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Superconductivity enhanced by d-density wave: A weak-coupling theory

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ABSTRACT

Making a revision of mistakes in Ref. [19], we present a detailed study of the competition and interplay between the d-density wave (DDW) and d-wave superconductivity (DSC) within the fluctuationexchange (FLEX) approximation for the two-dimensional (2D) Hubbard model. In order to stabilize the DDW state with respect to phase separation at lower dopings a small nearest-neighbor Coulomb repulsion is included within the Hartree-Fock approximation. We solve the coupled gap equations for the DDW, DSC, and π -pairing as the possible order parameters, which are caused by exchange of spin fluctuations, together with calculating the spin fluctuation pairing interaction self-consistently within the FLEX approximation. We show that even when nesting of the Fermi surface is perfect, as in a square lattice with only nearest-neighbor hopping, there is coexistence of DSC and DDW in a large region of dopings close to the quantum critical point (QCP) at which the DDW state vanishes. In particular, we find that in the presence of DDW order the superconducting transition temperature T_c can be much higher compared to pure superconductivity, since the pairing interaction is strongly enhanced due to the feedback effect on spin fluctuations of the DDW gap. π -pairing appears generically in the coexistence region, but its feedback on the other order parameters is very small. In the present work, we have developed a weak-coupling theory of the competition between DDW and DSC in 2D Hubbard model, using the static spin fluctuation obtained within FLEX approximation and ignoring the selfenergy effect of spin fluctuations. For our model calculations in the weak-coupling limit we have taken U/t=3.4, since the antiferromagnetic instability occurs for higher values of U/t.

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1. Introduction

It is one of the most interesting and important issues in condensed-matter physics to elucidate the mechanism of hightemperature superconductivity occurring in cuprates. Among a number of mechanisms proposed for the high-temperature superconductivity since its discovery in 1986 the spin-fluctuation mechanism has continued to be one of the most promising mechanisms [1]. Following systematic studies based on the parameterized spin fluctuation theory, more quantitative studies were carried out using the 2D Hubbard model within the FLEX approximation in which spin and charge fluctuations, the singleparticle spectrum, and superconducting gap function are determined self-consistently [2–7]. The results of these theories seem to be successful at least qualitatively in explaining not only dwave pairing but also a lot of unusual phenomena, which have been observed in high-temperature superconducting cuprates in the overdoped region. However, existing microscopic theories

have serious problems in explaining the underdoped region of the cuprates and instead many phenomenological approaches have been used. These problems are, in particular, the existence of a pseudogap [8,9], which appears to have the same symmetry as the superconducting gap, below a characteristic temperature T^* that is higher than the superconducting transition temperature T_c . This is unusual because the pseudogap is present in the normal state above T_c and coexists with the superconducting gap in the superconducting state below T_c . This striking pseudogap behavior initiated a variety of proposals [10–13] as to its origin, since the answer to this question may be a key ingredient for the understanding of high-temperature superconductivity. At present, there is no agreement as to which of these proposals is correct.

A natural explanation for the pseudogap behavior involves the discussion of the possible occurrence of a charge–density wave in the cuprates. Remarkably, it was shown that most of the observed properties referred to as a so-called pseudogap phenomenon can be naturally explained by introducing a charge–density wave having d-wave symmetry or d-density wave (d-CDW or DDW) [12]. Furthermore, as it is well known that the charge–density wave and superconductivity compete with each other in strongly correlated electron systems, such as high-temperature superconductors, a pseudogap arising from a DDW state therefore has immense appeal.

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Therefore, if the DDW state is responsible for the pseudogap behavior, its effect on DSC must be understood on the same microscopic level as the spin fluctuations. Most of previous studies for this problem has been almost restricted in the phenomenological or mean-field level [14–17]. Dahm et al. [18] have presented the general equations of the FLEX approximation for coexisting DDW and DSC gaps in the 2D Hubbard model, but these equations have not been solved yet because they are much more complicated than the pure superconducting equations.

In this paper, we present a detailed study of the competition and interplay between the DDW and DSC within the FLEX approximation for the 2D Hubbard model. In order to stabilize the DDW with respect to phase separation at lower dopings, a small nearest-neighbor Coulomb repulsion *V* is included within the Hartree-Fock approximation. The DDW state is described by singlet electron-hole pairing between the nested states above and below the Fermi sea and therefore the corresponding anomalous Green's functions contain the step function $\theta(|\varepsilon_{\mathbf{k}}| - |\varepsilon_F|)$, with an one-electron band energy $\varepsilon_{\mathbf{k}}$ and the Fermi energy ε_F . This step function plays an important role in our theory for the competition and interplay between the DDW and superconductivity. While in Refs. [14-17] without the step function the DDW transition temperature T^* as a function of doping after passing a large doping moves to lower dopings, in our calculation with this step function it decreases monotonously with increasing doping and goes toward larger dopings. This will result in the coexistence of the DDW and DSC in a broader region, even when nesting of the Fermi surface is perfect, as in a square lattice with only nearestneighbor hopping t. Most importantly, we find that the presence of a DDW leads to a large increase of the superconducting transition temperature T_c close to the QCP at which the DDW state vanishes, since the pairing interaction mediated by spin fluctuations is strongly enhanced due to the feedback effect of the DDW order parameter.

