A statistically consistent variational approach to the renormalized mean-field theory of the t-J model: critical hole concentrations for a paired state

Jakub Jędrak* and Jozef Spalek†
Marian Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland

Abstract
Recently, Fukushima [Phys. Rev. B 78 115105 (2008)] proposed a systematic derivation of the Gutzwiller approximation for the t-J model. In the present paper, using this approach we construct an effective single-particle Hamiltonian, which leads to a renormalized mean-field theory (RMFT). We also use the method proposed by us recently and based on the maximum entropy principle (MaxEnt), which in turn, yields a consistent statistical description of the problem. On the examples of non-magnetic superconducting d-wave resonating valence bond (dRVB) and normal staggered-flux (SF) solutions, we compare two selections of the Gutzwiller renormalization schemes, i.e. the one proposed by Fukushima with that used earlier by Sigrist et al. [Phys. Rev. B 49, 12 058 (1994)]. We also confront the results coming from our variational solutions with the self-consistency conditions build in, with those of the non-variational approach based on the Bogoliubov-de Gennes self-consistent equations. Combination of the present variational approach with the new renormalization scheme (taken from Fukushima’s work) provides, for $t/J = 3$, an upper critical hole concentration $x_c \approx 0.27$ for the disappearance of the d-wave superconductivity. Also, the hole concentration $x \approx 0.125$ is obtained for the optimal doping. These results are in rough accordance with experimental results for high-$T_c$ superconducting cuprates.

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1 Introduction
The t-J model [1] is commonly regarded as a minimal model capable of describing correctly the essential physics of the cuprate high-temperature superconductors. In its simplest form, used in the present paper, it is expressed by the following Hamiltonian

$$\hat{H}_{t-J} = \hat{P}_G (\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j) \hat{P}_G.$$  (1)
Here $\hat{P}_G = \prod_i (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$ is a Gutzwiller projection operator, ensuring that no doubly occupied sites are present.

Unfortunately, the rigorous treatment of the t-J model is limited to very special cases. This is both due to the interaction term ($\mathbf{S}_i \cdot \mathbf{S}_j$), as well as to the presence of $\hat{P}_G$ operators. Even in the $J = 0$ limit, Hamiltonian (1) is not an independent-particle one. To proceed further, (1) may be treated within the mean-field approximation. This procedure yields a single-particle Hamiltonian $\hat{H}$, being the mean-field analogue of $\hat{H}_{t-J}$ (1). The resulting effective description is termed the renormalized mean-field theory (RMFT) [2].

The crucial point in the construction of RMFT is an approximate treatment of the Gutzwiller projection. In a broader perspective, this problem is closely related to an analytic evaluation of the expectation values of operators with respect to the following variational state

$$|\Psi\rangle = \hat{P}_{GC}|\Psi_0\rangle = \prod_i \lambda_{i\uparrow}^{\hat{n}_{i\uparrow}} \lambda_{i\downarrow}^{\hat{n}_{i\downarrow}} (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}) |\Psi_0\rangle$$

In the above, $\hat{P}_G$ was replaced by a more general Gutzwiller correlator $\hat{P}_{GC}$, differing from $\hat{P}_G$ by the presence of the so-called fugacity factors $\lambda_{i\sigma}$ [3]. For $\lambda_{i\sigma} = 1$ we recover $\hat{P}_G$. $|\Psi_0\rangle$ is an uncorrelated single-particle state, which, within the framework of RMFT, is chosen as the eigenstate of the $\hat{H}$. Explicitly, we are interested in evaluation of the expressions like

$$\langle \hat{O} \rangle_G = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx g^O (\hat{A}) \langle \Psi_0 | \hat{O} | \Psi_0 \rangle \langle \Psi_0 | \Psi_0 \rangle$$

$\hat{O}$ is an arbitrary operator, $\{ A_s \} = A_1, A_2, \ldots, A_M (\equiv \hat{A})$ are the relevant mean-fields, i.e. the expectation values of the corresponding single-particle operators $\{ \hat{A}_s \} = \hat{A}_1, \ldots, \hat{A}_M$, and both $\hat{H}$ and $|\Psi_0\rangle$ are usually $\hat{A}$-dependent. Consequently, $f_O (\hat{A})$ is a $\mathbb{C}$-valued function of the mean-fields. Each prescription of the form (3) will be termed the renormalization scheme (RS).

Note, that usually the RS (3) may be given a more specific form

$$\langle \hat{O} \rangle_G \equiv \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx g^O (\hat{A}) \frac{\langle \Psi_0 | \hat{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \equiv g^O (\hat{A}) \langle \hat{O} \rangle.$$
advanced include also the inter-site quantities (mean fields defined on bonds, e.g. pairing amplitude), cf. the Refs. [3], [8]-[10]. In particular, the scheme of Ref. [8] has been used in Refs. [11] and [12] and also in our previous work, [13].

