1. Introduction

It is generally accepted that copper-oxide planes contain strongly correlated electronic states that are instrumental for achieving high-temperature superconductivity. The simplest models describing those states are the single-band $t$-$J$, Hubbard, and related extended models [1–5]. A standard treatment in this situation is the renormalized mean-field theory (RMFT), which describes the principal superconducting properties in a qualitative manner [6, 7]. In addition, a variational Monte-Carlo (VMC) approach provides a semi-quantitative description of selected properties, even through

Antiferromagnetism, charge density wave, and $d$-wave superconductivity in the extended $t$-$J$-$U$ model: role of intersite Coulomb interaction and a critical overview of renormalized mean field theory

M Abram¹, M Zegrodnik² and J Spalek¹

¹ Marian Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland
² Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Kraków, Poland

E-mail: jozef.spalek@uj.edu.pl

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Abstract

In the first part of the paper, we study the stability of antiferromagnetic (AF), charge density wave (CDW), and superconducting (SC) states within the $t$-$J$-$U$-$V$ model of strongly correlated electrons by using the statistically consistent Gutzwiller approximation (SGA). We concentrate on the role of the intersite Coulomb interaction term $V$ in stabilizing the CDW phase. In particular, we show that the charge ordering appears only above a critical value of $V$ in a limited hole-doping range $\delta$. The effect of the $V$ term on SC and AF phases is that a strong interaction suppresses SC, whereas the AF order is not significantly influenced by its presence. In the second part, separate calculations for the case of a pure SC phase have been carried out within an extended approach (the diagrammatic expansion for the Gutzwiller wave function, DE-GWF) in order to analyze the influence of the intersite Coulomb repulsion on the SC phase with the higher-order corrections included beyond the SGA method. The upper concentration for the SC disappearance decreases with increasing $V$, bringing the results closer to experiment. In appendices A and B we discuss the ambiguity connected with the choice of the Gutzwiller renormalization factors within the renormalized mean filed theory when either AF or CDW orders are considered. At the end, we overview briefly the possible extensions of the current models to put descriptions of the SC, AF, and CDW states on equal footing.

Keywords: $t$-$J$-$U$-$V$ model, charge density wave, antiferromagnetism, strong correlations, high temperature superconductivity

(Some figures may appear in colour only in the online journal)
the analysis is limited to systems of finite size [5, 7, 8]. Very recently, we have carried out [9, 10] an extensive analysis of
the universal properties of the cuprates for the case of a pure superconducting solution. As a result we have shown that a
very good agreement with principal experimental data can be achieved when including the higher-order terms within
the diagrammatic expansion of the Gutzwiller wave function (DE-GWF) method for the case of the $t$-$J$-$U$ model. In such
a picture the intra-atomic (Hubbard) interaction magnitude $U$ is not regarded as extremely strong, which means that the
limit $U/t \rightarrow \infty$ is not assumed at the start. In this situation, a straightforward decomposition of the narrow-band states
into the Hubbard sub-bands, with the upper sub-band (for the band filling $n \leq 1$) being unoccupied, is not physically
crucial, and in effect the $t$-$J$ model does not follow directly from the perturbation expansion of the Hubbard model in
powers of $\nu U$ [11–16]. Instead, the antiferromagnetic kinetic exchange interaction arises from the superexchange via $2p_\sigma$
states due to oxygen [17, 18]. Consequently, a small but non-
zero number of double occupancies is admissible for the non-
half-filled band case, and in such a situation the Hubbard
term $\sim U$ provides a direct contribution to the states. This
argument justifies the generalization of the $t$-$J$ model to the $t$-$J$-$U$ form. Originally, the Hubbard term has been added to the$t$-$J$ model when introducing the so-called Gossamer superconductivity (for detailed discussion see [19] and papers
cited therein; see also [20]).

Motivated by our previous results for the case of a pure SC phase [9, 10] and the antiferromagnetic phase [19], we focus here
on the one-band description of the Cu–O plane within the $t$-$J$-$U$-$V$ approach and analyze the three most important phases related to the copper-based high temperature superconducting (HTS) compounds: antiferromagnetic (AF), interunitcell charge ordered (CDW), and superconducting (SC) together. We mainly concentrate on the formation of the CDW state induced by the intersite Coulomb repulsion $\sim V$
as the most natural factor determining its appearance [21]. The inclusion of the $V$-term leads to the original $t$-$J$-$U$-$V$ model. We also analyze the influence of the modulation vector $Q$ on the charge ordering stability region in the phase diagram.

Interest in the field of charge ordered (CO) states within one-band models of Cu–O plane has revived in recent years
due to growing experimental evidence that the charge ordering appears spontaneously or in the presence of a magnetic field
in the underdoped region of high temperature cuprate superconductors [22–30]. For the La-based materials the NMR
experiments suggested a commensurate stripe-like charge order with a period of four unit cells [23]. For YBCO and
Bi-based materials it has been found that the CDW phase is characterized by the modulation vectors $(0, Q)$ and $(Q, 0)$ [24,
28, 31, 32] which are incommensurate with a weakly doping dependent period of $\sim 3.1$ for YBCO [28, 31, 33] and $Q \sim 2.6$
$(0, 3)$ for the single-layer (double-layered) Bi-based compounds [25, 26]. Another important conclusion is that, regardless of
the details of the charge ordered phase, a competition between superconductivity (SC) and CDW takes place in the cuprates.
Moreover, $T_{\text{CDW}}$ appears to be larger than $T_C$. Some analyses indicate that the charge order is located predominantly on the
bonds connecting the Cu sites [34, 35]. Such a scenario has been considered theoretically by Allais et al [36] by assuming a
proper $d$-formfactor of the CDW which leads to a modulation vector close to that observed experimentally [25, 26]. The $d$-wave symmetry of the CDW ordering has also been consid-
ered in [37, 38] to preserve the nodal nature of the $k_x = k_y$
direction at low temperature.

The research in this field is additionally motivated by the fact that there might be a connection between the pseudogap in the cuprates and the charge ordering [32, 39, 40]. It has also been suggested that for certain materials the CDW state may have a three-dimensional character in a nonzero applied magnetic field [41, 42]. A general form of CDW state has been considered many times earlier [43–45]. Furthermore, the appearance of the so-called pair-density-wave state has been proposed, which can coexist with the CDW state and may lead to the appearance of the pseudogap anomaly [46–48]. In such a state the SC order parameter has a nonzero Cooper pair momentum similar to that appearing in the Fulde–Ferrell–Larkin–Ovchinnikov phase.

Concerning the theoretical analysis, various calculation schemes have been applied to the (extended) Hubbard, $t$-$\J$,
and related models in seeking the stability of CO states [36, 49–54]. In contrast to some of those considerations, it has been suggested very recently [55] that the CDW solution for the $t$-$J$ model always has a slightly higher energy than the generic SC + AF solution. It is also not settled whether the simplified one-band approach can lead to the proper description of the charge-ordered phase in the cuprates. The STM experiments [56] point to the intrunitcell charge order which would require a three-band model of the Cu–O plane for a realistic theoretical analysis.