In Section 2 we will derive the coupled gap equations for the DDW, DSC, and π pairing as the possible order parameters, which are induced by exchange of spin fluctuations within the FLEX approximation. Results from solving these equations for the 2D Hubbard model will be presented in Section 3. We conclude with a summary of the main results in Section 4.

2. Gap equations for competing order parameters

Our starting point is the 2D extended Hubbard model with the onsite and nearest-neighbor Coulomb repulsions U and V

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle \sigma\sigma'} n_{i\sigma} n_{j\sigma'}, \tag{1}$$

The $c^+_{i\sigma}$ and $c^-_{i\sigma}$ are the usual creation and annihilation operators for an electron with spin σ at site i, respectively, and $n_{i\sigma}=c^+_{i\sigma}c_{i\sigma}$ is the number operator. The sum $\langle ij \rangle$ is over nearestneighbor pairs with hopping t, leading to the one-electron band dispersion $\varepsilon_{\bf k}=-2t(\cos k_x+\cos k_y)$. This dispersion has two important features: the nesting property $\varepsilon_{\bf k}=-\varepsilon_{\bf k+Q}$, with the antiferromagnetic wave vector ${\bf Q}=(\pi,\,\pi)$, and the Van Hove singularity in the density of states.

Due to nesting there will be a strong instability of the Fermi surface with respect to forming the DDW state with the order parameter $i\Delta_D(\mathbf{k}) \sim \langle c_{\mathbf{k}+\mathbf{Q}\sigma}^+ c_{\mathbf{k}\sigma} \rangle \theta(|\epsilon_{\mathbf{k}}|-|\epsilon_F|)$, which corresponds to condensation of singlet electron–hole pairs in nested states above and below the Fermi level ϵ_F . The Van Hove singularity can also result in the appearance of a superconducting state, which is described by the order parameter $\Delta_B(\mathbf{k}) \sim \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$ representing Cooper–pair formation of electrons having opposite spins and momenta. In the presence of two order parameters the operators

 $(c^+_{k\uparrow},c^+_{k+Q\uparrow},c_{-k\downarrow},c_{-k-Q\downarrow})$ are coupled leading to the following Green's function matrix:

$$\hat{G}^{-1}(k) = \begin{pmatrix} i\omega_n - \varepsilon_{\mathbf{k}} + \mu & -i\Delta_D(\mathbf{k}) & -\Delta_B(\mathbf{k}) & -i\Delta_H(\mathbf{k}) \\ -i\Delta_D(\mathbf{k} + \mathbf{Q}) & i\omega_n - \varepsilon_{\mathbf{k} + \mathbf{Q}} + \mu & -i\Delta_H(\mathbf{k} + \mathbf{Q}) & -\Delta_B(\mathbf{k} + \mathbf{Q}) \\ -\Delta_B(\mathbf{k}) & i\Delta_H(\mathbf{k} + \mathbf{Q}) & i\omega_n + \varepsilon_{-\mathbf{k}} - \mu & i\Delta_D(-\mathbf{k} - \mathbf{Q}) \\ i\Delta_H(\mathbf{k}) & -\Delta_B(\mathbf{k} + \mathbf{Q}) & i\Delta_D(-\mathbf{k}) & i\omega_n + \varepsilon_{-\mathbf{k} - \mathbf{Q}} - \mu \end{pmatrix},$$
(2)

where $k=(\mathbf{k},i\omega_n)$, with $\omega_n=(2n+1)\pi T$ being a fermion Matsubara frequency, μ is the chemical potential. Here, $i\Delta_H(\mathbf{k})$ is the π -pairing order parameter, which appears generically in the coexistence of the DDW and superconductivity. In Ref. [19] there was a sign mistake in the matrix elements G_{34}^{-1} and G_{43}^{-1} (see Ref. [21]).

