$d$-wave superconductivity and its coexistence with antiferromagnetism in $t-J-U$ model revisited: Statistically consistent Gutzwiller approach

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We discuss the coexistence of antiferromagnetism and $d$-wave superconductivity within the statistically-consistent Gutzwiller approximation (SGA) to the $t-J-U$ model. In this approach, the averages calculated in a self-consistent manner coincide with those determined variationally. Such consistency is not guaranteed within the standard Renormalized Mean Field Theory (RMFT).

With the help of SGA we show that the coexistence of antiferromagnetism (AF) and superconductivity (SC) appears only in a very narrow range of doping $\delta \leq 0.006$ in the vicinity of the Mott insulating state. The spin-singlet superconductivity disappears at the doping $\delta \approx 1/3$, in accordance with experiment for almost all cuprate high-temperature superconductors. In the coexistent AF+SC phase a very small staggered spin-triplet component of the superconducting gap appears also naturally.

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I. INTRODUCTION: RATIONALE FOR $t-J-U$ MODEL

High-temperature superconductivity is often described within the effective $t-J$ model12 when transformed to the form with the pairing operators in an explicit form (for the early review see Ref.13). It provides a successful rationalization of a number of experimental results such as dome-like shape of the superconductivity appearance on the phase diagram,14 non-Fermi liquid behavior of the normal state for the underdoped and optimally doped systems15,16,17 a disappearance of the pairing gap magnitude in the antiferromagnetic state, albeit only at the doping $\delta = 0.15$ and the doping dependence of the photoemission spectrum in the antinodal directions.9,10 All these features represent an attractive starting point for a further analysis (for a review see e.g. Ref.11).

In the effective $t-J$ model, the value of the kinetic exchange integral $J_{ij}$ does not necessarily coincide with the value $J_{ij} = 4\tilde{t}_{ij}/U$ obtained perturbationally from the Hubbard model. Instead, it expresses an effective coupling between the copper spins in the milieu of mixed copper-oxygen $2p-3d$ holes.12 Therefore, one may say that the values of the hopping integral $t_{ij}$ and that of antiferromagnetic exchange $J_{ij}$ in that model, are practically independent. Typically, the ratio $|t|/J \approx 3$ is taken what corresponds to the value $U/(8|t|) = 1.5$ in the context of the two-dimensional Hubbard model, i.e. after introducing the bare bandwidth $W = 8|t|$ in the tight-binding approximation for a square lattice, we obtain the ratio $U/W = 1.5$ which is not sufficiently large for the transformation of the original Hubbard model into the $t-J$ model to be valid to the low order. In that situation we are, strictly speaking, not in the strong correlation limit $U/W \gg 1$, in which the $t-J$ model was derived in the first place.12

In that situation, one may propose, that in order to account properly for the strong electronic correlations (the bare Hubbard parameter $U$ for Cu$^{2+}$ ion is 8-10 eV $\gg W \sim 2$ eV), we can add the Hubbard term $U\sum_i n_i \hat{n_i}$ to the $t-J$ model expression in the second order. In this manner, we regard in this still effective single-band model the exchange integral $J_{ij}$ as coming from full superexchange involving the oxygen ions rather than from the effective kinetic exchange only (for critical overview c.f. Ref.13). This argument may be regarded as one of the justifications for introducing the $t-J-U$ model (first used by Daul14 and Zhang15).

Antiferromagnetism (AF) and superconductivity (SC) can coexist in the electron doped cuprates17,18 but in the hole-doped cuprates the two phases are separated (cf. e.g. the review of Dagotto19). However, in the late nineties, reports of a possible coexistence in the cuprates appeared, first vague (cf. Kimura19 and his study of La$_2$−$x$Sr$_x$Cu$_{1-y}$Zn$_y$O$_4$), then more convincing (cf. e.g. Lee20 (study of La$_2$CuO$_{4+y}$)), Sidis21 (study of YBa$_2$Cu$_3$O$_{6.5}$), and Hodges22 (study of YBa$_2$(Cu$_{0.987}$Co$_{0.013}$)$_2$O$_{y+3}$)). Other systems, where the coexistence has been reported are the organic superconductors23 heavy-fermions systems24 iron-based superconductors such as Ba(Fe$_{1−x}$Ru$_x$)$_2$As$_2$ (studied by Ma25), Ba$_{0.77}$K$_{0.23}$Fe$_2$As$_2$ (studied by Ma25), Ba(Fe$_{1−x}$Co$_x$)$_2$As$_2$ (studied by Marsil25 and Bernhard25) and the graphene bilayer systems (cf. Milovanov26). Most of the listed works have been published in the last few years.

Our purpose is to undertake a detailed analysis of the paired (SC) state within the $t-J-U$ model and its coexistence with the two-sublattice antiferromagnetism in two dimensions. In this respect, detailed studies of the $t-J-U$ model have been carried out by Zhang27 Gan28 and Bernevig29 who described a transition from gossamer29
and $d$-wave superconductivity to the Mott insulator. However, the existence of AF order parameter was not examined there. Some attempts were made by Yuan and Heiselberg but in all those works one can raise the question concerning a mutual statistical consistency of the (mean-field) averages introduced in a self-consistent manner with those determined variationally. We show that the above problems appearing in the standard formulation, can be overcome by introducing, with the help of Lagrange multiplier method, the constraints assuring the equivalence of the two above ways of determining the mean-field values. This is the principal idea of our statistically consistent Gutzwiller approach (SGA) Using SGA, we obtain that AF is stable only in the presence of SC in a very narrow region close to the Mott-Hubbard insulating state, corresponding to the half-filled (undoped) situation. Additionally, in this AF-SC coexistent phase, a small staggered spin-triplet component of the superconducting gap appears naturally, in addition to the $d$-wave spin-singlet component. Furthermore, a universal upper-critical doping concentration $\delta = \delta_c \approx 1/3$ for the disappearance of the pure spin singlet superconductivity is obtained in the strong correlation limit, in agreement with the experimental data for the cuprates as well as with the recent statistically-consistent mean-field results for the $t$-$J$ model.