In the first part of the paper, our analysis is carried out with the use of the so-called statistically consistent Gutzwiller approximation (SGA), within which we can account for electron correlations in a reasonable computing time. (For the derivation of SGA method see [57, 58] and for its applications see [19, 59–63].) This approximation represents a consistent version of the RMFT, as explained in the papers just mentioned. In the second part of the paper (see section 4.3), we test the influence of the intersite Coulomb interaction on the robustness of the pure superconducting solution beyond SGA with the use of a systematic diagrammatic expansion for the Gutzwiller-wave function (DE-GWF method). (For details of this approach see [64] and for the application of this method to the $t$-$J$ model see [9, 10]) This last approach allows us to go beyond the SGA in a systematic manner and to take into account non-local correlations in higher orders of the expansion. The differences between the SGA and the DE-GWF solutions are specified there. Additionally, in Appendix A, we discuss an inherent ambiguity in choosing the Gutzwiller renormalization factors when either AF or CDW states are considered within SGA. Namely, we show that different calculation schemes used in the literature lead to different forms of the Gutzwiller factors, which results in different stability regimes of the AF phase.
2. t-J-U-V model

The starting Hamiltonian for the subsequent analysis has the following form,

\[
\hat{H}_{t-J-U-V} = t \sum_{\langle i,j \rangle, \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right) + t' \sum_{\langle i,j \rangle, \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right) + J \sum_{i} \hat{S}_i \cdot \hat{S}_j + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \left( \sum_i - \frac{V}{N} \right) \sum_{\langle i,j \rangle, \sigma, \sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'},
\]

(1)

where \(\sum_{\langle i,j \rangle}\) and \(\sum_{\langle i,j \rangle}\) denote summation up to all nearest and second-nearest neighbors. Furthermore, \(t\) and \(t'\) are respectively the hopping amplitudes between the nearest and the next nearest neighboring sites, \(J\) is the antiferromagnetic exchange integral, and \(U(V)\) is the onsite (inter-site) Coulomb repulsion magnitude. The standard notation is used, where \(\hat{c}_{i\sigma}^\dagger\) and \(\hat{c}_{i\sigma}\) are, respectively, the creation and the annihilation operators, for electron with spin quantum number \(\sigma = \pm 1\) located at site \(i\). Similarly, \(\hat{n}_{i\sigma} \equiv \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\) and \(\hat{S}_i \equiv \left( \hat{S}_i^+, \hat{S}_i^-, \hat{S}_i^z \right)\), where \(\hat{S}_i^z \equiv \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}\) and \(\hat{S}_i^z \equiv \frac{1}{2} \left( \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \right)\).

As has already been mentioned, the appearance of the \(J\) term in this approach is attributed mainly to the \(d-d\) superexchange via \(2p_{\sigma}\) states due to oxygen [17, 18]. The finite value of the Coulomb repulsion \(U\) leads to a relatively small but nonzero population of the upper Hubbard sub-band [2, 20, 65]. In such a situation the appearance of both the \(J\) and the \(U\) terms is physically admissible in the Hamiltonian. For \(V = 0\) and when \(U \to \infty\), the limit of the \(t-J\) model is recovered. On the other hand, for \(J = V = 0\), we obtain the limit of the Hubbard model. Nevertheless, the model is not only constructed as a formal generalization of those two limits. As can be seen from the numerous estimates of the model parameters, the typical values of the parameters of the one-band model are: \(t = -0.35\) eV, \(t' = 0.25|t|\) and \(U \approx 8-10\) eV, so that the ratio of \(U\) to the bare bandwidth \(W = 8|t|\) is \(U/W \approx 2.5-3\), i.e. only by a factor of about two higher than typically is required for Mott–Hubbard localization in the limit of a half-filled band [66]. As a consequence, the Hubbard gap is \(U - W \sim W\) and the double occupancy can be estimated as \(d^2 \lesssim \frac{1}{2} \delta \sim 10^{-2}\), where \(\delta\) is the hole doping. Additionally, the value of \(U\) is reduced to the value \(U - V \sim \frac{1}{2} U\) when the \(V\) term is present [11]. Also, as said above, the value of \(J\) cannot be regarded as resulting from the \(tU\) expansion of the (extended) Hubbard model [11–16, 67], and both \(J\) and \(U\) can be regarded as practically independent variables. The last term comes partially from the derivation of the \(t-J\) model from the Hubbard model (see [11–13, 15, 16, 67]) and partially (the part \(-V\)) represents an explicit intersite Coulomb repulsion of electrons located on the nearest neighboring sites. For simplicity, we denote \(V \equiv V - \frac{1}{2} J\).

3. Methods

3.1. Statistically consistent Gutzwiller approximation (SGA)

In this section we describe the principles of the statistically consistent Gutzwiller approximation (SGA) [57, 58, 69–71] which we use to solve the Hamiltonian (1). The phases which are of interest in our analysis are: the paired phase, the antiferromagnetic phase, and the charge ordered phase. We assume that the two last phases are in the simplest two-sublattice form with the modulation vector \(Q = (\pi, \pi)\). However, at the end we also show some results for the case of the CDW phase where \(Q = (2\pi/3, 0)\).

The main idea behind the Gutzwiller approach is to express the wave function of the system in the following manner:

\[
|\Psi\rangle = \tilde{P} |\Psi_0\rangle \equiv \prod_i \tilde{P}_i |\Psi_0\rangle,
\]

(2)

where the correlator \(\tilde{P}_i\) in its most general form is as follows:

\[
\tilde{P}_i = \sum_i \lambda_{i\Gamma} |\Gamma\rangle_i \langle \Gamma|.
\]

(3)

The variational parameters \(\lambda_{i\Gamma} \in \{\lambda_{i\uparrow}, \lambda_{i\downarrow}, \lambda_{i\uparrow\downarrow}, \lambda_{i\downarrow\uparrow}\}\) weight the configurations corresponding to states from the local basis: \(|\uparrow\rangle_i, |\downarrow\rangle_i, |\uparrow\downarrow\rangle_i\), and \(|\downarrow\uparrow\rangle_i\), respectively. The non-correlated wave function, \(|\Psi_0\rangle\), is taken as the broken-symmetry state of our choice. It has been shown by Bünemann et al [64], that it is convenient to choose the \(\tilde{P}_i\) operator that fulfills the following relation,

\[
\tilde{P}_i^2 = 1 + x_i \tilde{d}_i^{\text{HF}},
\]

(4)

where \(x_i\) is yet another variational parameter and \(\tilde{d}_i^{\text{HF}} = \hat{n}_{i\uparrow}^{\text{HF}} \hat{n}_{i\downarrow}^{\text{HF}}\), where \(\hat{n}_{i\sigma}^{\text{HF}} = \hat{n}_{i\sigma} - n_{i\sigma}\) with \(n_{i\sigma} = \langle \Psi_0 | \hat{n}_{i\sigma} | \Psi_0 \rangle\). The \(x_i\) parameter can be directly connected with the double occupancy probability \(d_i^2 = \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle\)

\[
x_i \equiv \frac{d_i^2 - n_{i\uparrow} n_{i\downarrow}}{n_{i\uparrow} n_{i\downarrow} (1 - n_{i\uparrow})(1 - n_{i\downarrow})}.
\]

(5)

The \(\lambda_{i\Gamma}\) parameters can be expressed with the use of \(x_i\) or \(d_i\), as we show in appendix A, therefore we are left always with only one local variational parameter.

As the operator \(\tilde{P}\) is in general not unitary, the expectation value of the ground-state energy of the system is expressed as follows,

\[
E \equiv \langle \hat{H} \rangle = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi_0 | \tilde{P} \hat{H} \tilde{P} | \Psi_0 \rangle}{\langle \Psi_0 | \tilde{P}^2 | \Psi_0 \rangle} \approx \langle \Psi_0 | \hat{H}_{\text{eff}} | \Psi_0 \rangle.
\]

(6)

In other words, instead of calculating the average of the initial Hamiltonian (1) with respect to a usually complicated, many-particle wave function \(|\Psi\rangle\), we choose to modify that Hamiltonian (presumably by making it more complicated) in order to have the relatively simple task of calculating its average with respect to the wave function \(|\Psi_0\rangle\) represented by a single Slater determinant. Within the SGA approach we make use of the following approximations while calculating \(E\): \(\langle \Psi | \hat{a}_i \hat{a}_j^{\dagger} | \Psi \rangle \approx \langle \Psi_0 | \tilde{P}_i \hat{a}_i \tilde{P}_j \hat{a}_j^{\dagger} | \Psi_0 \rangle\), \(\langle \Psi | \hat{a}_i^{\dagger} | \Psi \rangle \approx \langle \Psi_0 | \tilde{P}_i \hat{a}_i^{\dagger} | \Psi_0 \rangle\),

(7)

for any two local operators \(\hat{a}_i\) and \(\hat{a}_j^{\dagger}\) from our Hamiltonian. Such relations are exact in the infinite dimensions limit.

