Microscopic mean field theory of competing orders and inter-layer tunnelling in high-T_c superconductors

2006 J. Phys.: Condens. Matter 18 2635

(http://iopscience.iop.org/0953-8984/18/9/003)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **18** (2006) 2635–2640 doi:10.1088/0953-8984/18/9/003

Microscopic mean field theory of competing orders and inter-layer tunnelling in high-T_c superconductors

Xiang-Mei He and Qiang-Hua Wang

National Laboratory of Solid State Microstructures, Institute for Solid State Physics, Nanjing University, Nanjing 210093, People's Republic of China

Received 28 October 2005
Published 17 February 2006
Online at stacks.iop.org/JPhysCM/18/2635

Abstract

By using a microscopic mean field theory we investigate the effects of competing order (against the superconducting one) and inter-layer tunnelling on the transition temperature T_c of cuprate superconductors. We obtain the theoretical phase diagrams of mono- and bi-layer systems. For multi-layer systems we investigate T_c as a function of the layer number N (within a unit cell). It turns out that near optimal doping $T_c(N)$ is non-monotonic and peaks at $N = 3$, in qualitative agreement with existing experimental data. This arises from the cooperative effects of competing order, charge redistribution and inter-layer tunnelling. However, the dropping of T_c with increasing N in this case is not as significant as in experiments. We also predict that in the very under- and over-doped regimes T_c becomes a monotonic function of N and saturates for $N \to \infty$. This is because the competing order is either robust against thermal effects near T_c (in the very under-doped regime) or entirely absent (in the very over-doped regime), so that T_c as a function of N is solely enhanced by inter-layer tunnelling.

The transition temperature T_c of high-T_c superconductors is a dome-shaped function of the hole doping level x, and the normal state is pseudo-gapped in the under-doped region. The mechanism of the superconductivity remains unclear as yet. Regarding the pseudo-gap phase, there are two distinctly different scenarios according to their viewpoints on whether the pseudo-gap is independent of the pairing gap. In the phase-fluctuation scenario [1], it is speculated that the normal state contains preformed Cooper pairs under the pseudo-gap transition temperature, and the phase fluctuation of the pairing field destroys superconductivity. As the pairing gap has a d-wave symmetry in the internal momentum space, the d-wave-like dispersion of the pseudo-gap follows immediately. An advantage of the scenario is that it involves no symmetry breaking, and is adiabatically connected to the paramagnetic Mott insulator. Such a normal state is not a Fermi liquid. In the second scenario, a d-density-wave (DDW) order is proposed in the normal state which is regarded as a competitor of d-wave superconductivity when antiferromagnetism is absent [2]. The DDW state carries staggered orbital currents,

breaking parity and time-reversal symmetry. It creates four hole-like Fermi pockets in the nodal directions. The volume enclosed by the Fermi pockets scales exactly as the doping level x. Thus the pseudo-gap in the DDW scenario is from the band structure effect.

The second scenario has been further exploited recently by Chakravarty *et al* [3], who proposed a zero-temperature Landau theory to describe the competition between DDW order and superconducting order, and the effect of inter-layer tunnelling in multi-layer superconductors. By an *a priori* linear relation between T_c and zero-temperature order parameter (or the energy gap), T_c was extracted from such a zero-temperature theory. This idea is proposed to explain the other well known fact that in homologous series of cuprate superconductors, T_c depends non-monotonically on N, the number of CuO_2 layers within a unit cell [4]. While the success is remarkable, several points are debatable in this treatment. For example, it is not clear whether there is still a definite connection between the zero-temperature order parameter and the transition temperature when two orders compete with each other. In the case where the order parameters are modulated within a multi-layered sample, it is not clear which representative of the order parameters should be used in the extraction of T_c. Moreover, it is not clear why the zero-temperature pseudo-gap order parameter (or its energy scale) extrapolates to zero at a doping level of $x = 0.19$, whereas the pseudo-gap phenomenon certainly exists at $T \geqslant T_c$ even at the same doping [5]. Recently, a finite-temperature Landau theory was proposed [6]. It provides unambiguous T_c as functions of x and N, and also explains the above-mentioned puzzling relation between the pseudo-gap energy scale and the pseudo-gap temperature. The essence is that the DDW order vanishes near the critical doping due to the competing superconducting order instead of thermal suppression, and therefore even a tiny DDW order can survive up to T_c or even higher temperatures.