We have extended the FLEX approximation to the coexisting DDW and DSC state. We use here the weak-coupling gap equations for the competing order parameters $\Delta_{D,B,H}(\mathbf{k})$

$$i\Delta_D(\mathbf{k}) = \frac{T}{N} \sum_{k'} [U + 2V(0) - V(\mathbf{k} - \mathbf{k'}) + P_s(\mathbf{k} - \mathbf{k'}) + P_c(\mathbf{k} - \mathbf{k})] G_{12}(k'),$$
(3)

$$\Delta_B(\mathbf{k}) = \frac{T}{N} \sum_{k'} [U + V(\mathbf{k} - \mathbf{k}') + P_s(\mathbf{k} - \mathbf{k}') - P_c(\mathbf{k} - \mathbf{k}')] G_{13}(k'), \tag{4}$$

$$i\Delta_{H}(\mathbf{k}) = \frac{T}{N} \sum_{k'} [U + V(\mathbf{k} - \mathbf{k}') + P_{s}(\mathbf{k} - \mathbf{k}') - P_{c}(\mathbf{k} - \mathbf{k}')]G_{14}(k'), \tag{5}$$

with the static spin and charge fluctuation interactions $P_{s,c}(\mathbf{q}) = P_{s,c}(\mathbf{q}, iv_m = 0)$. The FLEX approximation yields

$$P_s(q) = \frac{1}{2}U^2 [3\chi_s(q) - \chi_s^0(q)]; \quad \chi_s = \chi_s^0 (1 - U\chi_s^0)^{-1}, \tag{6}$$

$$P_c(q) = \frac{1}{2}U^2 \left[\chi_c(q) - \chi_c^0(q) \right]; \quad \chi_c = \chi_c^0 (1 + U\chi_c^0)^{-1}, \tag{7}$$

The irreducible spin and charge susceptibilities are calculated from

$$\chi_{s,c}^{0}(q) = -\frac{T}{N} \sum_{\mathbf{k}} \sum_{\omega_{n}} [G_{11}(k+q)G_{11}(k) + G_{12}(k+q)G_{21}(k)$$

$$\pm G_{13}(k+q)G_{31}(k) \pm G_{14}(k+q)G_{41}(k)],$$
(8)

where $q=(\mathbf{q}, iv_m=0)$, with $v_m=2m\pi T$ being a boson Matsubara frequency. The plus sign is for the spin susceptibility χ_s^0 and the minus sign is for the charge susceptibility χ_c^0 . In Eqs. (3)–(5) we have taken account of the nearest-neighbor Coulomb repulsion $V(\mathbf{q})=2V(\cos q_x+\cos q_y)$ within the Hartree–Fock approximation.

In Eqs. (3)–(5) the effective interactions are dominated by the spin fluctuation interaction P_s due to the fact that the system is in the vicinity of an antiferromagnetic instability. Since the repulsive spin fluctuation interaction $P_s(q)$ has a large peak at $\mathbf{q} = \mathbf{Q}$, it is attractive in the $d_x 2_{-y} 2$ -wave channel and all the order parameters $\Delta_D(\mathbf{k})$, $\Delta_B(\mathbf{k})$, and $\Delta_H(\mathbf{k})$ have $d_x 2_{-y} 2$ -wave symmetry. Therefore, we assume that they have the simple form $\Delta_{D,B,H}(\mathbf{k}) = \Delta_{D,B,H} \cdot d_{\mathbf{k}}$, with $d_{\mathbf{k}} = \cos k_x - \cos k_y$. We use the fact that DSC order parameter $\Delta_B(\mathbf{k})$ can be chosen to be real. Then both the DDW and π -pairing order parameters, $i\Delta_D(\mathbf{k})$ and $i\Delta_H(\mathbf{k})$, must be purely imaginary because of their $d_x 2_{-y} 2$ -wave symmetry.

Eq. (2) can therefore easily be inverted and the sum over frequencies in Eqs. (3)–(5) carried out. Then we obtain the following coupled gap equations for competing $d_x 2_{-y} 2$ -wave

order parameters $\Delta_D(\mathbf{k})$, $\Delta_B(\mathbf{k})$, and $\Delta_H(\mathbf{k})$:

$$\frac{1}{V+P} = \frac{1}{N} \sum_{\mathbf{k}} \theta(|\varepsilon_{\mathbf{k}}| - |\varepsilon_{F}|) d_{\mathbf{k}}^2 \bigg\{ \frac{E_{\mathbf{k}} + \mu_{\mathbf{k}}}{4E_{\mathbf{k}}E_{\mathbf{k}+}} \tanh \frac{E_{\mathbf{k}+}}{2T} + \frac{E_{\mathbf{k}} - \mu_{\mathbf{k}}}{4E_{\mathbf{k}}E_{\mathbf{k}-}} \tanh \frac{E_{\mathbf{k}-}}{2T} \bigg\}, \tag{9}$$

$$\frac{1}{-V+P} = \frac{1}{N} \sum_{\mathbf{k}} d_{\mathbf{k}}^2 \left\{ \frac{1}{4E_{\mathbf{k}+}} \tanh \frac{E_{\mathbf{k}+}}{2T} + \frac{1}{4E_{\mathbf{k}-}} \tanh \frac{E_{\mathbf{k}-}}{2T} \right\}, \tag{10}$$

