the electrons, as emphasized firstly by Anderson. A theory in this line must go beyond the usual Bardeen-Cooper-Schrieffer mean field theory. However, there is also a possibility that the phenomenon is not that exotic, and a modification to the conventional theory by including a competing order may do the job. This is the attitude taken by Chakravarty, Kee and Völker, who proposed a zero temperature Landau theory to explain the general phase diagram, and in particular the copper-oxide layer-number $N$ (within a unit cell) dependence of superconducting transition temperature $T_c$ of homologous series of cuprate superconductors. The new ingredients are just a competing order, e.g., the d-density-wave (DDW), and inter-layer tunnelling that enhances superconductivity. It is therefore important to judge how robust the conclusions are against the weak points in the theory. Indeed, a few of them are debatable even within the mean field framework itself. 1) When two orders compete with each other, it is not clear whether there is still a definite connection between the zero temperature order parameter and the transition temperature even if this is the case in the absence of competition between the orders. 2) In the case of multi-layer systems, it is not clear which representative of the modulated order parameters (due to charge redistribution) is most appropriate to be related to the transition temperature, even if one assumes that the zero temperature order parameter scales with the transition temperature. 3) Moreover, the underlying motivation for a competing order to superconductivity is the fact that the normal state pseudo-gap seems to be independent of the pairing gap. From the elaborate collection of data in Ref. the pseudo-gap energy scale extrapolates to zero at a doping level of $x = 0.19$, while the pseudo-gap phenomena certainly exists at $T \geq T_c$ even at the same doping. This already indicates that the zero temperature value of the competing order, assumed to be responsible for the pseudo-gap, does not scale with the transition temperature for the pseudo-gap itself (if the pseudo-gap temperature crossover is a phase transition at all). As a compromise, the authors in Ref. defined a gap that is the root-sum-square of both order parameters, and used it to represent the pseudo-gap temperature. In general, there is no microscopic basis for this gap-combination. In a microscopic tight-binding model, the two gaps do not combine this way once the DDW bands is doped away from half filling. 4) Finally the weak points beyond the mean field theory is of course the ignorance of quantum or thermal fluctuation of the order parameters.

The last point can only be addressed by going beyond mean field theory, as in a recent spin wave analysis beyond mean field theory, as in a recent spin wave analysis of the anisotropic XY-model, which reproduces nicely the experimental $T_c(N)$ in homologous series of HBCO superconductors. In this paper, we address points 1)-3) listed above in the mean field framework under the motivation that the importance of a successful mean field theory should not be underestimated. In order to do so, we propose a finite temperature Landau theory, and determines the transition temperatures for both orders unambiguously. The structure of the rest of the paper is as follows. A finite temperature theory for the superconducting order or the DDW order alone is first proposed. We then introduce the coupling between these two orders, and discuss how competing orders in the case of mono-layer and double-layer systems, where no charge redistribution occurs, modify the relations between zero temperature order parameter and the transition temperature. By comparing the theoretical phase diagram with experiments we fix the parameter introduced in the finite
temperature theory. We also comment on point 3) raised above. Finally we extend the theory to the multi-layer systems, and calculate the \(T_c(N)\). We find that in a reasonable parameter space, the theoretical results are in agreement with experiment, and lend a support to the conjecture from the zero temperature Landau theory.

Let us begin with the simple case that the superconducting order is the only order parameter. It is known that \(2\sqrt{\psi_0/T_c} = 3.52\) in the weak coupling s-wave superconductor, where \(\psi_0\) is the zero temperature energy gap. For the case of weak coupling d-wave superconductor, this ratio is roughly 4.16. A Landau-type theory could be derived near the transition temperature from an effective microscopic model, but is a daunting task to access the zero temperature limit. We would therefore take a phenomenological attitude. We demand that the theory is of the form near \(T_c\), and while extended to lower temperatures should give a qualitative temperature dependence of the order parameter, and in particular, should yield a prescribed ratio of \(\psi_0/T_c\). Without loss of generality, we re-scale the temperature so that \(\psi_0/T_c = 1\). Under these conditions, a suitable finite temperature Landau free energy density is as follows,

\[
f_s = [\alpha(x) + \beta T^2]|\psi|^2 + \beta |\psi|^4.
\]

Henceforth we use arbitrary units, and borrow the parameterization in Ref.\[2\], with \(\alpha(x) = 10(x-0.3)\) and \(\beta = 2\). This simple model would yield \(T_c = \psi_0 = \sqrt{-\alpha(x)/\beta}\). We note that near \(T_c\) the coefficient of \(|\psi|^4\)-term can be approximated as \(2\beta T_c(T - T_c)\), which is of the desired form in a usual Landau theory.