The above theories are both phenomenological in nature. It is therefore pending to justify/falsify the phenomenological results using microscopic theories. In this paper, we perform microscopic mean field calculations and compare the results with the phenomenological ones. By comparing the theoretical phase diagrams with experiments in the case of mono- and bi-layer systems, we can fix all the parameters introduced in the microscopic theory. We then extend the theory to multi-layer systems, and calculate $T_c(N)$. It turns out that near optimal doping $T_c(N)$ is non-monotonic and peaks at $N = 3$, in qualitative agreement with existing experimental data. This arises from the cooperative effects of competing order, charge redistribution and inter-layer tunnelling. However, the dropping of T_c with increasing N is less significant than in experiments. We also predict that in the very under- and over-doped regimes T_c becomes a monotonic function of N and saturates for $N \to \infty$. This is because the competing order is either robust against thermal effects near T_c (in the very under-doped regime) or entirely absent (in the very over-doped regime), so that T_c as a function of N is solely determined by inter-layer tunnelling.

We begin with the mono-layer systems, in which d-wave pairing and DDW are assumed to be the two competing orders. The effective mean field Hamiltonian can be written as

$$H = \sum_{k\sigma}[(X_k - \mu)C^\dagger_{k\sigma}C_{k\sigma} - \mathrm{i}D_k C^\dagger_{k+Q\sigma}C_{k\sigma}] - \sum_k(\Delta_k C^\dagger_{k\uparrow}C^\dagger_{-k\downarrow} + \text{h.c.}). \tag{1}$$

Here $X_k = -2t(\cos k_x + \cos k_y)$ is the nearest-neighbour tight-binding dispersion relation, $D_k = 2V_d D(\cos k_x - \cos k_y)$ is the DDW gap function, $Q = (\pi, \pi)$, and $\Delta_k = 2V_s\Delta(\cos k_x - \cos k_y)$ is the d-wave pairing gap function. Here V_d and V_s are the effective interaction strengths in the DDW and pairing channels, respectively, and D and Δ are the corresponding order parameters. Because of the breaking of translation symmetry caused by the DDW order, the Brillouin zone is half of its original size. Using the facts that $X_{k+Q} = -X_k$, $\Delta_{k+Q} = -\Delta_k$, and $D_{k+Q} = -D_k$, the Hamiltonian can be rewritten as $H = \sum'_k \psi^\dagger_k h_k \psi_k$, where the primed summation over k is restricted to the reduced Brillouin

zone, $\psi_k = (C_{k\uparrow}, C^\dagger_{-k\downarrow}, C_{k+Q\uparrow}, C^\dagger_{-k+Q\downarrow})^T$ are Nambu–Anderson four-spinors, and h_k is a 4×4 single-particle Hamiltonian,

$$h_k = \begin{pmatrix} X_k - \mu & -\Delta_k & \mathrm{i}D_k & 0 \\ -\Delta_k^* & -X_k + \mu & 0 & \mathrm{i}D_k \\ -\mathrm{i}D_k & 0 & -X_k - \mu & \Delta_k \\ 0 & -\mathrm{i}D_k & \Delta_k^* & X_k + \mu \end{pmatrix}. \tag{2}$$