In our case, the resultant expectation value is dependent on a number of quantities,
\( \langle \Psi_0 | H_{\Sigma}^{\text{eff}} | \Psi_0 \rangle \equiv W(n, m, \delta_a, \delta_b, \chi_1, \chi_5, \chi_T, \Delta_S, \Delta_T) \),

(8)

where \( W(\ldots) \) is a functional of a number of mean-field averages that are explained below (for the explicit form of \( W \) and the details of the calculations, see section appendix A.). First, \( n \) is the average number of electrons per site, \( m \) is the magnitude of staggered magnetization in the AF state, and \( \delta_a \) is the order parameter for the CDW phase. Those three quantities can be combined by expressing the local occupancy in the following manner,

\[
n_{i\sigma} \equiv \langle \hat{c}_{i\sigma} \hat{c}_{i\sigma} \rangle_0 \equiv \frac{1}{2} \left( 1 + e^{\mathbf{Q} \cdot \mathbf{R}_i (\sigma m + \delta_a) \rangle} \right),
\]

(9)

where, for simplicity, we denote \( \langle \Psi_0 | \ldots | \Psi_0 \rangle \equiv \langle \ldots \rangle_0 \). The superlattice vector was first chosen to be \( \mathbf{Q} = (\pi, \pi) \), i.e. the lattice is naturally divided into two sublattices, A and B, such that one sublattice (A) has on average \( \frac{1}{2}(n + m + \delta_a) \) up \((\uparrow)\) electrons and \( \frac{1}{2}(n - m - \delta_a) \) down \((\downarrow)\) electrons, while the second sublattice (B) has on average \( \frac{1}{2}(n - m - \delta_a) \uparrow \) and \( \frac{1}{2}(n + m + \delta_a) \downarrow \) electrons. Second, the double occupancy probabilities on the sublattices are labelled as \( d_a \) and \( d_b \), respectively. Third, the average hopping amplitude for the first and the next nearest neighbors (1st and 2nd n.n.) are defined by

\[
\chi_{j\sigma} \equiv \langle \hat{c}_{j\sigma} \hat{c}_{j\sigma} \rangle_0 \equiv \begin{cases} 
\chi_\sigma \\
\chi_{SS,\sigma} + e^{\mathbf{Q} \cdot \mathbf{R}_j} \chi_{T,\sigma}
\end{cases} \text{for 1st n.n.},
\]

(10)

with \( \chi_{SS,\sigma} \equiv \frac{1}{2} \left( \chi_{\Lambda\Lambda\sigma} + \chi_{\Lambda\Sigma\sigma} \right) \), \( \chi_{T,\sigma} \equiv \frac{1}{2} \left( \chi_{\Lambda\Lambda\sigma} - \chi_{\Lambda\Sigma\sigma} \right) \), where \( \chi_{\Lambda\Lambda\sigma} \) and \( \chi_{\Lambda\Sigma\sigma} \) denote respectively the hopping of an electron with spin \( \sigma \) within sublattices A and B, and \( \chi_{\Lambda\Sigma\sigma} \equiv \chi_\sigma \) is the hopping between the sublattices (see figure I(a)). Fourth, the electron pairing amplitude between nearest neighbors, with spin-singlet and triplet components, \( \Delta_S \) and \( \Delta_T \), are defined by [19]

\[
\Delta_{j\sigma} \equiv \langle \hat{c}_{j\sigma} \hat{c}_{j\sigma} \rangle_0 = -\tau_{j\downarrow} (\sigma \Delta_S + e^{\mathbf{Q} \cdot \mathbf{R}_j} \Delta_T),
\]

(11)

where \( \tau_{j\downarrow} \equiv 1 \) for \( j = i \pm \hat{x} \) and \( \tau_{j\downarrow} \equiv -1 \) for \( j = i \pm \hat{y} \) to ensure the d-wave symmetry of \( \Delta_{j\sigma} \), and with \( \Delta_S \equiv \frac{1}{2} \left( \Delta_A + \Delta_B + \text{H.c.} \right) \) and \( \Delta_T \equiv \frac{1}{2} \left( \Delta_A - \Delta_B + \text{H.c.} \right) \) (see figure I(b)).

The mean-field order parameters defined above are determined numerically by minimizing the system’s ground-state energy. However, in order to be sure that the self-consistent equations for them are also fulfilled when carrying out the variational minimization procedure, we introduce additional constraints with the help of the Lagrange multiplier method (see [57, 58, 71]). The constraints form an essence of the statistically-consistent method, in addition to the standard Gutzwiller approximation elaborated in appendix A. Such an approach leads to the effective Hamiltonian of the following form:

\[
K = W(n, m, \ldots) - \sum_{\langle ij \rangle, \sigma} \left( \lambda_{i\sigma}^R \langle \hat{c}_{i\sigma} \hat{c}_{j\sigma} \rangle_0 - \chi_{j\sigma} \right) + \text{H.c.}
\]

- \sum_{\langle ij \rangle, \sigma} \left( \lambda_{i\sigma}^L \langle \hat{c}_{i\sigma} \hat{c}_{j\sigma} \rangle_0 - \chi_{j\sigma} \right) + \text{H.c.}
\]

- \sum_{\langle ij \rangle} \left( \delta_{ij} \langle \hat{n}_{i\sigma} \hat{n}_{i\sigma} \rangle - \mu \sum_{i\sigma} \hat{n}_{i\sigma} \right),
\]

(12)

Note that the constraints introduce the renormalizations of the hoppings \( \lambda_{i\sigma}^R \) and the pairing potential \( \lambda_{i\sigma}^L \) in real space as well as both the local molecular field \( \lambda_{i\sigma}^L \) and the chemical potential shift \( \lambda_{i\sigma}^L \).

Next we define the generalized grand potential function at temperature \( T > 0 \),

\[
F = -\frac{1}{\beta} \ln Z, \quad \text{with} \quad Z = \text{Tr} \left( e^{-\beta K} \right),
\]

(13)

with the Landau free energy equal to

\[
\frac{\partial F}{\partial A_\lambda} = 0, \quad \frac{\partial F}{\partial d_A} = 0, \quad \frac{\partial F}{\partial d_B} = 0. \quad \frac{\partial F}{\partial \lambda_i} = 0, \quad \frac{\partial F}{\partial A_\lambda} = 0, \quad \text{and} \quad \frac{\partial F}{\partial d_A} = 0, \quad \text{and} \quad \frac{\partial F}{\partial d_B} = 0.
\]

(15)

where \( \{ A_\lambda \} \) denotes the mean-field averages while \( \{ \lambda_i \} \) refers to the Lagrange multipliers. The set of equation (15) can be subsequently solved using numerical methods. The results are presented in section 4. In the SGA approximation, we regard all the local fields and mean-field averages as spatially homogeneous, dependent only on the sublattice index. After solving the set of equation (15) we can calculate the so-called correlated SC gap, which is the correspondent of \( \Delta_{j\sigma} \) in the Gutzwiller wave function approach (DE-GWF) [64, 72–75].

With this method one does not make use of the approximations (7) what lead beyond the RMFT or SGA. This can be done in a systematic manner by including the nonlocal correlations in higher orders and thus reaching asymptotically the full Gutzwiller wave function solution step by step. It is important to note that within the extended approach, the SGA is equivalent to the zeroth order form of the DE-GWF method. As the full approach is significantly more complicated than the SGA method, here we address the question of the full solution only for a pure superconducting phase, and analyze the influence of the intersite Coulomb repulsion on that phase. The determination of the full phase diagram, i.e. with the coexistent AF and CDW phases, is cumbersome within DE-GWF and must be discussed separately.