The structure of the paper is as follows. In Sec. II we define the model and provide the definition of the mean-field parameters. In Sec. III we introduce the constraints with the corresponding Lagrange multipliers to guarantee the consistency of the self-consistent and the variational procedures of determining those mean fields parameters. The full minimization procedure is also outlined there. In Sec. IV we discuss the numerical results, as well as provide the values of the introduced Lagrange multipliers. In Sec. V we summarize our results and compare them with those of other works. In Appendix A we discuss general form of the hopping amplitude and the superconducting gap, as well as some details of the analytic calculations required to determine the ground state energy. In Appendix B we present an alternative and equivalent procedure of introducing the Lagrange multipliers to that presented in the main text.

II. $t$-$J$-$U$ MODEL

We start from the $t$-$J$-$U$ model as represented by the Hamiltonian

$$\hat{H} = t \sum_{\langle ij \rangle, \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right) + J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

where $\sum_{\langle ij \rangle}$ denotes the summation over the nearest-neighboring sites, $t$ is the hopping integral, $J$ is the exchange coupling constant, $\hat{S}_i$ is the spin operator in the fermion representation and $U$ is the on-site Coulomb repulsion magnitude.

We study properties of the above Hamiltonian using the Gutzwiller variational approach, in which the trial wave function has the form $\Psi = \hat{P}_G \Psi_0$, where $\hat{P}_G$ is an operator reducing the contribution of configurations with double on-site occupancies and $|\Psi_0\rangle$ is an eigenstate of some single-particle Hamiltonian (not determined as yet). Since the correlated state $|\Psi\rangle$ is related to $|\Psi_0\rangle$, the average value of the Hamiltonian $\hat{H}$ can be expressed as

$$\langle \Psi | \hat{H} | \Psi \rangle = \frac{\langle \Psi_0 | \hat{P}_G \hat{H} \hat{P}_G | \Psi_0 \rangle}{\langle \Psi_0 | \hat{P}_G^2 | \Psi_0 \rangle} \approx \frac{\langle \Psi_0 | \hat{H}_{\text{eff}} | \Psi_0 \rangle}{\langle \Psi_0 | \hat{P}_G | \Psi_0 \rangle} \equiv \langle \hat{H}_{\text{eff}} \rangle_0,$$

where $\langle \ldots \rangle_0$ means the average evaluated with respect to $|\Psi_0\rangle$, and

$$\hat{H}_{\text{eff}} = g_t \sum_{\langle ij \rangle, \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right) + g_s J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j + U d^2$$

is the effective Hamiltonian resulting from the Gutzwiller Approximation (GA). In the above formula $d^2$ is the average double-occupancy probability, $g_t$ and $g_s$ are the Gutzwiller renormalization factors:

$$g_t = \frac{n - 2d^2}{n - 2w} \left( \frac{(1 - w)(1 - n + d^2)}{1 - r} + \sqrt{\frac{w d^2}{r}} \right) \times \left( \frac{(1 - r)(1 - n + d^2)}{1 - w} + \sqrt{\frac{r d^2}{w}} \right),$$

$$g_s = \left( \frac{n - 2d^2}{n - 2w} \right)^2,$$

where $n$ is the average number of electrons (occupancy) per site. To consider AF order the lattice is divided into two sublattices: $A$, where the majority of spins are $\uparrow$, and $B$, where the majority of spins are $\downarrow$. For $A$ sublattice, we have that $r \equiv \langle \hat{n}_i \rangle = \frac{1}{2} (n + m_{AF})$ and $w \equiv \langle \hat{n}_i \rangle = \frac{1}{2} (n - m_{AF})$, where $m_{AF}$ is the antiferromagnetic (staggered) spin polarization per site. For $B$ sublattice, the definitions of $w$ and $r$ are interchanged. Such division allows us to express the average number of electrons on site $i$ with spin $\sigma$ as

$$n_{i\sigma} \equiv \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \rangle_0 = \frac{1}{2} \left( n + \sigma e^{iQ \cdot R_i} m_{AF} \right),$$

with $Q \equiv (\pi, \pi)$, and with $R_i$ denoting position vector of site $i$. In order to evaluate $\langle \hat{H}_{\text{eff}} \rangle_0$ we define the following bare (nonrenormalized) quantities: the hopping amplitude for the nearest neighbors $\langle i, j \rangle$

$$\chi_{ij} \equiv \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \rangle_0 = \chi_{AB},$$

the pairing order parameter

$$\Delta_{ij} \equiv \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \rangle_0 = -\tau_{ij} (\sigma \Delta_S + e^{iQ \cdot R_i} \Delta_T),$$

where $\tau_{ij} \equiv 1$ for $j = i \pm \hat{x}$ and $\tau_{ij} \equiv -1$ for $j = i \pm \hat{y}$ (in order to ensure the $d$-wave symmetry). In consequence, the
defining a single order parameter in Fig. 1. In principle, where for the square lattice obtained in the form (cf. Eq. (A8) in Appendix A) of the gap are defined as