The self-consistent conditions for the order parameters are as follows:

$$\Delta = \frac{1}{N_\mathrm{L}} \sum_k{}' (\cos k_x - \cos k_y) \langle C_{-k\downarrow} C_{k\uparrow} - C_{-k+Q\downarrow} C_{k+Q\uparrow} \rangle, \tag{3}$$

$$D = \frac{\mathrm{i}}{N_\mathrm{L}} \sum_{k\sigma}{}' (\cos k_x - \cos k_y) \langle C^\dagger_{k+Q\sigma} C_{k\sigma} - C^\dagger_{k\sigma} C_{k+Q\sigma} \rangle, \tag{4}$$

where N_L is the number of lattice sites under consideration. The matrix h_k can be diagonalized exactly. Consequently, the self-consistent equations can be made more explicit,

$$\Delta = \frac{V_s \Delta}{N_\mathrm{L}} \sum_{k\nu}{}' \frac{(\cos k_x - \cos k_y)^2}{E_{k\nu}} \tanh \frac{\beta E_{k\nu}}{2}, \tag{5}$$

$$D = \frac{2V_d D}{N_\mathrm{L}} \sum_{k\nu}{}' \frac{(\cos k_x - \cos k_y)^2 \epsilon_{k\nu}}{\nu \xi_k E_{k\nu}} \tanh \frac{\beta E_{k\nu}}{2}, \tag{6}$$

where $\nu = \pm$, $E_{k\nu} = \sqrt{{\epsilon_{k\nu}}^2 + {\Delta_k}^2}$, $\epsilon_{k\nu} = \nu\xi_k - \mu$, and $\xi_k = \sqrt{{X_k}^2 + {D_k}^2}$. The chemical potential is determined by

$$1 - x = \frac{1}{N_\mathrm{L}} \sum_{k\sigma}{}' \langle C^\dagger_{k\sigma} C_{k\sigma} + C^\dagger_{k+Q\sigma} C_{k+Q\sigma} \rangle = 1 - \frac{1}{N_\mathrm{L}} \sum_{k\nu}{}' \frac{\epsilon_{k\nu}}{E_{k\nu}} \tanh \frac{\beta E_{k\nu}}{2}, \tag{7}$$

where x is the hole doping level. These equations can be used to calculate the doping dependence of the order parameters at any temperatures. As usual the transition temperature T_c for Δ is determined by the temperature that solves the linearized self-consistent equation for Δ, namely,

$$1 = \frac{V_s}{N_\mathrm{L}} \sum_{k\nu}{}' \frac{(\cos k_x - \cos k_y)^2}{\epsilon_{k\nu}} \tanh \frac{\beta \epsilon_{k\nu}}{2}, \tag{8}$$

and D is self-consistently calculated by setting $\Delta = 0$. Similarly, the transition temperature T_D for D is given by

$$1 = \frac{2V_d}{N_\mathrm{L}} \sum_{k\nu}{}' \nu \frac{(\cos k_x - \cos k_y)^2 \epsilon_{k\nu}}{\xi_k E_{k\nu}} \tanh \frac{\beta E_{k\nu}}{2}, \tag{9}$$

where $D = 0$ should be imposed in $E_{k\nu}$, $\epsilon_{k\nu}$, and ξ_k.

We first perform the calculation for mono-layered systems. By comparison with experiments we can fix the parameters V_s and V_d. In figure 1(a) we present T_c (thick solid line) and T_D (filled circles) and the zero-temperature order parameters Δ_0 (dotted line) and D_0 (open diamonds) as functions of doping level x in the mono-layer systems for $V_s = 0.8t$ and $V_d = 0.6t$. We note that similar results were reported in [7]. In order to see how Δ_0 and D_0 scale with the respective transition temperatures, we have re-scaled T_c and T_D so that $\Delta_0 = T_\mathrm{c}$ at the optimal doping $x = 0.2$ and $D_0 = T_D$ at the doping $x = 0$. By this means we observe that T_c and Δ_0 fall on top of each other approximately (except for the slightly under-doped regime), implying that $T_\mathrm{c} \propto \Delta_0$ applies approximately even in the presence of a competing DDW order. However, this is not true for T_D versus D_0. In fact, near $x = 0.174$, we have $D_0 = 0$ but a