The same consideration can be applied for the DDW order alone, with the free energy density

\[
f_D = [\alpha(x) + qbT^2]D^2 + \frac{b}{2}D^4,
\]

where \(\alpha(x) = 27(x-0.22)\), \(b = 2\), and \(q\) is a new phenomenological constant. The transition temperature for the DDW order alone is \(T_D = \sqrt{-\alpha(x)/qb} = D_0/\sqrt{q}\), where \(D_0\) is the bare zero temperature DDW order. Since we have taken the latitude to set \(\psi_0/T_c = 1\), there is no further freedom to set \(q = 1\). In fact the value of \(q\) is given by \(q = (D_0/T_D)^2/(\psi_0/T_c)^2\) independently of the temperature re-scaling. It is therefore understood that a smaller value of \(q\) means that the DDW order is more tolerant to thermal suppression, and vice versa. We take \(q\) as a new phenomenological parameter, which will be fixed by arguments below.

Let us now couple the two order parameters to form a theory describing mono-layer systems,

\[
f = \left[\alpha(x) + \beta T^2\right]|\psi|^2 + \frac{\beta}{2}|\psi|^4
\]

\[+ [\alpha(x) + qbT^2]D^2 + \frac{b}{2}D^4 + gD^2|\psi|^2, \quad (3)
\]

where \(g = 1.2\) is the coupling constant. As has been illustrated in Ref.\[2\], this theory yields zero temperature order parameters \(\psi_0(x)\) and \(D_0(x)\) that depends on the doping level \(x\) in very much the same way as the empirical \(T_c(x)\) and \(T_D(x)\), provided that one assumes that \(T_D \propto \sqrt{\psi_0^2 + D_0^2}\). Here \(T_D\) represents the pseudo-gap temperature scale. However, as has been pointed out, there is no microscopic basis for the gap-combination, and the relation between such a combined gap and the pseudo-gap temperature is not clear \textit{a priori}. In our case, the transition temperature \(T_c\) for \(\psi\) is determined by

\[
\alpha(x) + \beta T_c^2 + gD^2 = 0, \quad (4)
\]

where \(D = \sqrt{-[\alpha(x) + qbT_c^2]/\beta}\) is the value of \(D\) at \(T = T_c\). Similarly, the transition temperature \(T_D\) for \(D\) is given by

\[
\alpha(x) + bqT_D^2 + g\psi^2 = 0, \quad (5)
\]

where \(\psi = \sqrt{-[\alpha(x) + qbT_D^2]/\beta}\) is the value of \(\psi\) at \(T = T_D\). Explicit expressions for \(T_c\) and \(T_D\) are not provided because \(D \geq 0\) and \(\psi \geq 0\) have to be imposed in the above equations. We present \(T_c\) (thick solid lines) and \(T_D\) (thin solid lines) for typical cases, with \(q = 0.1, 0.6, 1, 1.5\) in Figs.1(a)-(d) respectively. We have also shown \(\psi_0\) (thick dotted lines) and \(D_0\) (thin dotted lines) in each figure for comparison to the transition temperatures. We observe that \(\psi_0/T_c = 1\) for all doping levels in Fig.1(b). However, this does not hold in the other cases. Moreover, in the same case \(D_0/T_D\) is apparently not a constant. The reason why Fig.1(b) is a special case is because the parameters satisfy \(qb - g = 0\), which gives rise to a line of critical temperatures for DDW at the zero-temperature critical doping level. For \(q < 0.6\), as in Fig.1(a), we observe a lobe-shaped DDW phase transition line near \(x = 0.198\), namely, two \(T_D\)'s at a given doping. This is best understood in the limit of \(q = 0\). Under this assumption DDW order is not suppressed by thermal effects but by the superconducting order. Near \(T_c\) the latter is small and DDW may survive. However, with lowering temperature the superconducting order increases and eventually squeeze the DDW order. With a finite but small \(q\) the qualitative behavior is the same. Because such a feature is not observed yet, it is very unlikely that \(q < 0.6\). For larger values of \(q\) as in Figs.1(c) and (d), the resulting doping dependence of \(T_c\) is very oblique, a feature that does not seem to appear in high-\(T_c\) phenomenology. Basing on these judgements we believe a reasonable regime is given by \(0.6 \leq q < 1\). We emphasize an interesting feature in Fig.1(b), where \(T_D\) survives above \(T_c\) in the under-doped regime and drops abruptly to zero at \(x = 0.198\), whereas \(D_0\) vanishes nearby. The reason for this to occur is because \(D\) vanishes here not because of thermal suppression but the competing order \(\psi\). This seems to account for the puzzling fact that even though pseudo-gap behavior is observed at relatively high...
temperatures, but the associated energy scale extrapolates to zero near $x = 0.19$. We regard this as yet another successful aspect of this mean field theory.