$$\frac{1}{-V+P} = \frac{1}{N} \sum_{\mathbf{k}} d_{\mathbf{k}}^2 \left\{ \frac{\mu_{\mathbf{k}} + E_{\mathbf{k}}}{\mu_{\mathbf{k}}} \frac{1}{4E_{\mathbf{k}+}} \tanh \frac{E_{\mathbf{k}+}}{2T} + \frac{\mu_{\mathbf{k}} - E_{\mathbf{k}}}{\mu_{\mathbf{k}}} \frac{1}{4E_{\mathbf{k}-}} \tanh \frac{E_{\mathbf{k}-}}{2T} \right\}, \tag{11}$$

with $E_{\mathbf{k}\pm}=[(\mu_{\mathbf{k}}\pm E_{\mathbf{k}})^2+\varDelta_B^2(\mathbf{k})]^{1/2}$, $E_{\mathbf{k}}=[\varepsilon_{\mathbf{k}}^2+\varDelta_D^2(\mathbf{k})]^{1/2}$, and $\mu_{\mathbf{k}}=[\mu^2+\varDelta_H^2(\mathbf{k})]^{1/2}$. Here $E_{\mathbf{k}\pm}$ are quasiparticle energies in the coexistent state of the DDW and superconductivity. The coupling parameter P is given by

$$P = \frac{2}{\pi} \int_0^\infty dv \frac{1}{v} N^{-2} \sum_{\mathbf{k}, \mathbf{k'}} d_{\mathbf{k}} \text{Im} P_s(\mathbf{k} - \mathbf{k'}, v + i0^+) d_{\mathbf{k'}},$$
 (12)

which characterizes the strength of the pairing interaction in the $d_x 2_{-y} 2$ -wave channel mediated by spin fluctuations. The charge fluctuation interaction P_c has been neglected from its weakness compared to the spin fluctuation interaction P_s . Since Im P_s has a large peak at $\mathbf{k} - \mathbf{k}' = \mathbf{Q}$, Eq. (12) yields P > 0, i.e., a $d_x 2_{-y} 2$ -wave attraction. Note that the nearest-neighbor Coulomb interaction V is attractive in Eq. (9) for the DDW gap $\Delta_D(\mathbf{k})$ corresponding to electron-hole pairing, but it is repulsive in Eqs. (10) and (11) for the superconducting gaps $\Delta_B(\mathbf{k})$ and $\Delta_H(\mathbf{k})$ described by electron-electron pairing.

We perform calculations as a function of hole doping $\delta=1-n$, with $n=1/N\Sigma_i\langle n_i\rangle$ being the band filling. The chemical potential μ is related to the band filling n by

$$n = \frac{1}{N} \sum_{\mathbf{k}} \left[1 + \frac{\mu + E_{\mathbf{k}}}{E_{\mathbf{k}+}} \tanh \frac{E_{\mathbf{k}+}}{2T} + \frac{\mu - E_{\mathbf{k}}}{E_{\mathbf{k}-}} \tanh \frac{E_{\mathbf{k}-}}{2T} \right], \tag{13}$$

At half filling (δ =0) $E_{\mathbf{k}+}$ = $E_{\mathbf{k}-}$ and μ =0, as it should.

Our Eqs. (9)–(11) look similar to the equations presented in Ref. [14] with some important differences. First, Eq. (9) contains the step function $\theta(|\varepsilon_{\mathbf{k}}| - |\varepsilon_F|)$, which means that the formation of electron–hole pairs takes place only between the nested states above and below the Fermi see. Here, ε_F is the Fermi energy for the noninteracting case and is calculated from the relation $n=1/N\Sigma_{\mathbf{k}}\theta(\varepsilon_F-\varepsilon_{\mathbf{k}})$. At half filling (n=1) $\varepsilon_F=0$ and the step function becomes unity. Second, the gap parameters $\Delta_{D,B,H}$ are related to the coupling constant P via the irreducible susceptibilities χ_s^0 . Thus P must be calculated self-consistently together with $\Delta_{D,B,H}$.

Our calculations are carried out as follows: starting with initial values of $\Delta_{D,B,H}$, the parameters $P_{s,c}$ are calculated from Eqs. (6)–(8) and (12). This is used in finding the solutions of the Eqs. (9)–(11) to get the updated $\Delta_{D,B,H}$. This procedure is repeated until convergence is achieved. It is important to note that P is recalculated in every iteration. In contrast to the conventional mean-field theory, in which the coupling parameter P is fixed, it must be calculated self-consistently, taking account of the feedback effect on spin fluctuations of the gaps $\Delta_{D,B,H}$. This will be especially important in explaining our mechanism of high-temperature superconductivity induced by the DDW as discussed below.

3. Results and discussion

In this section we present results obtained from solving the coupled gap equations for the DDW, DSC, and π -pairing order parameters, which are induced by spin fluctuations in the 2D Hubbard model. We will first discuss pure DDW states in the

absence of superconductivity, then the superconducting transition in the DDW state, and finally the competition between order parameters and the influence on the phase diagram of the nearest-neighbor Coulomb repulsion. All results will be presented for t=1, that is, all quantities are given in units of t. We will present the results for a fixed U=3.4 and several values of V.