\[ \tau_{ij} \Delta_S = \frac{1}{4} \left( \langle \hat{c}_{ij} \hat{c}_{ji} \rangle_0 + \langle \hat{c}_{ij} \hat{c}_{ji} \rangle_0 + \text{H.c.} \right) \]

\[ = \frac{1}{4} \tau_{ij} (\Delta_A + \Delta_B + \text{H.c.}) , \tag{8a} \]

\[ \tau_{ij} \Delta_T = \frac{1}{4} \left( \langle \hat{c}_{ij} \hat{c}_{ji} \rangle_0 - \langle \hat{c}_{ij} \hat{c}_{ji} \rangle_0 + \text{H.c.} \right) \]

\[ = \frac{1}{4} \tau_{ij} (\Delta_A - \Delta_B + \text{H.c.}) . \tag{8b} \]

The graphical representation of \( \Delta_A \) and \( \Delta_B \) is provided in Fig. 1. In principle, \( \Delta_A \) and \( \Delta_B \) can be different, so defining a single order parameter \( \Delta = \Delta_{ij} \) for SC phase is insufficient (cf. Tsonis and Aperis). Applying the Wick’s theorem and the definitions introduced above, the expectation value of \( \langle \hat{H}_{\text{eff}} \rangle_0 \) \( \equiv \hat{W} \) is obtained in the form (cf. Eq. (A8) in Appendix A)

\[ \hat{W} = 8g_t \chi_{AB} + Ud^2 - \lambda_{\chi} \left( \frac{1}{2} m_{AF}^2 + 3x_{AB}^2 + 3\Delta_S^2 - \Delta_T^2 \right) , \tag{9} \]

where \( \lambda_{\chi} \) is the number of atomic sites in the system. In what follows, we incorporate the statistical-consistency constraints into the present formulation and determine the physical ground-state energy as limiting value (for temperature \( T \to 0 \)) of the grand thermodynamic potential.

### III. QUASIPARTICLE STATES AND MINIMIZATION PROCEDURE FOR THE GROUND STATE

Following Refs. [10, 12, 49, and 50] we write the mean-field grand Hamiltonian in the form

\[ \hat{K} \equiv \hat{W} - \sum_{(ij),\sigma} (\lambda^{ij}_{\sigma} (\hat{c}_{ij} \hat{c}_{ji} - \chi_{ij}) + \text{H.c.}) \]

\[ - \sum_{(ij),\sigma} (\lambda^{ij}_{\sigma} (\hat{c}_{ij} \hat{c}_{ji} - \chi_{ij} \sigma) + \text{H.c.}) \]

\[ - \sum_{i\sigma} (\hat{\lambda}^{i\sigma} (\hat{n}_{i\sigma} - n_{i\sigma})) - \mu \sum_{i\sigma} \hat{n}_{i\sigma} , \tag{10} \]

with \( \mu \) being the chemical potential, and the Lagrange multipliers \( \{ \lambda^{ij}_{\sigma} \} \) are introduced in general for each operator whose average appears in \( \hat{W} \) (Eq. (9)). The Lagrange multipliers can be interpreted as the correlation-induced effective fields. Those fields are assumed to have the same symmetry as corresponding to them averages (cf. Eqs. (5), (6), and (7)), namely

\[ \lambda^{i\sigma}_{n} = \frac{1}{2} (\lambda_{\chi} + \text{e}^{iQ_{\chi}} \lambda_{m}) , \tag{11a} \]

\[ \lambda^{i\sigma}_{\chi} = \lambda_{\chi} , \tag{11b} \]

\[ \lambda^{i\sigma}_{\lambda} = -\tau_{ij} \left( \sigma \lambda_{\Delta} + \text{e}^{iQ_{\lambda}} \lambda_{\Delta T} \right) . \tag{11c} \]

The effective Hamiltonian in form (10) and the constraints (11a)–(11c) constitute the statistically consistent Gutzwiller approach (SGA) discussed in the remaining part of the paper.

To diagonalize \( \hat{K} \), we perform first the space Fourier transform. The result can be rewritten in the following \( 4 \times 4 \) matrix form

\[ \hat{K} = \hat{W} + \sum_{\epsilon} \hat{\psi}_{k}^\dagger \hat{M}_{k} \hat{\psi}_{k} + \frac{1}{2} \Lambda (\lambda_{\chi}(n-1) + \lambda_{m} m_{AF}) \]

\[ - \Lambda \mu + 8 \lambda_{\chi} \chi_{AB} + 8 \lambda_{\chi} (\lambda_{\Delta S} + \lambda_{\Delta T}) , \tag{12} \]

where \( \hat{\psi}_{k}^\dagger = (\hat{c}_{k\uparrow}, \hat{c}_{-k\uparrow}, \hat{c}_{k+Q_{\uparrow}}, \hat{c}_{-k+Q_{\uparrow}}) \), the sum is evaluated over the reduced (magnetic) Brillouin zone \(|k_x| + |k_y| \leq \pi\), and