Similar to before, in the DE-GWF method we are looking for the ground state of the system in the form given by equation (2). Using the condition (4), we can write all the
relevant expectation values which appear during the evaluation of equation (6) in the form of a power series with respect to the parameter $x$ (we assume the spatial homogeneity of the paired solution, so $x \equiv x_0$), without the use of the approximations (7). As an example, we show below the power series for the hopping probability and the intersite Coulomb interactions (7). As an example, we show below the power series expressions, e.g.

\[
\langle \Psi | \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} | \Psi \rangle = q_i \langle \Psi | \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} | \Psi_0 \rangle, 
\]

are no longer valid due to the appearance of the nonlocal correlations of increased range (caused by the appearance of the $\hat{d}_{k_{\text{HF}}}$ terms inside the expectation values $\langle \cdots \rangle_0$ in equation (17)).

By using Wick's theorem for the averages in the non-correlated state appearing in (17), one can express the average value of the system energy in terms of the paramagnetic and superconducting lines, i.e. the correlation functions that connect particular lattice sites

\[
P_{ij} \equiv \langle \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} \rangle_0, \quad S_{ij} \equiv \langle \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} \rangle_0, 
\]

respectively. As we are considering only the pure SC phase in this extended approach, the anomalous average corresponding to the paired state is purely of a spin-singlet character. Such a procedure leads to a natural manner to the diagrammatic representation of the energy expectation value, in which the lattice sites play the role of the vertices of the diagrams and the paramagnetic or superconducting lines are interpreted as their edges.

The minimization condition of the ground state energy (6) can be evaluated by introducing the effective single-particle Hamiltonian of the form (see [9])

\[
\hat{H}_{\text{eff}} = \sum_{ij} t_{ij} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \sum_{ij} (\Delta_{ij}^{\text{eff}} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma}^{\dagger} + \text{H.c.}), 
\]

where the effective parameters appearing in this Hamiltonian are defined as

\[
r_{ij}^{\text{eff}} \equiv \frac{\partial F}{\partial P_{ij}}, \quad \Delta_{ij}^{\text{eff}} \equiv \frac{\partial F}{\partial S_{ij}}. 
\]

By using the above concept of the effective Hamiltonian one can derive self-consistent equations for $P_{ij}$ and $S_{ij}$, which can then be solved numerically (see [73]). Such a procedure has to be supplemented with the concomitant energy minimization with respect to the wave-function variational parameter $x$. After determination of the value of $x$, together with those of the paramagnetic and superconducting lines, one can evaluate the so-called correlated superconducting gap in the Gutzwiller state, defined as $\Delta_{G_{ij}} \equiv \langle \Psi | \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma}^{\dagger} | \Psi \rangle / \langle \Psi | \Psi \rangle$, which represents the physical order parameter.

It should be noted that during the calculations one may limit the terms with lines that correspond to distances smaller than $R_{\text{max}}$, as $P_{ij}$ and $S_{ij}$ with increasing distance $|\Delta R_{ij}| = |R_i - R_j|$ lead to systematically smaller contributions [74]. In our calculations we have taken $\Delta R_{\text{max}} = 10$, which for the case of a square lattice in a spatially homogeneous state and for the $d$-wave pairing symmetry, leads to five different superconducting lines. Each of those lines has its correspondent in the correlated state. The following notation is used in the subsequent discussion:
where $a$ is the lattice constant. Again, because we are now considering the pure SC phase, the gap parameters correspond to the creation of spin-singlet Cooper pairs, without the admixture of spin-triplet pairing which appears in the coexistent AF + SC phase.

4. Results

4.1. SC versus CDW stability in the statistically consistent Gutzwiller approximation (SGA)

The numerical calculations were carried out for the planar square lattice. Unless stated otherwise, the following values of the microscopic parameters have been taken: $t = -0.35$ eV, $J = |t|/3$, $U = 20|t| \approx 2.5W$, and $\beta = 1500/|t|$, where $\beta = 1/k_B T$ ($T$ is the absolute temperature, $k_B$ is the Boltzmann constant). We have checked that for such a choice of $\beta$, we reproduce accurately the $T = 0$ limit values. In the following, all the energies are given in units of $|t|$. As shown in [9], similar values of $t$, $J$, and $U$ as those chosen here lead to good agreement between the DE-GWF results for the $t$-$J$-$U$ model and the principal experimental data for the SC phase in the cuprates. The GSL library [76] has been used to solve the system up to 13 self-consistent equations. The typical accuracy of solution was $10^{-10}$ for dimensionless quantities ($\chi_{\sigma\sigma}, \chi_{\tau\tau}, \chi_{\sigma\tau}, \Delta S, \Delta T$, etc.)

In figure 2 we present the order parameters of the phases AF, CDW, and SC, as well as the double occupancy, $d$ (or $d_A$ and $d_B$ where necessary), all as a function of doping, $\delta \equiv 1 - n$. The staggered magnetization, $m$, and the difference between the average number of electrons for sublattices A and B, $\delta_\sigma$, are the order parameters for the AF and CDW phases, respectively. In the case of SC, there are two order parameters (see [78, 79]), namely the singlet $\Delta S$ and the triplet $\Delta T$ gap parameters. Note that $\Delta T \neq 0$ only if $m \neq 0$ and $d$ splits to $d_A \neq d_B$ only if $\delta_\sigma \neq 0$ (indices $A$ and $B$ refer to different sublattices).

In figure 2, we display the phase diagrams for two values of the intersite Coulomb interaction term ($V = 0$ and $V = 2.5$). For $V = 0$ the SC phase appears for $\delta \lesssim 0.45$ with the coexisting AF + SC phase for $\delta \lesssim 0.25$ in which both the spin-singlet and the spin-triplet contributions to the pairing are present. As one can see, for a relatively large value of $V = 2.5$ the SC order no longer appears on the phase diagram, while the CDW phase stability region is broad. Note that the AF region is barely affected by the change of the $V$ value.

It should be noted that the suppression of $T_C$ with increasing $V$ has been discussed within the Green function approach [86, 87]. However, the scaling of the superconducting gap solution with $V$ obtained here differs from that of [86, 87]. This may be due to the circumstance that we start from the $t$-$J$-$U$ model, in which the $J$ term originates from the superexchange via the oxygen states, and is not purely due to the large-$U$ limit. This conclusion is supported by the full DE-GWF solution going beyond any renormalized mean-field treatment, as shown in section 4.3.

In figures 3(a) and (b) we show the effect of $V$ on the SC order parameters as we increase it gradually, from 0 to 1.5. One can see that with the increasing value of $V$ the SC order parameters are suppressed, and in the highly underdoped region only a pure AF phase survives. In figure 3(c), the range of the CDW ordering (with the order parameter - $\delta_\sigma$) is specified. For $V < 1.85$, no stable CDW phase is observed, but when $V$ reaches the critical value around 1.85, a region of a stable CDW order appears at $\delta \approx 0.47$. Upon increasing further the value of $V$, the CDW phase regime broadens. Note that here the AF and CDW states have the same modulation vector $Q = (\pi, \pi)$.

It is foreseeable that for a large enough value of $V$ the stability region of the CDW phase should be centered around $\delta = n = 0.5$ on the phase diagram. This is because for this particular value of $\delta$ a given occupied atomic site is always surrounded by empty sites in the CDW phase with $Q = (\pi, \pi)$ for $\delta_\sigma = n$. As a result, the gain of the system energy resulting from the intersite Coulomb repulsion is reduced drastically.
When it comes to the influence of the intersite Coulomb repulsion on the pairing, with increasing $V$ the upper concentration of the superconductivity disappearance is reduced (from $\delta = 0.45$ to $0.3$, as observed in HTS), as well as the paired phase being destroyed in the highly underdoped region ($\delta < 0.1$). In effect, the pure AF phase becomes stable very close to half-filling. Unfortunately, for the considered modulation vector $Q = (\pi, \pi)$ higher values of $V$ are required to obtain the stability of the CDW phase, which means that the experimentally observed phase diagram cannot be reproduced. Moreover, in the presented results the CDW phase appears for relatively large values of dopings. Thus, it is necessary to investigate the problem further by taking a CDW modulation vector similar to that reported in the experiment. Such an analysis is carried out in the next section.