In this paper we focus our attention mainly on the renormalization scheme of Ref. [3], which, in our opinion, is the most promising one devised so far. First, due to the presence of fugacity factors in (2), the Gutzwiller projection does not change the local densities of spin up (down) electrons, i.e. \( \langle \hat{n}_{i\sigma} \rangle_G = \langle \hat{n}_{i\sigma} \rangle \equiv n_{i\sigma} \). Next, this formalism may, in principle, be systematically extended beyond the second order in the inter-site quantities (formulas of Ref. [3] are provided up to this order). Also, it can be relatively easily applied to the extensions of Hamiltonian (1), or to the more complicated symmetry - breaking situations.

Suppose, that we have constructed the RMFT specifying appropriate single-particle mean-field Hamiltonian \( \hat{H} \). Next, we have to determine the optimal values of mean-fields appearing in a model. One possibility is an application of the non-variational self-consistent approach based on the Bogoliubov-de Gennes (BdG) equations. However, this route, apart from its other drawbacks, [14], encounters a serious difficulty in the following sense. Namely, the renormalization scheme of that Ref. [3] is in general not of the form (4). This feature does not allow for an unambiguous identification of the renormalization factors and hence the construction of the effective MF Hamiltonian. Namely, there is no clear way to ascribe the corresponding single-particle operator expression to the expectation values (3). Even if some way of replacing \( \langle \hat{O} \rangle_3 \) by the operator counterpart may seem more natural than others, there is in fact no unique way of carrying out such procedure. Also, different such ways obviously yield different versions of RMFT Hamiltonians and consequently different BdG self-consistent equations, hence different predictions of the model.

This lack of uniqueness does not appear within the variational method proposed by us recently [14], as will be discussed in detail below.

The main aim of the present paper is twofold. First, we compare different renormalization schemes within the RMFT effective single-particle picture for the t-J model. Moreover, as in to Ref. [13], we compare two distinct methods of solving such MF models: the present variational approach (labeled as \( \text{var} \)) and a non-variational one, based on the Bogoliubov-de Gennes self-consistent equations (labeled as \( s-c \)).

The paper is organized as follows. In Section 2 we present those parts of our approach which are relevant to the present discussion. In Section 3 we present our numerical results, first for the d-wave superconducting (dRVB), \( 3.1 \) and \( 3.2 \), and then for the staggered-flux (SF) solutions \( 3.3 \), respec-
tively. In Appendix A we provide some of the technical details omitted in main text. Section 4 contains a concluding remarks.

2 Formalism: the method

2.1 Self-consistent variational approach to the mean-field models

The most of standard mean-field models may be solved by employing two methods. First, we may invoke the variational procedure, i.e. minimization of the MF grand potential or ground state energy, with respect to the values of the order parameters (mean fields). Secondly, by using the self-consistency (Bogoliubov-de Gennes) equations, expressing the basic fact that the mean-fields are averages of the corresponding operators. However, those two routes are equivalent only for MF Hamiltonians of the Hartree-Fock type (e.g. the BCS Hamiltonian) \[14\] \[15\]. In the case of RMFT for the t-J model, the self-consistency of the MF formalism may be spoiled by unwary application of such variational procedure, for both nonzero temperatures and for \(T = 0\). This due to the non-Hartree character of the RMFT Hamiltonian, caused by MF treatment of the Gutzwiller projection.

In such situation, the non variational self-consistent method based on the Bogoliubov-de Gennes (BdG) equations is usually applied to those advanced versions of RMFT, \[4\] \[8\] \[7\] \[11\] \[12\]. However, this route suffers from serious drawbacks \[14\].

The other solution is the appropriate modification of the variational method. Examples of such self-consistent variational MF approach may be found in Refs. \[5\] \[6\] \[10\], \[16\]-\[18\]. The approaches of those References exhibit various degree of generality, and differ from each other with respect to technical details. Yet, all are based on the variational principle of quantum mechanics (minimization of the expectation value of the Hamiltonian), applied to the MF case. As such, they are applicable to \(T = 0\) situation only.

Our point of departure is different. We base our approach \([13\] \[14\]) on the maximum entropy principle (MaxEnt) \[19\], which is the basis of Bayesian mathematical statistics. In particular, it may be viewed also as the basis of the standard (non mean-field) statistical mechanics \[19\] \[20\]. The application of MaxEnt inference to the non-standard case of MF statistical-mechanical description is a natural extension of this fundamental principle \((14\), c.f. also \[21\]). To ensure the self consistency of MF description, it is necessary to introduce additional constraints, not present in the standard statistical mechanics. This could be achieved in the most natural manner by the Lagrange
multiplier method. Explicitly, starting from an arbitrary MF Hamiltonian \( \hat{H}(\vec{A}) \), we define yet another MF Hamilton operator \( \hat{H}_\lambda \) according to

\[
\hat{H} \rightarrow \hat{H}_\lambda = \hat{H} - \sum_{s=1}^{M} \lambda_s (\hat{A}_s - A_s).
\]  

(5)