\[ \hat{M}_{k} = \begin{pmatrix} -\lambda_{\chi} \epsilon_{k} - \frac{1}{2} \lambda_{\mu} - \lambda_{\Delta S} \eta_{k} & -\lambda_{\Delta S} \eta_{k} & -\frac{1}{2} \lambda_{m} & \lambda_{\Delta T} \eta_{k} \\
-\lambda_{\Delta S} \eta_{k} & \lambda_{\chi} \epsilon_{k} + \frac{1}{2} \lambda_{\mu} + \mu & -\lambda_{\Delta T} \eta_{k} & -\frac{1}{2} \lambda_{m} \\
-\frac{1}{2} \lambda_{m} & -\lambda_{\Delta T} \eta_{k} & \lambda_{\chi} \epsilon_{k} - \frac{1}{2} \lambda_{\mu} - \mu & \lambda_{\Delta S} \eta_{k} \\
\lambda_{\Delta T} \eta_{k} & -\frac{1}{2} \lambda_{m} & -\lambda_{\Delta S} \eta_{k} & -\lambda_{\chi} \epsilon_{k} + \frac{1}{2} \lambda_{\mu} + \mu \end{pmatrix} , \tag{13} \]

where for the square lattice

\[ \epsilon_{k} \equiv 2 (\cos k_{x} + \cos k_{y}) , \tag{14a} \]

\[ \eta_{k} \equiv 2 (\cos k_{x} - \cos k_{y}) . \tag{14b} \]

Diagonalization of \( \hat{M}_{k} \) yields four branches of eigenvalues.
with their explicit form

$$E_{lk} = E_{l+1,k} = \frac{1}{2} \sqrt{K_{lk} + 2K_{kl}}, \quad (15)$$

where \(l = 1, \ldots, 4\), and

$$K_{lk} = 4e_k^2 \lambda^2 + (\lambda_n + 2\mu)^2 + 4\eta_k^2 (\lambda_{\Delta s}^2 + \lambda_{\Delta T}^2) + \lambda_n^2,$$  

$$K_{kl} = 4(4\eta_k^2 \lambda_{\Delta s} \lambda_{\Delta T} + \lambda_n (\lambda_n + 2\mu))^2 + 4e_k^2 \lambda^2 (4\eta_k^2 \lambda_{\Delta T}^2 + (\lambda_n + 2\mu)^2). \quad (16a)$$

The energies \(\{E_{lk}\}_{l=1,\ldots,4}\) represent quasiparticle bands after all the parameters (mean-fields, parameters, the Lagrange multipliers, and \(d\)), are determined variationally.

Next, we define the generalized grand potential functional at temperature \(T > 0\) as given by

$$\mathcal{F} = -\frac{1}{\beta} \ln Z, \quad \text{with} \quad Z = \text{Tr} \left( e^{-\beta \hat{K}} \right), \quad (17)$$

and \(\beta \equiv 1/k_B T\). As we are interested in the ground-state properties (\(T = 0\)), we take the \(T \to 0\) limit. We have checked that taking \(k_B T = 0.002|t|\) is sufficient for the practical purposes. Explicitly, \(\mathcal{F}\) has then the following form

$$\mathcal{F}/\Lambda = 8g_t \chi_{\Delta s} - g_s J \left( \frac{1}{2} m_{AF}^2 + 3\lambda_{\Delta s}^2 + 3\lambda_{\Delta T}^2 \right) + \frac{1}{\beta} \lambda_\beta (n-1) + \frac{1}{2} \lambda_m m_{AF} + 8 (\lambda_\chi \chi_{\Delta s} + \lambda_{\Delta s} \Delta s + \lambda_{\Delta T} \Delta T) \right) - \frac{1}{\Lambda \beta} \sum_{l,k} \ln (1 + e^{-\beta E_{lk}}) + Ud^2 - \mu. \quad (18)$$

The necessary conditions for the minimum of \(\mathcal{F}\) subject to constraints (5), (6), (7) are

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = 0, \quad \frac{\partial \mathcal{F}}{\partial \lambda_\beta} = 0, \quad \text{and} \quad \frac{\partial \mathcal{F}}{\partial d} = 0, \quad (19)$$

where the five mean-field parameters are labeled collectively as \(\Lambda\), and the Lagrange multipliers as \(\lambda\). Explicitly, we obtain the following set of equations

$$\lambda_\chi = -g_t \frac{3}{4} g_s \chi_{\Delta s}, \quad (20a)$$

$$\lambda_{\Delta s} = \frac{3}{4} g_s \chi_{\Delta s}, \quad (20b)$$

$$\lambda_{\Delta T} = -\frac{1}{4} g_s \chi_{\Delta T}, \quad (20c)$$

$$\lambda_n = -16t \chi_{\Delta s} \chi_{\Delta T} \frac{\partial g_s}{\partial n},$$

$$-2J \left( \frac{1}{2} m_{AF}^2 - 3\chi_{\Delta s}^2 - 3\Delta s^2 + \Delta T^2 \right) \frac{\partial g_s}{\partial n} \quad (20d)$$

$$\lambda_m = 2g_t m_{AF} - 16t \chi_{\Delta s} \chi_{\Delta T} \frac{\partial g_s}{\partial m_{AF}},$$

$$-2J \left( \frac{1}{2} m_{AF}^2 - 3\chi_{\Delta s}^2 - 3\Delta s^2 + \Delta T^2 \right) \frac{\partial g_s}{\partial m_{AF}} \quad (20e)$$

$$\frac{1}{\Lambda} \sum_{k,l} f(E_{lk}) \frac{\partial \mathcal{F}}{\partial \lambda_\chi_{lk}} + 8 \chi_{\Delta s} = 0, \quad (20f)$$

$$\frac{1}{\Lambda} \sum_{k,l} f(E_{lk}) \frac{\partial \mathcal{F}}{\partial \lambda_{\Delta s}^k l} + 8 \Delta s = 0, \quad (20g)$$