4.2. CDW versus AF stability with the modulation vector $Q_{\text{CDW}} = (\frac{2}{3}\pi, 0)$

Here we discuss the effect of choice of the CDW modulation vector. So far we have assumed the simplest form of modulation vector $Q = (\pi, \pi)$, whereas the modulation vector reported in experiments is closer to $Q_{\text{CDW}} = (\frac{2}{3}\pi, 0)$ [32, 41], where the CDW order parameter $\delta_n$ is defined for arbitrary $Q$ in equation (9). A more realistic such situation is considered next, though without including the SC phase, while the analysis of all the considered phases simultaneously is quite cumbersome and should be discussed separately. By applying equation (9) with $Q_{\text{CDW}} = (\frac{2}{3}\pi, 0)$ and $m = 0$ (no AF ordering), one can see that the average number of particles per spin on an atomic site ($n_\sigma$) changes in the $x$ direction with a period of $3a$, where $a$ is the lattice constant. From the results depicted in figure 4, we see that in this case the maximum of the CDW order parameter is shifted towards the smaller dopings with respect to the case considered previously. This is an important result, since it is observed in experiments that the CDW appears in the underdoped regime, close to the boundary of the AF phase [32, 80]. This in turn suggests that the full description including all phases (and their possible coexistence), with such a choice of the CDW modulation vector might bring the theory closer to experiment. Such a study may constitute a firm test of the one-band model applicability to HTS as far as quantitative discussion is concerned. It should be noted that the AF solution presented in figure 4 appears still in the too-wide range of the doping $\delta$. The direct influence of the magnitude of $V$ on the SC phase stability is discussed in the following section.

4.3. SC stability beyond SGA: effect of intersite Coulomb interaction

For the sake of completeness, in this section we discuss the robustness of the pure superconducting phase within the DE-GWF method, with the intersite Coulomb repulsion included, when going beyond SGA (of RMFT type) approach. First, we show the differences between the SGA and the DE-GWF for the selected set of model parameters. The magnitudes of the intersite correlated gap parameters (see equation (22)), in an exemplary situation, obtained in the diagrammatic approach, are displayed in figure 5(a). It should be noted that for the case of the pure SC phase we have only the singlet SC gap which we denote $\Delta_G \equiv \Delta_G^S$ here. As one can see, the nearest neighbor pairing amplitude $\Delta_G^{(10)}$ is by far the dominant one. Nonetheless, the remaining larger-distance contributions may also become significant. Note that in some doping regions different contributions can change their signs. For example, in the underdoped regime both $\Delta_G^{(10)}$ and $\Delta_G^{(30)}$
obey exactly the $d$-wave symmetry, but with opposite signs. The situation is different within the SGA method, where the only nonzero pairing contribution taken into account is the nearest neighboring one. In figure 5(b) we present the evolution of the nearest-neighbor correlated gap $\Delta_{10}^G$ with the increasing order of the calculations. The lowest dotted—dashed line corresponds to the SGA method, which is also equivalent to the zeroth order DE-GWF approach. The differences between the green dotted line (the fourth order) and the black solid line (the fifth order) are very small, which means that we have achieved a convergence with the assumed accuracy. As one can see, the two methods, SGA and DE-GWF, are qualitatively similar when it comes to the doping dependence of the correlated gap, but the correlations increase the pairing amplitude by $30\%$–$40\%$ in the latter case as it encompasses also the more distant pairing amplitudes. It should be noted that qualitative differences between the two methods appear when it comes to the appearance of the non-BCS regime, as discussed in the remaining part of this work. Also, a more detailed comparison of DE-GWF and SGA is presented in [9] for the case of the $t$-$J$-$U$ model.

In figure 6 we illustrate the influence of the intersite Coulomb repulsion on the stability of the paired phase within the DE-GWF method. As one can see, the upper critical doping for the disappearance of the superconducting phase decreases significantly when the value of $V$ increases, bringing the critical doping closer to the experimental value for $V \sim |t|$. The case of the SGA calculations is similar. One of the differences between the two considered methods is that the inclusion of the higher order contributions leads to the appearance of the so-called non-BCS region in the considered model, which is manifested by the kinetic energy gain at the transition to the SC phase. The kinetic energy gain is defined by

$$\Delta E_{\text{kin}} = E_{\text{SC}}^G - E_{\text{PM}}^G, \quad E_G = \frac{1}{N} \sum_{\sigma} \sum_{\alpha} \epsilon_{\alpha} c_{\alpha \sigma}^\dagger c_{\alpha \sigma},$$

where $E_{\text{SC}}^G$ and $E_{\text{PM}}^G$ correspond to the kinetic energies in the SC and normal (paramagnetic, PM) phases, respectively.
In the BCS-like region $\Delta E_{\text{kin}} > 0$, which is also true for the BCS theory of the phonon-mediated superconductivity, whereas $\Delta E_{\text{kin}} < 0$ for the non-BCS region. It should be noted that the non-BCS behavior has been detected experimentally [81, 82] for the overdoped samples of the cuprate compounds. This very feature highlights the necessity of including the higher orders to describe this important aspect of cuprate superconductivity.

We show here also that the intersite Coulomb repulsion promotes the non-BCS behavior by pushing it to higher doping values (see figure 6(a)) with a concomitant decrease of the correlated gap magnitude.

Therefore, even though the intersite Coulomb interaction has a destructive effect by diminishing the condensation energy (see figure 6(b)), it extends the region of the non-BCS state at the same time. In figures 6(b) and (c) we plot explicitly the contributions to the condensation energy that originate from either the intersite Coulomb repulsion term (b) or the exchange interaction term (c). The intersite Coulomb repulsion term increases the energy of the SC phase with respect to the normal (PM) state, which means that it has a negative influence on the pairing strength. The opposite is true for the case of the exchange term.

5. A critical overview

In the first part we have analyzed the stability of AF, SC, CDW (and some of the possible coexistent phases) within the $t$-$J$-$U$-$V$ model. For this purpose we have used both the SGA and the DE-GWF methods. By using the former approach we have shown that the CDW phase with $Q = (\pi, \pi)$ is stable only above a critical value of $V$ (the intersite Coulomb repulsion), and is detrimental to SC phase stability. With increasing $V$, the CDW stability range broadens, whereas the SC phase is gradually suppressed. Such behavior is consistent with the experimental findings, according to which CDW and SC compete with each other. However, it should be mentioned that according to our calculations the CDW $(\pi, \pi)$ phase becomes stable in the overdoped regime, with maximal order parameter for $\delta \approx 0.5$, while in the experiment this phase is observed for smaller doping values. By changing the modulation vector to $Q = (\frac{\pi}{2}, 0)$, which is close to the one detected experimentally, we have obtained a shift of the CDW order parameter maximum towards the smaller dopings. Nevertheless, the region of stability of CDW is still too wide, even for moderate values of $V$. An interesting question arises as to whether such a situation could change if we included in figure 4 the SC phase and/or went beyond the RMFT approach.

In the second part of the article, we have analyzed first the influence of the higher-order terms on the pure SC phase within the DE-GWF method. This was motivated by the question about the extent to which the former results, obtained within the $t$-$J$-$U$ model [9, 13], are robust in the presence of the intersite Coulomb interaction. One of the differences between the DE-GWF and SGA is that in the former approach the larger-distance contributions to the pairing in real space do appear (see figure 5), whereas in SGA only the nearest neighbor SC gap appears. Secondly, the magnitude of the SC order parameter in DE-GWF is enhanced by up to 40% as compared to the zeroth-order calculations (SGA).