3.1. Pure DDW state

In the absence of superconductivity, the gap equation for the DDW order parameter Δ_D can be written as

$$\frac{1}{V+P} = \frac{1}{N} \sum_{\mathbf{k}} \theta(|\varepsilon_{\mathbf{k}}| - |\varepsilon_{F}|) \frac{d_{\mathbf{k}}^{2}}{4E_{\mathbf{k}}} \left\{ \tanh \frac{E_{\mathbf{k}} + \mu}{2T} + \tanh \frac{E_{\mathbf{k}} - \mu}{2T} \right\}, \tag{14}$$

with $E_{\mathbf{k}} = [\varepsilon_{\mathbf{k}}^2 + \Delta_D^2(\mathbf{k})]^{1/2}$. In the DDW state the energy dispersion splits into two branches $\pm E_{\mathbf{k}}$ with the $d_x 2_{-y} 2$ -wave gap $\Delta_D(\mathbf{k}) = \Delta_D(\cos k_x - \cos k_y)$. They are connected with each other at the nodal points ($\pm \pi/2$, $\pm \pi/2$) and separated by the maximum gap $2\Delta_D$ at the points ($\pm \pi$, 0) and (0, $\pm \pi$). The equations $E_{\mathbf{k}} \pm \mu = 0$ define effective Fermi surface of the DDW state. For hole doping the effective Fermi surface consists of hole pockets around the nodal points ($\pm \pi/2$, $\pm \pi/2$).

The DDW transition temperature T^* is defined as the temperature at which $\Delta_D(T) \rightarrow 0$. In this case, $E_{\mathbf{k}} \rightarrow |\varepsilon_{\mathbf{k}}|$, all the quantities become the same as in the normal state. Thus, T^* is found by solving Eq. (14) with $\Delta_D(T) \rightarrow 0$ and P in the normal state. In Fig. 1 we show our results for T^* as a function of the hole doping δ for U=3.4 and V=0.9. With increasing doping δ , T^* first decreases slowly in the small doping region and then vanishes rapidly at a doping δ_c , which is called the quantum critical point (QCP) of the DDW state. The dashed line shows the result of previous studies (Refs. [14–16]) calculated from Eq. (14) without regard to the step function. In our calculation taking account of the step function the DDW transition temperature T^* as a function of doping decreases monotonously with increasing doping and goes towards the larger dopings, which is similar to the phenomenological result of Ref. [12], while in Refs. [14–17] taking not into account the step function it moves to lower dopings after passing a large doping. This step function plays an important role in our theory for the competition and interplay between the DDW and superconductivity, for they can coexist below the dished line as shown below.

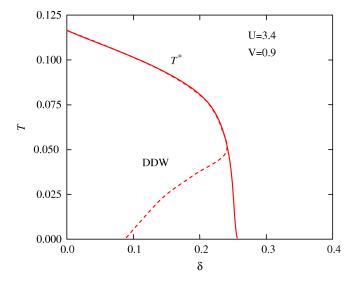


Fig. 1. Phase diagram for the pure DDW state in the absence of superconductivity. The dashed line denotes the result calculated without taking account of the step function $\theta(|\varepsilon_{\mathbf{k}}| - |\varepsilon_{F}|)$.

For comparison we discuss the pure superconducting transition in the absence of DDW order. In this case the gap equation for the DSC order parameter Δ_B can be written as

$$\frac{1}{-V+P} = \frac{1}{N} \sum_{\mathbf{k}} \frac{d_{\mathbf{k}}^2}{2[(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_B^2(\mathbf{k})]^{1/2}} \tanh \frac{[(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_B^2(\mathbf{k})]^{1/2}}{2T}, \tag{15}$$

This is the well-known BCS equation for the DSC gap induced by spin fluctuations. In the limit of V=0 and at half-filling ($\mu=0$) two Eqs. (14) and (15) are the same with each other, yielding $T^*=T_c$. For a finite repulsion V, T^* is higher than T_c at small dopings. Therefore, the introduction of the nearest-neighbor Coulomb repulsion V yields a possibility of the DDW state dominating in the small region of doping. In Fig. 2 we present the doping dependence of the temperatures T^* and T_c for V=0.0 and 0.9 in the uncoupled case. T^* decreases rapidly with increase in doping. For V=0.9 T_c is lower than T^* at lower dopings $\delta < \delta_c$, whereas it decreases so rather slowly to become nonzero at large dopings $\delta > \delta_c$ where $T^*=0$. Note that with the increase of V the DDW-transition temperature T^* is much higher and the corresponding QCP δ_c shifts slightly to higher dopings.