$$\frac{1}{\Lambda} \sum_{k,l} f(E_{lk}) \frac{\partial \mathcal{F}}{\partial \lambda_{\Delta T}^k l} + 8 \Delta T = 0, \quad (20h)$$

$$\frac{1}{\Lambda} \sum_{k,l} f(E_{lk}) \frac{\partial \mathcal{F}}{\partial \lambda_n^k l} + 8 \lambda_n = 0, \quad (20i)$$

$$\frac{1}{\Lambda} \sum_{k,l} f(E_{lk}) \frac{\partial \mathcal{F}}{\partial \lambda_m^k l} + 8 \lambda_m = 0, \quad (20j)$$

$$\begin{align*}
2Ud + 8t \chi_{\Delta s} \frac{\partial g_s}{\partial d}
+ J \left( \frac{1}{2} m_{AF}^2 - 3\chi_{\Delta s}^2 - 3\Delta s^2 + \Delta T^2 \right) \frac{\partial g_s}{\partial d} = 0, \quad (20k)
\end{align*}$$

where \(f(E_{lk}) \equiv 1/\left(1 + e^{\beta E_{lk}}\right)\). Eqs. (20a)-(20e) can be used to eliminate the parameters \(\lambda\) from the numerical solution procedure, what reduces the number of algebraic equations to be solved numerically to six. In this manner, we are left with Eqs. (20f)-(20j) (the conditions \(\partial \mathcal{F}/\partial \lambda_\beta = 0\)) and Eq. (20k) (\(\partial \mathcal{F}/\partial d = 0\)).

The stable phase is determined by the solution which has the lowest physical free energy defined by

$$F = \mathcal{F}_0 + \mu \Lambda n, \quad (21)$$

where \(\mathcal{F}_0\) denotes the value of \(\mathcal{F}\) obtained at the minimum.

Eqs. (20a)-(20e) are solved numerically using GNU Scientific Library (GSL)\(^{31}\). For selected analytic tasks Mathematica v. 7 has been used. Unless stated otherwise, we present the results for \(t = -1\), \(J = |t|/3\), \(\beta |t| = 500\) on a two-dimensional square-lattice of size \(\Lambda = 512 \times 512\) with periodic boundary conditions.

### IV. RESULTS: PHASE DIAGRAM AND MICROSCOPIC CHARACTERISTICS

A representative phase diagram on the Coulomb repulsion \(U\) – hole doping \(\delta\) plane is exhibited in Fig. 2. We find three stable phases: paramagnetic (PM), superconducting (SC) and phase with coexisting SC and antiferromagnetic order (AF+SC). The pure AF stable phase is found only for \(\delta = 1 - n = 0\) and \(U/|t| > 10.6\). The region where the AF+SC appears is limited to a very close vicinity of the Mott insulating state (hole doping range \(\delta \in (0, 0.006)\)). The result is in qualitatively agreement with some experimental works where the region of AF+SC was reported to be narrow (cf. e.g. Bernhard\(^{28}\) (study of Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\)) where the coexistence region is not wider than 0.02 (of the hole doping range).

For further analysis we restrict ourselves to \(U/|t| = 12\), as marked by the dashed vertical line in Fig. 2. In Figs. 2 and 3, we plot the doping dependence of the mean-fields and the correlation fields, as marked in the Figures. The...
Figure 2. (Color online) Representative phase diagram for the $t$-$J$-$U$ model on the Coulomb repulsion – hole doping plane. The phases are labeled as follows: PM – paramagnetic metallic phase, SC – superconducting phase, AF+SC – phase with coexisting superconducting and antiferromagnetic orders. The pure AF stable phase is found only for $\delta = 0$ and for $U > 10.6|t|$. The bottom part is an enlargement of the region with the stable AF+SC phase. The value $U/|t| = 12$ marked by the dashed vertical line is taken in the subsequent analysis.

The magnitude of $\Delta_T$ is non-zero only in the region with AF order (i.e., $m_{AF} \neq 0$).

The correlated spin-singlet gap parameter in real space is defined as

$$\Delta_S^c = \frac{1}{4}(\langle c_{itA\uparrow}c_{jtB\downarrow}\rangle - \langle c_{itA\uparrow}c_{jtB\downarrow}\rangle + \text{H.c.})$$

where the average is calculated using the Gutzwiller wave function $|\Psi\rangle$, instead of $|\Psi_0\rangle$. Approximately (within GA), the correlated (physical) SC order parameters can be expressed as

$$\Delta_S = g_\Delta \Delta_S, \quad \text{and} \quad \Delta_T = g_\Delta \Delta_T,$$

where

$$g_\Delta = \frac{n - 2d^2}{2(n - 2r w)} \left[ \frac{\sqrt{(1 - w)(1 - n + d^2)(1 - r)}}{1 - r} + \sqrt{\frac{w d^2}{r}} \right] + \frac{\sqrt{(1 - r)(1 - n + d^2)(1 - w)}}{1 - w} + \sqrt{\frac{r d^2}{w}}.$$  

Figure 3. (Color online) Selected bare physical quantities $\chi_{AB}$, $\Delta_S$, $\Delta_T$, $m_{AF}$, and $d^2$, all as a function of doping $\delta$ and for $U/|t| = 12$. In the coexistent AF+SC phase we have $\Delta_S \neq 0$, $\Delta_T \neq 0$, and $m_{AF} \neq 0$. Such phase is stable only in the vicinity of the half filling, as detailed in the left panel where $\delta \in [0, 0.01]$. On the right panel we present an overall behavior in wider range of the doping. The spin-singlet component of the superconducting gap disappears at $\delta = 1/3$ (this point depends only weekly on $U/|t|$ ratio for $U/|t| \gg 1$).