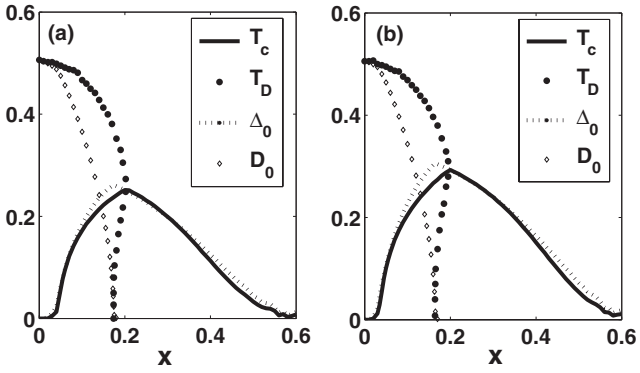

Figure 1. T_c (thick solid line), T_D (filled circles), Δ_0 (dotted line) and D_0 (open diamonds) as functions of doping level x in the (a) mono-layer systems with channel interaction $V_s = 0.8t$ and $V_d = 0.6t$ and (b) bi-layer systems with $V_s = 0.8t$, $V_d = 0.6t$ and $J = 0.07t$. All quantities are in arbitrary units.

very large T_D. Moreover, for $0.174 < x < 0.2$ we find two T_D values for each doping whereas $D_0 = 0$. This feature nicely explains the puzzle that the pseudo-gap transition temperature can be high even though the associated zero-temperature energy scale extrapolates to zero [5]. The mechanism is as follows. At zero temperature, D_0 already vanishes at $x \geqslant 0.174$ because of the suppression of the strong pairing order Δ_0. With increasing temperature, the pairing order is thermally suppressed so that the DDW order reappears and survives up to T_c. This behaviour was also found in the finite temperature Landau theory [6].

We now generalize the theory to multi-layer systems. The effective Hamiltonian is written as

$$H = \sum_{n=1}^{N}\Bigg\{\sum_{k\sigma}(X_k - \mu_n)C^{\dagger}_{n,k\sigma}C_{n,k\sigma} - \sum_{k\sigma}\mathrm{i}D_{n,k}C^{\dagger}_{n,k+Q\sigma}C_{n,k\sigma} - \sum_{k}(\Delta_{n,k}C^{\dagger}_{n,k\uparrow}C^{\dagger}_{n,-k\downarrow} + \text{h.c.})\Bigg\}, \tag{10}$$

where n is the layer index and N is the total number of layers in a unit cell of the homologous series of superconductors, $D_{n,k} = 2V_dD_n(\cos k_x - \cos k_y)$, $\Delta_{n,k} = 2[V_s\Delta_n + J(\Delta_{n-1} + \Delta_{n+1})](\cos k_x - \cos k_y)$. Here J is the Josephson coupling energy and D_n and Δ_n are the layer-dependent order parameters. We neglect the single-particle tunnelling, assuming that such processes are largely incoherent. We also assume that the DDW order decouples in different layers, and that the d-wave pairing symmetry is preserved in the presence of Josephson tunnelling. An open boundary condition is implied so that any terms involving layer indices $n < 1$ and $n > N$ are excluded from the Hamiltonian. For $N \geqslant 3$, it is found experimentally that there exists a charge redistribution so that the hole density changes in different layers [8]. This is because of the Coulomb interaction from the apical oxygen atoms surrounding the outer layers. Therefore, the chemical potential μ_n (and consequently D_n and Δ_n) may depend on the layer index. 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) [3, 8]. Here $\epsilon = 0$, 0.085, 0.39 and 0.61 for the $N = 2, 3, 4, 5$ respectively. We note that the hole distribution was measured experimentally mainly in the doping regime $x \geqslant 0.18$ [8]. Anticipating that ϵ does not change appreciably with doping (for a fixed N), we shall extrapolate to obtain the hole distribution in the under-doped regime.