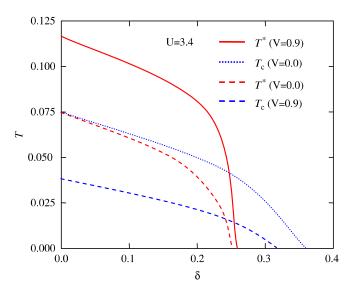


Fig. 2. Phase diagram for the uncoupled superconducting and DDW state for V=0.0 and 0.9.

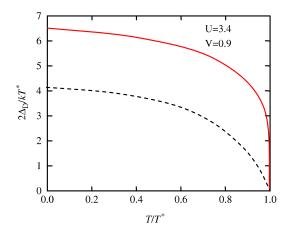


Fig. 3. Temperature dependence of the DDW gap $2\Delta_D/kT^*$ at a doping δ =0.21. Dashed line is the result of the conventional weak-coupling theory.

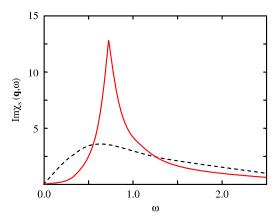


Fig. 4. Spin susceptibility Im $\chi_s(\mathbf{q}, \omega)$ at a doping δ =0.21. The dashed line and solid line correspond to T/T^* =1.5 (normal state) and T/T^* =0.1(DDW state), respectively.

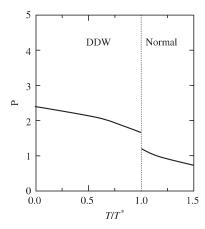


Fig. 5. Temperature dependence of the pairing interaction strength *P*.

Below T^* we calculate the DDW gap parameter Δ_D , the spin fluctuation spectrum Im $\chi_s(\mathbf{q}, \mathbf{v})$, and the coupling parameter P by solving the Eqs. (14) and (12) self-consistently within the FLEX approximation. The resulting temperature dependence of Δ_D is shown in Fig. 3 along with the one of the conventional weak-coupling theory where the coupling parameter is constant. We find that the DDW gap develops much more rapidly within the FLEX approximation (solid line) as compared with the weak-coupling theory (dashed line). This behavior is associated with the feedback effect on spin fluctuations of the DDW gap.

Fig. 4 shows a typical result for the spin fluctuation spectrum Im $\chi_s(\mathbf{Q}, \mathbf{v})$ at the antiferromagnetic wave vector obtained within FLEX approximation. In the normal state the spectrum is comparatively structureless, as shown by the dashed line. The solid line shows results in the DDW state. The opening of the DDW gap leads to a suppression of spectral weight at low frequencies, but at higher frequencies a strong resonance-like peak appears in Im $\gamma_s(\mathbf{Q}, \mathbf{v})$. The appearance of such a strong peak in the spin fluctuation spectrum yields an enhancement of the coupling parameter P in Eq. (15), as shown in Fig. 5. This in turn leads to an increase of the DDW gap, resulting in a positive feedback effect. This is the reason for the almost jump-like increase of the DDW gap in company with the pairing interaction below T^* . Such a strong enhancement of the spin fluctuation pairing interaction due to feedback of the DDW gap will especially important in explaining high-temperature superconductivity induced by DDW as shown below.

3.2. Superconducting transition from the DDW state

We now study the superconducting transition from the DDW state within FLEX theory, neglecting the π -pairing order parameter. In the DDW state the equation for the superconducting transition temperature T_c is given from Eq. (10) as follows:

$$\frac{1}{-V+P} = \frac{1}{N} \sum_{\mathbf{k}} \frac{d_{\mathbf{k}}^2}{4} \left(\frac{1}{E_{\mathbf{k}} + \mu} \tanh \frac{E_{\mathbf{k}} + \mu}{2T_c} + \frac{1}{E_{\mathbf{k}} - \mu} \tanh \frac{E_{\mathbf{k}} - \mu}{2T_c} \right), \quad (16)$$

where $E_{\mathbf{k}} = [\varepsilon_{\mathbf{k}}^2 + \Delta_D^2(\mathbf{k})]^{1/2}$ is the quasiparticle energy in the DDW state. Here, we use the DDW gap Δ_D and the coupling parameter P calculated in the pure DDW state by solving Eqs. (14) and (12) self-consistently. Since the coupling parameter P is strongly enhanced due to the feedback effect on spin fluctuations of the DDW gap as shown above, the superconducting transition temperature T_c in the DDW state can be much larger than expected in the spin fluctuation theory without DDW order.

In Fig. 6 we show the result for the T_c calculated from Eq. (16) in the DDW state. Near half-filling T_c is zero. With increasing doping T_c starts to increase at a finite doping δ_1 , reaching a maximum at an optimal doping δ_m , then decreases with further increase of doping as $T_c = T^*$ as far as the QCP δ_c . After passing δ_c , T_c becomes the pure superconducting transition temperature in the absence of DDW order.