Furthermore, the non-BCS region appears only after the inclusion of the higher-order terms within the DE-GWF and the $V$ term pushes it to higher dopings (see figure 6). The observation of non-BCS behavior in the experiment for the cuprates [81–84] clearly shows the necessity of including the higher-order terms in the calculations for the considered model.

In the experiment, it is observed that CDW and SC phases can coexist [22, 25, 26, 31, 32, 80, 85]. However, in SGA the increase of the $V$ parameter suppresses SC before CDW appears. Therefore, the inclusion of the higher-order terms, which also results in the increase of the pairing amplitude, can lead to the stability of the coexistent SC-CDW phase. The DE-GWF calculations for the CDW phase within the one-band approach, even though significantly more complicated, can still be carried out. We should see progress along this line in the near future. Moreover, it would be interesting to explore the possibility of the intraunitcell charge ordering appearance within the three-band, Emery-type or related models by using the same method [77]. The combined exact diagonalization- *ab initio* approach [89, 90] for the Cu–O clusters could also bring some new insights in the field of charge ordered states of the cuprates.

Very recently, we have extended our DE-GWF approach to study pure SC phase for both hole- and electron-doped systems within the most general single-narrow-band model of strongly correlated electrons [88]. Such a study confirms again the applicability of the model, albeit discussed within DE-GWF, i.e. beyond SGA.

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Appendix A. Form of the $W$ function and mean-field renormalization factors

The central problem within the SGA approach is to calculate the expectation value of the system energy $\langle \Psi | \mathcal{H}_{t-J-U-V} | \Psi \rangle$ (see equation (6)), namely

$$W = \langle \mathcal{H}_{t-J-U-V} \rangle = t \sum_{(i,j), \sigma} \left( \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \rangle + \text{H.c.} \right) + \frac{t'}{4} \sum_{(i,j)} \left( \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j'\sigma'} \rangle + \text{H.c.} \right) + J \sum_{(i,j)} (\hat{S}_i \cdot \hat{S}_j) + U \sum_i (\hat{n}_{i\uparrow} \hat{r}_{i\uparrow} + \hat{r}_{i\uparrow} \hat{n}_{i\uparrow}) \left( \frac{1}{4} - \frac{1}{J} \right) \sum_{(i,j), \sigma, \sigma'} \langle \hat{r}_{i\sigma}^\dagger \hat{r}_{j\sigma'} \rangle,$$

(A.1) where for simplicity we denote $\langle \Psi | \ldots | \Psi \rangle \equiv \langle \ldots \rangle$ and the wave function is taken in the form $| \Psi \rangle = \tilde{P} | \Psi_0 \rangle$ [69, 70], where $| \Psi_0 \rangle$ is a simple, non-correlated wave function, and $\tilde{P} = \prod_i \tilde{P}_i$ is the operator, which changes the probability of local states appearing at atomic sites. The most general form of $\tilde{P}_i$ is
\[ P_t = \sum_{\Gamma} \lambda_{\Gamma} | \Gamma \rangle i_{\Gamma}(\Gamma) = \lambda_{\Gamma} \,(1 - \hat{n}_{\Gamma}) \,(1 - \hat{n}_{\Gamma}) \]
\[ + \lambda_{\delta} \hat{n}_{\Gamma} \,(1 - \hat{n}_{\Gamma}) + \lambda_{\delta} \,(1 - \hat{n}_{\Gamma}) \hat{n}_{\Gamma} + \lambda_{\delta} \hat{n}_{\Gamma} \hat{n}_{\Gamma}. \quad (A.2) \]

Following [64], we assume that \( P_t = 1 + x_i \hat{n}_{\Gamma}^{HF} \hat{n}_{\Gamma}^{HF} \), with \( \hat{n}_{\Gamma}^{HF} \equiv \hat{n}_{\Gamma} - n_{\Gamma} \). Next, by acting with \( \hat{P}_t \) on the states from the local basis \(| \delta \rangle, | \uparrow \rangle, \| \uparrow \rangle, | \uparrow \rangle | \uparrow \rangle \), one yields:
\[
\begin{align*}
\lambda_{\delta 0}^2 &= 1 + x_i n_{\Gamma} n_{\Gamma}, \\
\lambda_{\delta \sigma}^2 &= 1 - x_i (1 - n_{\Gamma}) n_{\Gamma}, \\
\lambda_{\delta \sigma}^2 &= 1 + x_i (1 - n_{\Gamma}) (1 - n_{\Gamma}). \quad (A.3)
\end{align*}
\]

where \( x_i \) is a variational parameter. When \( \forall \, i, x_i = 0 \), then the operator \( P = 1 \) and \( | \Psi \rangle = | \Psi_0 \rangle \), but when \( \exists, x_i < 0 \), then the probability of double occupancy on site \( i \) is reduced. Since the average number of electrons in the system should remain constant, \( x_i < 0 \) requires that the number of single occupied sites is increased and the number of empty sites is reduced at the same time.

A direct meaning of parameter \( x_i \) is not easy to provide. Therefore we introduce \( d_i^2 \) as the double-occupancy probability at site \( i \), namely,
\[ \langle \Psi | \hat{n}_{\Gamma} \hat{n}_{\Gamma} | \Psi \rangle \equiv d_i^2. \quad (A.4) \]

We can relate \( d_i^2 \) to the \( x_i \) parameter, since
\[ d_i^2 = \langle \Psi | \hat{n}_{\Gamma} \hat{n}_{\Gamma} | \Psi \rangle = \langle \Psi_0 | \hat{n}_{\Gamma} \hat{n}_{\Gamma} | \Psi_0 \rangle = \lambda_{\delta 0}^2 n_{\Gamma} n_{\Gamma}, \quad (A.5) \]

where we have assumed that \( \langle \Psi_0 | \hat{n}_{\Gamma} \hat{n}_{\Gamma} | \Psi_0 \rangle \equiv \langle \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 = n_{\Gamma} n_{\Gamma}, \) i.e. that the following averages \( \langle \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 \) and \( \langle \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 \) are zero. Using equations (A.3)–(A.5), we can show that
\[ x_i = \frac{d_i^2 - n_{\Gamma} n_{\Gamma}}{n_{\Gamma} (1 - n_{\Gamma}) (1 - n_{\Gamma})}, \]

and as a result, we can rewrite the expressions (A.3) in the form:
\[
\begin{align*}
\lambda_{\sigma 0}^2 &= \frac{1 + d_i^2 - n_{\Gamma} - n_{\Gamma}}{1 - n_{\Gamma} (1 - n_{\Gamma})}, \\
\lambda_{\delta \sigma}^2 &= \frac{n_{\Gamma} - d_i^2}{n_{\Gamma} (1 - n_{\Gamma})}, \\
\lambda_{\delta \sigma}^2 &= \frac{d_i^2}{n_{\Gamma} n_{\Gamma}}. \quad (A.9)
\end{align*}
\]

To calculate the averages appearing in equation (A.1), we need one more (partial) result, namely
\[
\tilde{\hat{P}} \hat{c}_{\sigma} \hat{c}_{\sigma} \tilde{\hat{P}} = (\lambda_{\sigma} \hat{n}_{\Gamma} (1 - \hat{n}_{\Gamma}) + \lambda_{\delta} \hat{n}_{\Gamma} \hat{n}_{\Gamma}) \hat{c}_{\sigma} \hat{c}_{\sigma} (\lambda_{\sigma} \hat{n}_{\Gamma} (1 - \hat{n}_{\Gamma}) + \lambda_{\delta} \hat{n}_{\Gamma} \hat{n}_{\Gamma})
\]
\[ = (\alpha_{\sigma} + \beta_{\sigma} \hat{n}_{\Gamma}) \hat{c}_{\sigma} \hat{c}_{\sigma}. \quad (A.10) \]

where
\[ \alpha_{\sigma} = \sqrt{\frac{n_{\Gamma} - d_i^2}{n_{\Gamma} (1 - n_{\Gamma})}} | d_i | \sqrt{\frac{n_{\Gamma} - d_i^2}{n_{\Gamma} (1 - n_{\Gamma})}}. \quad (A.11) \]