We now consider a double-layer system, where the only modification to the theory is the inter-layer tunnelling,

$$ f = \sum_{n=1}^{2} \left( [\alpha(x) + \beta T^2]|\psi_n|^2 + \frac{\beta}{2} |\psi_n|^4 ight) $$

$$ + \left[ a(x) + q b T^2 D_n^2 + \frac{b}{2} D_n^4 + g D_n^2 |\psi_n|^2 \right] $n \geq 1$$

$$ - J(|\psi_1|^2 + |\psi_2|^2 + c.c.), $$

(6)

where $\psi_n$ and $D_n$ represents the order parameters on the $n$-th layer, and $J = 0.3$ is the tunnelling energy scale. By symmetry the equilibrium values of the order parameters are independent of the layer index. Therefore the analysis can be proceeded in very much the same way as for the mono-layer case. The effect of the inter-layer tunnelling can be included into a modification of the upper doping limit of the superconducting order, so that $\alpha(x) - J \to 10(x - 0.33)$. The discussion then follows closely the case of mono-layer. Figs.2 present the zero temperature order parameters and the transition temperatures for the corresponding values of $q$ used in Figs.1. Because of interlayer tunnelling that enhances superconducting order, the onset doping for the zero temperature DDW order is reduced slightly to $x = 0.188$. Except from such details, we find that the qualitative behavior is the same as in a mono-layer. In particular $b q - g = 0$ remains to be the special case.

Given the success of the theory in dealing with mono- and double-layer systems, generalization to more layers seems natural and reasonable. The free energy density is now written as,

$$ f = \sum_{n=1}^{N} \left( [\alpha(x_n) + \beta T^2]|\psi_n|^2 + \frac{\beta}{2} |\psi_n|^4 ight) $$

$$ - J(|\psi_n|^2 + |\psi_{n+1}|^2 + c.c.) $$

$$ + [a(x) + q b T^2 D_n^2 + \frac{b}{2} D_n^4 + g D_n^2 |\psi_n|^2], $$

(7)

where $N$ is the total number of layers, and $x_n$ is the doping level on the $n$-th layer, which is different from the mean doping level $x$ because of the charge redistribution effect. The hole distribution can be roughly described by $x_n = [1 - \epsilon/(N - 2)]x$ for the inner layers $1 < n < N$ and $x_n = [1 + \epsilon/2]x$ for the outer layers ($n = 1$ and $n = N$). Here $\epsilon = 0.085, 0.39$ and 0.61 for the $N = 3, 4, 5$ respectively. We note that the hole distribution was measured experimentally mainly in the doping regime $x \geq 0.18$. Anticipating that $\epsilon$ does not change appreciably with doping (for a fixed $N$), we shall extrapolate to obtain the hole distribution in the under-doped regime. With the present finite temperature theory, we can calculate $T_c$ directly from the secular problem in the linearized Landau equations,

$$ [\alpha(x_n) + \beta T^2 + g D_n^2]|\psi_n| - J(|\psi_{n+1}| + |\psi_{n-1}|) = 0, $$