In order to get better understanding of this behavior, we take a look at the integral in Eq. (16). The dominant contribution to the integral arises from the vicinity of the effective Fermi surface defined by the equations $E_{\mathbf{k}} \pm \mu = 0$. For hole doping $(\mu < 0)$ the Fermi surface $E_{\mathbf{k}} + \mu = 0$ consists of hole pockets around the nodal points ($\pm \pi/2$, $\pm \pi/2$). At small dopings, since small hole pockets are opened around the nodal points and there $d_{\mathbf{k}}^2 \rightarrow 0$, Eq. (14) yields $T_c \rightarrow 0$. When the hole pockets are large enough, for large doping, $d_{\mathbf{k}}^2$ has a finite value near the Fermi surface, resulting in a finite T_c . This is the reason for the increase of T_c with increasing doping. Close to the QCP δ_c , where the DDW gap vanishes, the density of states is closer to the one for the normal state, so that the transition temperature T_c for the DDW-induced superconductivity is much higher than expected for the pure superconductivity induced by spin fluctuations because the coupling parameter P is strongly enhanced due to the feedback effect on spin fluctuations of the DDW gap. A further result of this feedback effect is $T_c = T^*$ close to the QCP δ_c . This is caused by the jump-like increase of both the DDW gap and coupling parameter below T^* .

It should be pointed out that such a strong enhancement of the superconducting transition temperature T_c in the DDW state close

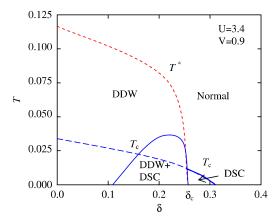


Fig. 6. Phase diagram of the hole-doped 2D Hubbard model with U=3.4 and V=0.9. The dashed–dotted line shows the DDW temperature T^* , the solid and dashed lines show the superconducting T_c in the presence and absence of DDW order, respectively. δ_c is the QCP at which the DDW state vanishes.

to the QCP is quite a new phenomenon and to the best of our knowledge no such theoretical demonstration exists. Our result is obtained from the following two facts. The first is the introduction of the step function $\theta(|\varepsilon_{\mathbf{k}}|-|\varepsilon_F|)$ in Eq. (14) for the DDW gap, which yields the coexistence region of the DDW and DSC close to the QCP at which the DDW state vanishes. Without taking account of this step function, no coexistence is found between the DDW and DSC because the boundary of the DDW state is given as the dashed line in Fig. 1. The second is the feedback effect on spin fluctuations of the DDW gap, which leads to a strong enhancement of the coupling parameter P in Eq. (16) for the superconducting transition temperature T_c in the DDW state.

3.3. Competition between order parameters

Here, we discuss the results obtained from self-consistently solving the coupled gap Eqs. (9)–(11) for competing DDW, DSC, and π -pairing as the possible order parameters within the FLEX approximation. When the DDW and superconductivity coexist π pairing appears generically, the corresponding order parameter Δ_H is usually tiny. The reason is that since the factor $(\mu_{\bf k}-E_{\bf k})/\mu_{\bf k}$ in Eq. (11) is smaller than one, Cooper pairing is dominant and suppresses π pairing strongly. Hence the π -pairing order parameter is very small compared to the others, such that its feedback into the gap equations for Δ_D and Δ_B can be neglected. Similar results are obtained in the renormalized mean-field analysis of antiferromagnetism and superconductivity [20].

In Fig. 7 we show the temperature dependence of the DDW and DSC gaps Δ_D and Δ_B , calculated at a fixed δ =0.21. The dotted and dashed lines show the results for uncoupled Δ_D and Δ_B ,

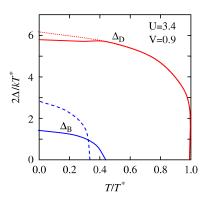


Fig. 7. Temperature dependence of competing DDW and DSC order parameters Δ_D (two outer lines) and Δ_B (two inner lines) calculated at δ = 0.21. Dotted and dashed lines are the corresponding results for uncoupled case.

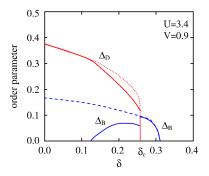


Fig. 8. Doping dependence of the order parameters \varDelta_D and \varDelta , calculated at $T/T^* = 0.02$.

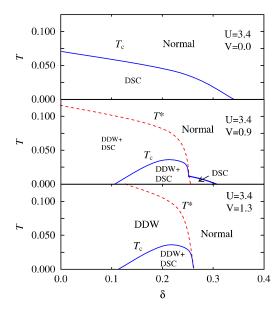


Fig. 9. Evaluation of the phase diagram for U=3.4 and different nearest-neighbor Coulomb repulsions.

respectively. After the growth of the DSC gap below T_c , the DDW gap is slightly suppressed and remains almost constant with lowing temperature. The DDW-induced-DSC gap develops at higher temperature, but its magnitude is small compared to the pure DSC gap. Below T_c the DDW and DSC gaps coexist.