The AF order parameter, and the renormalized hopping parameter are defined in a similar manner, namely

$$m_{AF}^c = g_m m_{AF},$$

$$\chi_{AB}^c = g_\chi \chi_{AB},$$

where $g_\chi$ is presented in Eq. (4a) and

$$g_m = \frac{n - 2d^2}{n - 2r w}.$$
Figure 5. (Color online) Order parameters of SC and AF states in the correlated state versus doping $\delta$ and for $U/|t| = 12$. AF disappears for $\delta \approx 6 \cdot 10^{-3}$, whereas the spin-singlet superconducting state for $\delta = 1/3$. In the limit $\delta = 0$ the state transforms into AF insulator. For $\delta \geq 0.1$ the hopping probability $\chi_{AB}$ grows spectacularly. Inset: dependence of $\Delta_T^c$ in the vicinity of the half filling. Note, that the value of $\Delta_T^c$ is about $10^4$ times smaller than the value of $\Delta_S^c$.

The doping dependence of $\chi_{AB}^c$, $\Delta_S^c$, and $\Delta_T^c$ for $U/|t| = 12$ is shown in Fig. 5. The magnitude of $\Delta_T^c$ is about $10^4$ times smaller than the magnitude of $\Delta_S^c$, so most probably, it may not be observable. Note a spectacular increase of the hopping probability $\chi_{AB}^c$ with the increasing doping leading to an effective Fermi liquid state for $\delta \geq 1/3$.

The non-zero correlated gap at $n = 1$ for low-$U$ values provides an evidence for a gossamer superconductivity. It appears when the pure SC phase is stable at the half filling. For $U/|t| = 10.6$ and $n = 1$, where AF+SC phase sets in, the correlated gap $\Delta_S^c$ vanishes. Details of the transition are presented in Fig. 6 in the bottom panel. The critical $U/|t|$ value for the disappearance of $\Delta_S^c$ is marked by the dotted vertical line.

For the sake of completeness, in Fig. 7 we present the dependencies of the renormalization factors $g_t$, $g_s$, $g_\Delta$, and $g_m$, and in Table I we list representative values of the parameters calculated for the following phases: PM ($U/|t| = 5$, $\delta = 0.1$), SC ($U/|t| = 12$, $\delta = 0.03$), and AF+SC ($U/|t| = 12$, $\delta = 0.001$). The energies in the columns should not be compared directly as they correspond to different set of parameters. Numerical accuracy is at the level of the last digit specified.

V. CONCLUSION AND COMMENTS

We have analyzed in detail the effective Hamiltonian considered previously in Refs. [36, 37] and [39] in the statistically-consistent Gutzwiller approximation (SGA). However, in contrast to those references we consider a richer structure of the SC gap (the components $\Delta_S$ and $\Delta_T$). As a result, a much narrower region of the coexistence of AF and SC is obtained for $U \geq 10|t|$. We have checked that the bare amplitude $\Delta_T$ is about $10^3$ times smaller than that of $\Delta_S$ (similarly, $\Delta_T/\Delta_S \approx 10^{-3}$), so the presence of the triplet gap component does not change the results in any significant manner, and most probably, is not detectable experimentally. Therefore, the large coexistence region obtained previously in Refs. [36, 37] and [39] may be an artifact of the non-statistically-consistent RMFT approach used. To show it explicitly: e.g., in Ref. [36] the minimization procedure is formulated by setting $\partial E_{\text{var}}/\partial m = 0$ what yields Eq. (21 in Ref. [36]) for $m$ which is different than that Eq. (16 in Ref. [36]) defining $m$. It results in having two different equations for one quan-
Table I. Values of the parameters obtained for the PM phase \((U/|t| = 5)\) and \(\delta = 0.3\), for SC phase \((U/|t| = 12\) and \(\delta = 0.03\), and for the AF+SC phase \((U/|t| = 12\) and \(\delta = 0.001\)). The calculations were made for the lattice with \(\Lambda = 1024 \times 1024\) sites. The numerical accuracy is at the last digit specified.

| Variable       | PM          | SC          | AF+SC       |
|----------------|-------------|-------------|-------------|
| \(\chi_{AB}\) | 0.1907587   | 0.1887189   | 0.1693210   |
| \(\Delta_S\)  | 0           | 0.138176    | 0.166906    |
| \(\Delta_T\)  | 0           | 0           | 1.9227 \times 10^{-3} |
| \(\mu\)       | 0.56643     | 3.55703     | 3.71541     |
| \(m_{AF}\)    | 0           | 0           | 0.13194     |
| \(d^2\)       | 5.2226 \times 10^{-2} | 8.16196 \times 10^{-3} | 2.2406 \times 10^{-4} |
| \(\lambda_\chi\) | 0.9661403   | 0.327769    | 0.168074    |
| \(\lambda_{\Delta_S}\) | 0           | 0.1258974   | 0.160777    |
| \(\lambda_{\Delta_T}\) | 0           | 0           | 1.2595 \times 10^{-5} |
| \(\lambda_\eta\) | -2.526087   | -7.176836   | -6.744724   |
| \(\lambda_\mu\) | 0           | 0           | 0.100911    |
| \(W\)         | -1.1509250  | -0.33669191 | -0.233031   |
| \(g_t\)       | 0.8844382   | 0.1558210   | 4.97139 \times 10^{-3} |
| \(g_s\)       | 1.713292    | 3.644459    | 3.85310     |
| \(g_\Delta\)  | 0.9661403   | 0.1558210   | 4.99012 \times 10^{-3} |
| \(g_{m}\)     | 1.3088937   | 1.9090702   | 1.96293     |
| \(\chi_{AB}^\tau\) | 0.1687143   | 2.94064 \times 10^{-2} | 8.41761 \times 10^{-4} |
| \(\Delta_{\chi}^\mu\) | 0           | 2.15306 \times 10^{-2} | 8.343884 \times 10^{-4} |
| \(\Delta_{\chi}^\tau\) | 0           | 0           | 1.9610 \times 10^{-7} |
| \(m_{AF}^c\)  | 0           | 0           | 0.25900     |