Since the mean field Hamiltonian for the fermions is layer diagonal, the self-consistent equations described previously can be extended straightforwardly to the multi-layered case as

$$\Delta_n = \frac{V_s\Delta_n + J(\Delta_{n-1} + \Delta_{n+1})}{N_L} \times {\sum_{k\nu}}' \frac{(\cos k_x - \cos k_y)^2}{E_{n,k\nu}} \tanh\frac{\beta E_{n,k\nu}}{2}, \tag{11}$$

$$D_n = \frac{2V_d D_n}{N_L} \times \sum_{kv}{}' \frac{(\cos k_x - \cos k_y)^2 \epsilon_{n,kv}}{v\xi_{n,k} E_{n,kv}} \tanh \frac{\beta E_{n,kv}}{2}. \tag{12}$$

The chemical potentials μ_n are determined by

$$1 - x_n = 1 - \frac{1}{N_L} \sum_{kv}{}' \frac{\epsilon_{n,kv}}{E_{n,kv}} \tanh \frac{\beta E_{n,kv}}{2}. \tag{13}$$

Here $E_{n,kv} = \sqrt{{\epsilon_{n,kv}}^2 + {\Delta_{n,k}}^2}$, $\epsilon_{n,kv} = v\xi_{n,k} - \mu_n$, and $\xi_{n,k} = \sqrt{{X_k}^2 + {D_{n,k}}^2}$. The layer-dependent order parameters are coupled through the self-consistent equations.

For $N = 2$ the apical oxygen appears symmetrically with respect to the two layers, so that the hole density is still the same in the two layers. The order parameters in equilibrium are thus independent of the layer index. The effect of the inter-layer tunnelling can be included into a modification of the pairing interaction, $V_s \to V_s + J$. The remaining discussion then follows closely the case of the mono-layer. Figure 1(b) presents the zero-temperature order parameters and the transition temperature for $V_s = 0.8t$, $V_d = 0.6t$ and $J = 0.07t$. Because of inter-layer tunnelling that enhances superconducting order, the upper doping limit for the superconducting order increases, and the onset doping for the zero-temperature DDW order is reduced slightly to $x = 0.165$. Except for such details, we find that the qualitative behaviour is the same as in the mono-layered case.

We will now be mainly interested in the N dependence of T_c in various doping regimes. For this purpose, it suffices to consider the linearized self-consistent equations for Δ_n (while D_n is self-consistently calculated by setting $\Delta_n = 0$). These can be formally written as $\Delta_n = \sum_{n'} B_{n,n'} \Delta_{n'}$. The matrix B is calculated by setting $\Delta_n = 0$ in $E_{n,kv}$. The condition for a nontrivial solution to these linear equations is $\det(B - I) = 0$, which determines T_c exactly. We seek symmetric solutions for the order parameters as a function of n, as this yields the highest T_c. This reduces the number of independent layers so that up to $N = 5$ we only have to deal with a 3×3 matrix B.

In figure 2 we show T_c as a function of N in the (a) under-doped region $x = 0.1$ and $x = 0.12$, (b) optimally doped region $x = 0.175$ and $x = 0.2$, and (c) over-doped region $x = 0.28$ and $x = 0.3$. We find that T_c peaks at $N = 3$ in the optimally doped region, in qualitative agreement with experiments and previous phenomenological theories. However, it increases monotonically in the under-doped and over-doped regions (and saturates in the limit of $N \to \infty$). The N dependence of T_c is determined by the joint effects of competing order, inter-layer tunnelling, and charge redistribution. Suppose at first 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 $2 - 2/N$. This accounts for the initial enhancement in $T_c(N)$ for all doping levels. In the very under-doped region the hole density is low despite the charge redistribution effect. In such cases, the competing DDW order is robust and does not change appreciably. On the other hand, in the very over-doped region the hole density is so high that DDW order is absent (at least up to T_c). In these two extremes, only the inter-layer tunnelling contributes to influence T_c, yielding an increasing $T_c(N)$ as in figures 2(a) and (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 figure 2(b). The physics is first discussed in the phenomenological Landau theory [6], for which the present results provide support.