In Fig. 8 we show the doping dependence of the gap parameters Δ_D and Δ_B , calculated at $T/T^* = 0.02$. The uncoupled DDW gap (dotted line) first decreases monotonically with increasing δ , then vanishing rapidly at the QCP δ_c =0.26. The uncoupled DSC gap (dashed line) is smaller than the DDW gap at lower dopings $\delta < \delta_c$ due to the nearest-neighbor Coulomb repulsion V, but it decreases so rather slowly to become nonzero up to large dopings $\delta_c < \delta_2 = 0.32$. The solid lines show the doping dependence of competing gap parameters Δ_D and Δ_B . Near half filling the DSC gap Δ_B is completely suppressed due to the strong competition with the DDW gap Δ_D . Upon further doping, Δ_B first appears at a doping δ_1 = 0.12 and increases with increasing δ , coexisting with the DDW gap up to δ_c . The DDW gap is slightly suppressed by the appearance of the DSC gap in the doping region $\delta_1 < \delta < \delta_c$. After passing δ_c the DDW gap is zero and only the pure DSC gap exists. Thus the QCP δ_c separates a pure superconducting state at large dopings from a ground state containing both the DDW and superconducting gaps.

Finally we discuss the dependence of the phase diagram on the nearest-neighbor Coulomb repulsion V. Fig. 9 shows the phase diagrams calculated for V=0.0, 0.9, and 1.3. The solid line shows the superconducting transition temperature T_c . The dasheddotted line describes the DDW transition temperature T^* . In the case of negligible Coulomb repulsion, i.e., V=0.0, the superconducting phase is dominant in the whole region of doping and wipes out the DDW phase as shown in the upper panel of Fig. 9. Lowering the temperature from high values one crosses the solid line and enters the pure superconducting region. Increasing Vthe pure superconducting state is more and more suppressed whereas the DDW state becomes dominant at lower dopings. This is shown in the middle panel of Fig. 9 for V=0.9, which is the same diagram as Fig. 6. Moreover, the superconducting region is now split into two regions. In the overdoped region only a pure superconducting phase exists, whereas in the underdoped region the superconducting and DDW phases coexist with each other. In the underdoped region a pure DDW phase exists above T_c with a pseudogap of d-wave symmetry in the excitation spectrum. When V exceeds a threshold, i.e., V > 1.3, the total effective interaction -V+P becomes repulsive and the pure superconducting phase is completely suppressed in the overdoped region, as shown in the lower panel of Fig. 9.

As shown above, it is in general necessary to include the nearest-neighbor Coulomb repulsion V in order to stabilize the DDW, which gives a good description of the pseudogap behavior in the underdoped region. Note that the DDW-induced-superconducting T_c remains almost constant even with increase of the Coulomb repulsion V, as shown in the middle and lower panels of Fig. 9. This behavior may be explained as follows: the increase of V leads to an enhancement of the coupling parameter P due to the feedback effect of the enhanced DDW gap, which gives compensation for a decrease in T_c due to the increase of V. The position of the maximum T_c is close to the QCP of the DDW state and also does hardly move with increasing V.

4. Conclusion

We have found that high-temperature superconductivity is induced due to the feedback effect on spin fluctuations of the DDW in the 2D Hubbard model. Using the FLEX approximation we have derived the coupled gap equations for the DDW, DSC, and π pairing as the possible order parameters induced by exchange of spin fluctuations. In order to stabilize the DDW state with respect to phase separation in the underdoped region, we have included a small nearest-neighbor Coulomb repulsion within the Hartree-Fock approximation. Calculating the strength of the pairing interaction in the $d_x 2_{-y} 2$ -wave channel mediated by spin fluctuations self-consistently, the coupled gap equations for competing order parameters have been solved and the corresponding transition temperatures have been found. Our principle findings are: (1) Even when nesting of the Fermi surface is perfect, as in a square lattice with only nearest-neighbor hopping t, due to the feedback effect on spin fluctuations the DDW and DSC can coexist in the relatively large region of doping close to the QCP at which the DDW state vanishes. (2) The superconducting transition temperature T_c in the DDW state can be much higher compared to pure superconductivity, since the pairing interaction strength is enhanced strongly due to the feedback of the DDW gap. (3) With an increase of the Coulomb repulsion the DDWinduced-superconducting T_c remains almost constant whereas the pure T_c decreases strongly. (4) By the QCP the phase diagram is split into two regions: in the overdoped region only a pure superconducting phase exists, whereas in the under- and optimally doped region the superconducting and the DDW order parameters coexist. Our results give a good explanation for high-temperature superconductivity and pseudogap phenomena in cuprates.

In the present work, we have developed a weak-coupling theory of the competition between DDW and DSC in 2D Hubbard model, using the static spin fluctuation obtained within FLEX approximation and ignoring the self-energy effect of spin fluctuations. For our model calculations in the weak-coupling limit we have taken U/t = 3.4, since the antiferromagnetic instability occurs for higher values of U/t.

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