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**Appendix A: Definitions of the mean-fields and evaluation of \(\langle \hat{H}_{eff} \rangle_0\)**

In the main text, the uniform bond order parameter for \(i\) and \(j\) sites indicating the nearest neighbors is defined as \(\langle \hat{c}_{i\uparrow} \hat{c}_{j\uparrow} \rangle_0 \equiv \chi_{AB}\), i.e., it was assumed that \(\langle \hat{c}_{i\uparrow} \hat{c}_{j\uparrow} \rangle_0 = 0\). More generally, since the sublattice \(A\) contains the sites, where the majority spin is \(\uparrow\) and the sublattice \(B\) the sites, where majority spin is \(\downarrow\), it should have been written (for \(i\) and \(j\) being the nearest neighbors) in the form

\[
\langle \hat{c}_i^{\uparrow} \hat{c}_j^{\uparrow} \hat{c}_k^{\downarrow} \hat{c}_l^{\downarrow} \rangle_0 = \langle \hat{c}_i^{\uparrow} \hat{c}_k^{\downarrow} \rangle_0 \chi_{\sigma=c},
\]

(A1)

\[
\langle \hat{c}_j^{\uparrow} \hat{c}_k^{\downarrow} \hat{c}_l^{\uparrow} \hat{c}_m^{\uparrow} \rangle_0 = \langle \hat{c}_j^{\uparrow} \hat{c}_l^{\uparrow} \rangle_0 \chi_{\sigma=\sigma},
\]

(A2)

where \(\chi_{\sigma=\sigma}\) is an average of the operator describing the hopping of an electron from a site which belongs to the sublattice, where the average spin is opposite to the spin of the electron, to the site which belongs to the sublattice, where average spin is congruent to the spin of the electron. \(\chi_{\sigma-c}\) describes opposite situation. It brings us to the general expression that

\[
\chi_{ij\sigma} \equiv \langle \hat{c}_i^{\uparrow} \hat{c}_j^{\sigma} \rangle_0 = \chi_{AB} + i\sigma e^{i\mathbf{Q} \cdot \mathbf{r}} \delta_{\chi_{AB}},
\]

(A3)

where \(\chi_{AB} = \frac{1}{2} \left( \chi_{\sigma-c} + \chi_{\sigma=\sigma} \right) \) and \(\delta_{\chi_{AB}} = \frac{1}{2} \left( \chi_{\sigma-c} - \chi_{\sigma=\sigma} \right)\).

The electron-pairing order parameter for the nearest neighbors is defined as

\[
\langle \hat{c}_i \hat{c}_j \rangle_0 = \begin{cases} 
\tau_{ij} \Delta_A, & \text{for } i \in A, \\
\tau_{ij} \Delta_B, & \text{for } i \in B,
\end{cases}
\]

(A4)

where \(\tau_{ij} = 1\) for \(j = i \pm \hat{x}\) and \(\tau_{ij} = -1\) for \(j = i \pm \hat{y}\). For the staggered magnetic moment \(m_{AF} \neq 0\) one can assume that \(\Delta_A \equiv \Delta_B\). However, when \(m_{AF} = 0\), the order parameter \(\Delta_A\) is a product of two operators which both annihilate electrons whose spin is congruent to the average spin of individual sites. On the contrary, \(\Delta_B\) is a product of two operators annihilating electrons whose spin is opposite to the average spin of individual sites. Hence, \(\Delta_A\) and \(\Delta_B\) could be, in general, complex numbers. Let us indicate \(\Delta_A \equiv (\Delta_A, \delta \Delta_A)\) and \(\Delta_B \equiv (\Delta_B, \delta \Delta_B)\), where in the brackets there are provided the real and imaginary parts of the corresponding gaps, respectively.

The only part of \(\langle \hat{H}_{eff} \rangle_0\) which is dependent on \(\Delta_A\) and \(\Delta_B\) is \(\langle \hat{S}_i \cdot \hat{S}_j \rangle_0\) which can be evaluated in the form

\[
4 \langle \hat{S}_i \cdot \hat{S}_j \rangle_0 \approx -\left( \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle_0 - \langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle_0 \right)^2.
\]
- \left( \langle \hat{c}_{i}^{\dagger} \hat{c}_{j} \rangle_{0} + 2 \langle \hat{c}_{i}^{\dagger} \hat{c}_{j} \rangle_{0} \right) \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0}

- \left( 2 \langle \hat{c}_{i}^{\dagger} \hat{c}_{i} \rangle_{0} + \langle \hat{c}_{i} \hat{c}_{j} \rangle_{0} \right) \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0}

- \left( -\langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} + 2 \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} \right) \langle \hat{c}_{i}^{\dagger} \hat{c}_{j} \rangle_{0}

- \left( 2 \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} - \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} \right) \langle \hat{c}_{i}^{\dagger} \hat{c}_{j} \rangle_{0}

\right). \quad (A5)

where we have applied the Wick’s theorem and we have assumed that \langle \hat{c}_{i}^{\dagger} \hat{c}_{i} \rangle_{0} \equiv 0, \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} \equiv 0, and \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} = \langle \hat{c}_{i} \hat{c}_{i} \rangle_{0} \equiv 0.