Note that for \( \tilde{\hat{P}} \hat{c}_{\sigma} \hat{c}_{\sigma} \tilde{\hat{P}} \) we would obtain the same result as above. Using the obtained expressions, one can calculate other averages, e.g. the average of the hopping term is then
\[
\langle \hat{c}_{\sigma} \hat{c}_{\sigma} \rangle = \langle \tilde{\hat{P}} \hat{P}_t \hat{c}_{\sigma} \hat{c}_{\sigma} \tilde{\hat{P}} \hat{P}_t \rangle = \langle \tilde{\hat{P}} \hat{P}_t \hat{c}_{\sigma} \hat{c}_{\sigma} \tilde{\hat{P}} \hat{P}_t \rangle_0
\]
\[ = \alpha_{\sigma} \hat{\alpha}_{\sigma} \hat{c}_{\sigma} \hat{c}_{\sigma} \alpha_{\sigma} + \beta_{\sigma} \hat{\alpha}_{\sigma} \hat{c}_{\sigma} \hat{c}_{\sigma} \beta_{\sigma} + \alpha_{\sigma} \hat{\alpha}_{\sigma} \hat{\beta}_{\sigma} \hat{c}_{\sigma} \hat{c}_{\sigma} \beta_{\sigma} + \beta_{\sigma} \hat{\alpha}_{\sigma} \hat{\beta}_{\sigma} \hat{c}_{\sigma} \hat{c}_{\sigma} \beta_{\sigma}. \quad (A.13) \]

Using Wick’s theorem we can check that \( \langle \hat{c}_{\sigma} \hat{c}_{\sigma} \rangle = 0 \) and \( \langle \hat{c}_{\sigma} \hat{c}_{\sigma} \rangle = 0 \), as far as we assume that there is no onsite pairing of electrons, \( \langle \hat{c}_{\sigma} \hat{c}_{\sigma} \rangle = 0 \), and hopping does not change spin, \( \langle \hat{c}_{\sigma} \hat{c}_{\sigma} \rangle = 0 \). The last average in equation (A.13) is usually non-zero, but small, therefore it can be neglected here. Hence, we are left with
\[ \langle \hat{c}_{\sigma} \hat{c}_{\sigma} \rangle \approx \alpha_{\sigma} \hat{\alpha}_{\sigma} \hat{c}_{\sigma} \hat{c}_{\sigma} \alpha_{\sigma}. \quad (A.14) \]

In the simplest case, where neither AF nor CDW orderings are present, we have \( \alpha_{\sigma} = \alpha_{\sigma} = \alpha \) and thus
\[ \alpha^2 = \gamma = \frac{n - 2d^2}{n(1 - n/2)} \left( \sqrt{1 - n + d^2 + |d|} \right)^2, \quad (A.15) \]

which is the Gutzwiller factor for the hopping part, well known from the literature, see [2, 4, 91, 92].

In a similar manner, the other averages appearing in equation (A.1) can also be calculated. To provide one more example, we show here explicitly how to calculate the last term, \( \langle \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 \), requiring perhaps the most non-trivial calculations, rarely discussed in the literature. To abbreviate the length of the expressions, we assume here for a moment that we are interested only in the AF order. The generalization to the case of CDW order (or others) is not difficult and it can be left to the reader. Note that in the simplest two-sublattice AF ordering it is required that \( n_{\sigma} \) on A sublattice is equal to \( n_{\sigma} \) on the B sublattice. In such a case,
\[ \Lambda^{-1} \sum_{(\delta), \sigma} \langle \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 = \Lambda^{-1} \sum_{(\delta), \sigma} \langle \hat{P}_t \hat{c}_{\sigma} \hat{c}_{\sigma} \hat{P} \rangle_0 \]
\[ = \Lambda^{-1} \sum_{(\delta), \sigma} \left( \langle \hat{n}_{\Gamma} + (\lambda_{\sigma}^2 - \lambda_{\delta}^2) \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 \langle \hat{n}_{\Gamma} + \lambda_{\delta}^2 \hat{n}_{\Gamma} \hat{n}_{\Gamma} \rangle_0 \right)_0 \]
\[ = \Lambda^{-1} \sum_{(\delta), \sigma} \left( \langle \hat{n}_{\Gamma} \rangle_0 \langle \hat{n}_{\Gamma} \rangle_0 \right) \left( \lambda_{\sigma}^2 - \lambda_{\delta}^2 \right) \]
\[ + \left( \langle \hat{n}_{\Gamma} \rangle_0 \langle \hat{n}_{\Gamma} \rangle_0 \right) \lambda_{\sigma}^2 \lambda_{\sigma}^2 \]
\[ + \left( \langle \hat{n}_{\Gamma} \rangle_0 \langle \hat{n}_{\Gamma} \rangle_0 \right) \lambda_{\sigma}^2 \lambda_{\sigma}^2 \]
\[ + \left( \langle \hat{n}_{\Gamma} \rangle_0 \langle \hat{n}_{\Gamma} \rangle_0 \right) \lambda_{\sigma}^2 \lambda_{\sigma}^2 \]
\[ = 2n^2 + 4n^2 (\Delta_2^2 - 2\Delta_2^2) + 4n^2 \left( \Delta_2^2 - 4\Delta_2^2 \right) \]
\[ = 2n^2 + 4n^2 (-2\Delta_2^2) + 4n^2 (\Delta_2^2 + \Delta_2^2). \quad (A.16) \]
where
\[ g_\uparrow^2 = \left(1 + n_\sigma (\lambda_\uparrow^2 - \lambda_\downarrow^2) + n_\sigma (\lambda_\downarrow^2 - \lambda_\uparrow^2) + n_\sigma (\lambda_\uparrow^2 - \lambda_\downarrow^2) n_\sigma (\lambda_\downarrow^2 - \lambda_\uparrow^2)\right), \]
\[ g_\downarrow^2 = \left(1 + n_\sigma (\lambda_\downarrow^2 - \lambda_\uparrow^2) + n_\sigma (\lambda_\uparrow^2 - \lambda_\downarrow^2) + n_\sigma (\lambda_\downarrow^2 - \lambda_\uparrow^2) n_\sigma (\lambda_\uparrow^2 - \lambda_\downarrow^2)\right) + \frac{1}{2} \left(n_\sigma (\lambda_\downarrow^2 - \lambda_\uparrow^2)^2 + n_\sigma (\lambda_\uparrow^2 - \lambda_\downarrow^2)^2\right). \] (A.17)

The ‘\(\approx\)’ sign in equation (A.16) results from the fact that we neglected terms proportional to \(\lambda_\downarrow^2\), \(\Delta_\downarrow^2\), \(\Delta_\uparrow^2\) and \(n_\sigma n_\sigma \lambda^2\). Note that if no AF order is considered \((m = 0)\), then \(n_\sigma = n_\sigma = n/2\) and then
\[ g_\lambda^2 = g_\lambda^2 = \left(\frac{2d^2 + n(1-n)}{m(1-n/2)}\right)^2. \] (A.18)

Appendix B. Two ways of defining the Gutzwiller factor in the presence of extra orderings

In this appendix we show that the introduction of extra orderings, such as AF or CDW, can lead to a specific ambiguity in determining the final form of the Gutzwiller renormalization factors. We explain also how we have decided to select a particular form used in the main text.

For simplicity, we assume here that \(U \rightarrow \infty\), resulting in \(d \rightarrow 0\). Furthermore, to make our arguments easy to follow, we consider only the AF order and focus on the example of the Gutzwiller factor for the hopping term that has been already discussed in the foregoing appendix (see equation (A.15)). The generalization to other states and to other averages is straightforward.