(8)

where $D_n^2 = \max(0, -[a(x_n) + q b T^2]/b)$ and $n = 1, 2, ..., N$. The condition for the existence of a nontrivial solution to the linear homogeneous Eqs. gives uniquely $T = T_c$. We seek symmetric solutions for $\psi_n$ as a function of $n$, as this yields the highest $T_c$. This reduces
the number of independent variables $\psi_n$, so that $N = 5$ we only have to deal with a $3 \times 3$ matrix determinant. The algebra is straightforward. The numerical result of $T_c$ as a function of $N$ is presented in Figs. 3(a) the cases of (a) $x = 0.14$ (under-doped), (b) $x = (\text{optimally doped})$ and (c) $x = 0.25$ (over-doped) each case we used $q = 0.6 - 1$, as argued to be re: able previously. In Fig.3(a) $T_c$ peaks broadly at $N$ for $q = 1$. We have checked that for even lower ing levels $T_c(N)$ increases monotonically (and event saturates), to which we shall return shortly. Homok serious in this doping region is not available to the of our knowledge but is desirable to check the predic In Fig.3(b) $T_c$ peaks at $N = 3$ (4) for $q = 0.6$ and explains nicely the data reported in Ref.[5] [8] Fig.3(c) $T_c$ increases monotonically again. This is consistent with experimental data. Indeed, $T_c(3) =$ and $T_c(4) = 117K$ at $x = 0.25$ in Table 1 of ref.[5] perconductors with $N \geq 5$ and $x \geq 0.25$ are not avai in Ref.[8].

The non-monotonic dependence in $T_c(N)$ is under- stood as a cooperative effect from inter-layer tunnelling, charge redistribution, and the competing order. For a uniform hole distribution, the effect of inter-layer tunnelling is to enhance superconductivity so that $T_c$ increases with the average layer-coordination number $2 - 2/N$ (as has been checked but not shown here). This ac- counts for the initial enhancement in $T_c(N)$ for all doping levels. In the very under-doped region the hole density is low despite of the charge redistribution effect. In such cases, the competing DDW order is robust and does not change appreciably. Therefore, apart from a global sup- pression by DDW, $T_c$ should increase with $N$. This is the case in Fig.3(a) if one takes $q = 0.6$ as the appropri- ate parameter. In the very over-doped region, the hole density is so high that DDW order is absent (at least up to $T_c$), and only the inter-layer tunnelling matters, yielding an increasing $T_c(N)$ again, as in Fig.3(c). The situation is quite different near the optimal doping. At the average doping, DDW is weak or absent. But with increasing $N$, charge redistribution introduces hole-poor inner layers with DDW order, counteracting the effect of inter-layer tunnelling and eventually suppressing $T_c$, as in Fig.3(b).

To summarize, we proposed a finite temperature Lan- dau theory that describes competing orders and inter- layer tunnelling in cuprate superconductors as an im- portant extension to a corresponding theory at zero temperature.[2] For given parameters, our theory deter- mines $T_c$ without any ambiguity. In mono- and double- layer systems we discuss the relation between zero tem- perature order parameter and the associated transition temperature in the presence of competing orders, and discuss the puzzling experimental fact that the pseudo- gap temperature is much higher than the corresponding energy scale near optimum doping. Applying the the- ory to multi-layer systems, we calculate the layer-number dependence of $T_c$. In a reasonable parameter space the result turns out to be in agreement with experiments.

We should emphasize that just as in Ref.[2] DDW is used as an example of the competing order to superconductivity. The discussion in this paper holds for any other forms of competing orders. However, DDW has the special property that it yields a band-gap with d-wave symmetry in the moment- space,[4] in accordance with angle-resolved-photoemission measurement.[9] While this seems to be appealing, other consequences that follow the DDW pic- ture are still in debates. For example, the temperature derivative of the superfluid density at low temperatures was claimed to be insensitive to the doping deep in the under-doped limit of YBCO thin films,[10] but another group reported that in YBCO crystals it tends to di- verge with under-doping.[11] While DDW picture is consistent with the latter, it can not account for the former results.[12] The fate of the DDW picture depends on fur- ther experimental clarification.

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