Using the notation introduced above we write that

\[ 4\langle \hat{S}_{i} \hat{S}_{j} \rangle_{0} = -m_{AF}^{2} - 6\chi_{AB}^{2} + 2(\delta\chi_{AB})^{2} \]

- |\Delta_{A}|^{2} - |\Delta_{B}|^{2} - 4\Delta_{A}\Delta_{B}. \quad (A6)

Since the above expression is invariant with respect to the same rotations of both vectors \Delta_{A} and \Delta_{B}, one component of the vectors can be assumed as vanishing. With the choice \delta\Delta_{A} = 0, we have

\[ \Delta_{ij\sigma} \equiv \langle \hat{c}_{i\sigma} \hat{c}_{j\sigma} \rangle_{0} \equiv -\tau_{ij} \left( \sigma \Delta_{S} + e^{iQ_{r\sigma}} \Delta_{T} \right) \]

- \tau_{ij} \frac{1}{2} (\sigma - e^{iQ_{r\sigma}}) \delta\Delta_{B}. \quad (A7)

where \Delta_{S} \equiv \Delta_{A} + \Delta_{B} and \Delta_{T} \equiv \Delta_{A} - \Delta_{B}.

Using the notation above the \langle \hat{H}_{\text{eff}} \rangle_{0} \equiv W can be presented in the form:

\[ \frac{W}{\Lambda} = 8\nu t\chi_{AB} + Ud^{2} - g_{s}J \left( \frac{1}{2} m_{AF}^{2} + 3\chi_{AB}^{2} - (\delta\chi_{AB})^{2} \right) \]

- 3\Delta_{S}^{2} - \Delta_{T}^{2} + \frac{1}{2} (\delta\Delta_{B})^{2}. \quad (A8)

Introduction of \delta\chi_{AB} and \delta\Delta_{B} affects the form of selecting the correlated fields \lambda_{ij\sigma} and \lambda_{ij\sigma}', and the final set of necessary conditions for a local minimum of the free energy. It was found that the state with the lowest energy has always been that with \delta\chi_{AB} \equiv 0 and \delta\Delta_{B} \equiv 0.

Hence, it is acceptable to neglect both terms, what is equivalent to assuming that \Delta_{ij\sigma} and \chi_{ij\sigma} are both real. Under such conditions Eq. (A7) is reduced to Eq. (7), Eq. (A3) to Eq. (6), and Eq. (9) to Eq. (A8).

**Appendix B: An alternative procedure of introducing the constraints via Lagrange multipliers**

In the main text we define \hat{H}_{\text{eff}} (cf. Eq. (3)), we calculate \[ W \equiv \langle \hat{H}_{\text{eff}} \rangle_{0} \quad (cf. Eq. (4)), \]

we construct \[ \hat{K} \equiv W - \sum_{i} \left( \lambda_{i} (\hat{O}_{i} - \hat{O}) + \text{H.c.} \right) - \mu N, \]

where \lambda_{i} are the Lagrange multipliers for the corresponding operator. We calculate the grand potential functional \( F = -\int \ln Z \) where \Z = Tr \( e^{-\beta K} \) (cf. Eq. (17)) which is minimized subject to constraints included in \( K \).

An alternative procedure to the above is to introduce the Lagrange multipliers directly to \hat{H}_{\text{eff}}^{MF} which represents a mean-field approximation of \hat{H}_{\text{eff}}. There should be a separate Lagrange multiplier \lambda_{ij}^{\text{MF}} to each mean-field average \( \langle \hat{O}_{ij} \rangle \) present in \hat{H}_{\text{eff}}^{MF}. In effect, we construct the effective mean-field Hamiltonian

\[ \hat{H}_{\text{eff}}^{MF} = \sum_{i} \lambda_{i} \langle \hat{O}_{ij} \rangle + \text{H.c.} \]

and only then define \[ \hat{K}' \equiv \hat{H}_{\text{eff}}^{MF} - \mu N \] and subsequently calculate \( F' \) (as above). We minimize \( F' \) subject to constraints included in \hat{H}_{\text{eff}}^{MF}, and as a result, we obtain a different set of the equations than represented by Eqs. (2a)-(2k). However, we have checked numerically that the values of the variables, corresponding to the minimum of the \( F' \) subject to the same constraints coincide. The difference occurs only in the values of the Lagrange multipliers what, however, does not affect the values of the calculated physical quantities. Hence two approaches are equivalent. The Lagrange multipliers are obviously different in such two formulations, because in one of them they describe the whole dynamics in the system (e.g. the eigenvalues in Eqs. (16a)-(16f) are function of only \lambda) whereas in the alternative schema they are introduced to \hat{H}_{\text{eff}}^{MF} on top of the dynamics described in this Hamiltonian.

A second difference between the two approaches is an implementation. In the first procedure discussed in the main text we extract directly the conditions for the constraints \lambda_{ij} (as it is shown in Eqs. (2a)-(2k)) and in this manner reduce the number of equations to be solved numerically. In the second approach discussed here, the conditions for the constraints \lambda_{ij}' are much more complicated and there is no easy way to separate the equations which increases the effort and numerical cost of solving the model. This is even though the latter method sounds as more intuitively appealing. This is the reason why we have used the former method in the main text.

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