Within the SGA approach one expresses the average from the hopping term in the following manner
\[ \langle \Psi | \hat{c}_i^\dagger \hat{c}_j \rangle \Psi \rangle = \langle \Psi_0 | \hat{P}_i \hat{c}_i^\dagger \hat{P}_j \hat{c}_j \Psi_0 \rangle \] (B.1)

The renormalization factor for particular processes can be defined in the following manner
\[ g_0(n_{\sigma\sigma}, n_{\sigma\sigma}, \ldots) = \frac{\langle \Psi | \hat{c}_i^\dagger \hat{c}_j | \Psi \rangle}{\langle \Psi_0 | \hat{P}_i \hat{c}_i^\dagger \hat{P}_j \hat{c}_j | \Psi_0 \rangle}. \] (B.2)

Let us assume that the average number of electrons per atomic site is \(n\) and the staggered magnetization is equal to \(m\). In the non-correlated case \((U = 0)\), there is on average \(n_\sigma \equiv n_{\sigma\sigma} = \frac{1}{2}(n + s m)\) electrons with spin \(\sigma\) per site for the A sublattice and \(n_\sigma \equiv n_{\sigma\sigma} = \frac{1}{2}(n - s m)\) for the B sublattice. Additionally, on average, \(n_{\sigma\sigma} = n_{\sigma\sigma} = n_{\sigma\sigma} = n_{\sigma\sigma}\) and consequently, \(n_{\sigma\sigma} = (1 - n_{\sigma\sigma})(1 - n_{\sigma\sigma}) = (1 - n_{\sigma\sigma})(1 - n_{\sigma\sigma})\) (see table B1).

In the correlated state \(|\Psi\rangle\) the double occupancy \(d^2\) is reduced with respect to \(|\Psi_0\rangle\) due to the presence of the onsite Coulomb repulsion. The adjustment of \(d^2\) is made by selecting a proper form of \(\hat{P}\) operator (see [69, 70]). In the limiting case of \(U \rightarrow \infty\), the double occupancies are removed in \(|\Psi\rangle\), which results in \(\forall \lambda_\downarrow, \lambda_\downarrow = 0\) (see the general form of \(\hat{P}\), equation (A.2)). However, by removing the double occupancies (by changing the \(\lambda_\downarrow, \lambda_\downarrow\) parameters) we also change the average number of electrons in the system. To avoid this, the weights \(\lambda_\downarrow, \lambda_\downarrow\), and \(\lambda_\downarrow, \lambda_\downarrow\) must be modified as well.

There are two intuitive ways in which this can be achieved.

(i) We can ‘split’ every double occupancy, separating the electrons (one \(\uparrow\) and one \(\downarrow\)) to different, previously empty sites. Such an operation would not change the global magnetization of the system \((m = n_\uparrow - n_\downarrow)\) but it would modify the proportion between the number of sites occupied by spin-up and down electrons.

(ii) We can ‘erase’ the double occupancies. However, such an action would change the number of electrons in the system. Therefore, to restore the previous number of electrons, we can proportionally add up and down electrons to previously empty sites. This operation would maintain the proportion of the number of single occupied states with the spin up to those with the spin down, but it would modify the global magnetization of the system.

Both of the presented schemes lead to a different probability of sites to be in a certain state, as displayed in the table B2. Note that in the first scheme, the proportion of \(|\uparrow\rangle\) states is the same as \(|\downarrow\rangle\) or \(|\downarrow\rangle\) states in the table B1. In the second scheme, after erasing the doubly occupied states, the number of electrons has changed from \(n\) to \(n - n_{\sigma\sigma}n_{\sigma\sigma}\) in the A sublattice and to \(n - n_{\sigma\sigma}n_{\sigma\sigma}\) in the B sublattice. Therefore, to restore the previous number of electrons in the system, the probability that the state will have a single electron \(\sigma\) was renormalized by the factor \(n/(n - 2n_{\sigma\sigma}n_{\sigma\sigma})\).

Next, it is possible to derive the \(g_{\lambda\lambda}\) Gutzwiller factor for the hopping term in both schemes. For the hopping to occur in the correlated state, there needs to be a site occupied by a single electron with the spin \(\sigma\), while the neighboring site needs to be empty. Therefore, by comparing the amplitudes of the bra and the ket contributions of \(\langle \Psi | \hat{c}_i^\dagger \hat{c}_j | \Psi \rangle\), and with the help of table B2, we can write that in the first scheme,
\[
\langle \Psi | \hat{c}_i^{\dagger} \hat{c}_j \Psi \rangle \equiv \sqrt{n_{A\sigma} n_{B\sigma}} (1 - n).
\]  
(B.3)

whereas in the second scheme,
\[
\langle \Psi | \hat{c}_i^{\dagger} \hat{c}_j \Psi \rangle \equiv \sqrt{n_{A\sigma} (1 - n_{A\sigma})} n_{B\sigma} (1 - n_{B\sigma}) \frac{n}{(n - 2n_{A\uparrow} n_{A\downarrow})(n - 2n_{B\uparrow} n_{B\downarrow})} r(1 - n).
\]  
(B.4)

Analogically, we can calculate the hopping probability in the uncorrelated state. Hopping can occur when either site has an electron with the spin \(\sigma\) or it is doubly occupied, and when either the neighboring site is empty or has one electron with the spin \(\overline{\sigma}\) (see also [7]). Using table B1, we obtain
\[
\langle \Psi_0 | \hat{c}_i^{\dagger} \hat{c}_j \Psi_0 \rangle = \sqrt{n_{A\sigma} (1 - n_{B\sigma})} n_{B\sigma} (1 - n_{A\sigma}).
\]  
(B.5)

In effect, by using equation (B.2), we obtain either
\[
g_1^{(1)} = \frac{1 - n}{\sqrt{(1 - n_1)(1 - n_1)}},
\]  
(B.6)
or
\[
g_1^{(2)} = \frac{1 - n}{1 - 2n_{n\downarrow}},
\]  
(B.7)

where we denoted \(n_{1\sigma} = n_{A\sigma} n_{B\sigma}\). Both \(g_1^{(1)}\) and \(g_1^{(2)}\) are present in the literature, for example \(g_1^{(2)}\) in [2, 4, 21, 91], whereas \(g_1^{(3)}\) is identical with the zero-order renormalization factors of the DE-GWF method [64, 72–74, 93].

Note that if no AF order is present,
\[
g_1^{(1)} = g_1^{(2)} \equiv g_1 = \frac{1 - n}{1 - n/2}.
\]  
(B.8)

and there is no difference between \(g_1^{(1)}\) and \(g_1^{(2)}\) (see also equation (A.15) and take \(d = 0\)). For the case of CDW ordering (without AF), one should take in equations (B.3)–(B.5) \(n_{A\sigma} = n_{A\downarrow}\) and \(n_{B\sigma} = n_{B\downarrow}\), so that \(n_{A\uparrow} \neq n_{B\uparrow}\). In such a situation we have also \(g_1^{(1)} \neq g_1^{(2)}\).

The above discussion can be easily carried out for other Gutzwiller factors that renormalize the averages from the remaining energy terms. In effect, the results will become method dependent. Explicitly, it has also been checked that the two schemes lead to substantially different outputs, especially regarding the stability of the AF phase. In the first scheme (used in the main text of this paper), the AF phase is stable in a wide range of doping, from 0 to about \(d_{\text{max}} = 0.27\) (see figure 2) On the other hand, by using the second scheme one obtains AF phase stability very close to the half-filling with \(d_{\text{max}} < 0.006\) (see our previous paper [19]).

In this paper, we have decided to use the first scheme, since it is consistent with the SGA method which in turn is equivalent to the the zero order DE-GWF approach.

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