There are differences between the present results and the phenomenological ones [3, 6], however. The dropping of T_c from $N = 3$ to 5 in our case is quite limited as shown in figure 2(b). The details depend on the value of J we used. We find that a larger value of

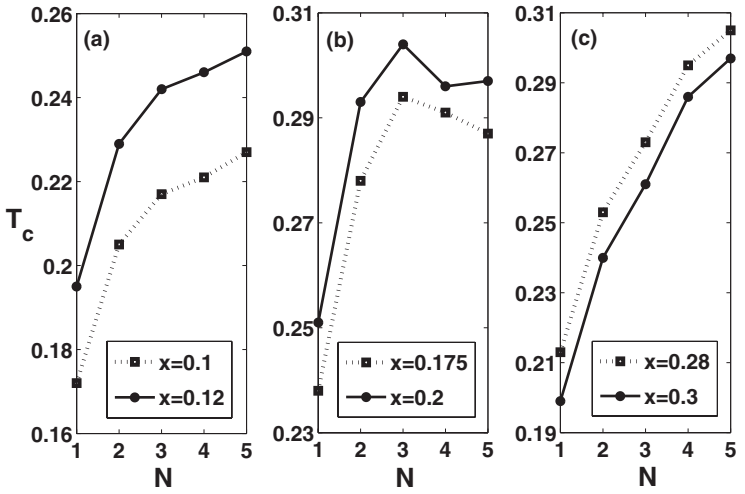

Figure 2. N dependence of T_c (in arbitrary units) in the (a) under-doped region $x = 0.1$ and 0.12, (b) optimally doped region $x = 0.175$ and 0.2, and (c) over-doped region $x = 0.28$ and 0.3.

J would eliminate the non-monotonic $T_c(N)$ near the optimal doping, so that it is monotonic in all doping regimes, whereas a smaller value of J would cause insignificant enhancement of T_c from $N = 1$ to 3. This cautions that the model proposed in [3] may not be as universal as anticipated.

In conclusion, we performed mean field microscopic investigation on the effects of competing order, Josephson inter-layer tunnelling and the charge redistribution in homologous series of cuprate superconductors. The parameters in the theory are set by comparing the theoretical phase diagrams of the mono- and bi-layer systems with experiments. We find that $T_c(N)$ near the optimal doping is non-monotonic, in agreement with experiments. We also predict that it becomes monotonic in the very under-doped and over-doped regions. Comparison with Landau theories are made.

Acknowledgments

This work was supported by NSFC 10325416 and 10021001, the Fok Ying Tung Education Foundation No 91009, and the Ministry of Science and Technology of China (973 project No 2006CB601002).

References

[1] Emery V and Kivelson S A 1995 *Nature* **374** 434
[2] Chakravarty S, Laughlin R B, Morr D K and Nayak C 2001 *Phys. Rev.* B **63** 094503
[3] Chakravarty S, Kee H Y and Völker K 2004 *Nature* **428** 53
[4] Scott B A, Suard E Y, Tsuei C C, Mitzi D G, McGuire T R, Chen B-H and Walker D 1994 *Physica* C **230** 239
Kuzemskaya I G, Kuzemsky A L and Cheglokov A A 2000 *J. Low Temp. Phys.* **118** 147
[5] Tallon J L, Williams G V M and Loram J W 2000 *Physica* C **338** 9
[6] Wu J-B, Pei M-X and Wang Q-H 2005 *Phys. Rev.* B **71** 172507
[7] Zhu J-X, Kim W, Ting C S and Carbotte J P 2001 *Phys. Rev. Lett.* **87** 197001
[8] Kotegawa H, Tokunaga Y, Ishida K, Zheng G-Q, Kitaoka Y, Kito H, Iyo A, Tokiwa K, Watanabe T and Ihara H 2001 *Phys. Rev.* B **64** 064515
Kotegawa H, Tokunaga Y, Ishida K, Zheng G-Q, Kitaoka Y, Asayama K, Kito H, Iyo A, Ihara H, Tanaka K, Tokiwa K and Watanabe T 2001 *J. Phys. Chem. Solids* **62** 171