The correct grand-canonical MF density operator is then given by

\[
\hat{\rho}_\lambda = \frac{1}{Z_\lambda} \exp\left(-\beta(\hat{H}_\lambda - \mu \hat{N})\right), \quad Z_\lambda = \text{Tr}\left[\exp\left(-\beta(\hat{H}_\lambda - \mu \hat{N})\right)\right].
\]  

(6)

Next, the generalized grand-potential Landau functional is defined as

\[
\mathcal{F}(\vec{A}, \vec{\lambda}) \equiv -\frac{1}{\beta} \ln(\text{Tr}[\exp(-\beta(\hat{H}_\lambda - \mu \hat{N}))]) = -\frac{1}{\beta} \ln(Z_\lambda),
\]  

(7)

with the inverse temperature \( \beta = 1/k_B T \). The equilibrium values of \( \vec{A} = \vec{A}_0 \), \( \vec{\lambda} = \vec{\lambda}_0 \) are the solution of the set of equations

\[
\nabla_A \mathcal{F} = 0, \quad \nabla_\lambda \mathcal{F} = 0,
\]  

(8)

for which \( \mathcal{F}(\vec{A}, \vec{\lambda}) \) has the lowest value. By taking the derivatives with respect to \( \vec{\lambda} \) only, and subsequently putting \( \vec{\lambda} = \vec{0} \),

\[
\nabla_\lambda \mathcal{F} = 0, \quad \vec{\lambda} = \vec{0},
\]  

(9)

we obtain standard Bogoliubov-de Genes (BdG) self-consistent equations. In such a case we denote the chemical potential \( \tilde{\mu} = \mu_s - c \), which corresponds to \( \tilde{\mu} = \mu + \lambda \) for the var method. The thermodynamical grand potential \( \Omega \) and the free energy \( F \) are defined respectively as

\[
\Omega(T, V, \mu) = \mathcal{F}(T, V, \mu; \vec{A}_0(T, V, \mu), \vec{\lambda}_0(T, V, \mu)), \quad F = \Omega + \mu N
\]  

(10)

for var, and similarly (with \( \mu_s - c, \vec{\lambda}_0 = \vec{0} \)) for s-c method.

Obviously, the present formalism is valid for any non-zero temperature, but not for \( T = 0 \). Consequently, we should replace pure states \( |\psi_0\rangle \) in Eqs. (2) - (4) by mixed ones (6), \( \hat{\rho}_\lambda \).

On the other hand, the Gutzwiller approximation in a form (3) or (4) is devised for a ground state, hence for temperature \( T = 0 \). However, the solutions of the mean field models (and the RMFT of the t-J model in particular), obtained for non-zero, but sufficiently low \( T \) are practically identical to those of the real \( T = 0 \) analysis. Consequently, \( \hat{\rho}_\lambda \) is practically indistinguishable

\footnote{Lagrange multipliers \( \lambda_s \) appearing in (3) should not be confused with the fugacity factors \( \lambda_{\alpha\sigma} \) appearing in Eqn. (2).}
from $|\psi_0\rangle$, and thus the application of the finite-temperature formalism in the $\beta \to \infty$ limit is fully justified.

Reader interested in details of our method may consult Ref. [14]. Below we recall some of its features, which are important from the point of view of the present application. They are justified in the Appendix A.

First, the $\vec{A}$-dependence of the nontrivial part of the Hamiltonian $\hat{H}_\lambda(\vec{A})$ is completely determined by the set of the single-particle operators out of which $\hat{H}_\lambda(\vec{A})$ and $\hat{H}(\vec{A})$ are composed.

Moreover, two MF Hamiltonians $\hat{H}^{(1)}$ and $\hat{H}^{(2)}$ (or $\hat{H}_\lambda^{(1)}$ and $\hat{H}_\lambda^{(2)}$), having the same nontrivial operator part and the same $\vec{A}$-dependence of the expectation value, i.e. $\langle \hat{H}^{(1)} \rangle = \langle \hat{H}^{(2)} \rangle = \langle \hat{H}(\vec{A}) \rangle$, are equivalent. Namely, they yield identical equilibrium values of mean fields, quasi-particle energies, thermodynamic potentials etc. This feature guarantees that, when constructing RMFT Hamiltonian, different assignments of the operator expression to the expectation values (13) lead to identical results.

Parenthetically, the values of the Lagrange multipliers $\vec{\lambda}$ may differ between two such equivalent MF Hamiltonians $\hat{H}_\lambda^{(1)}$, $\hat{H}_\lambda^{(2)}$. This indicates, that $\vec{\lambda}$ have no unambiguous physical interpretation by themselves, but only in the certain combinations with the mean fields. Only the Lagrange multipliers related to the quantities of a priori known average values, e.g. particle number $N$, are identical for all such equivalent Hamiltonians.

### 2.2 Application to the renormalized mean-field t-J model

For the RS that can be given the form (11), with $\lambda_i^{\sigma} = 1$ in (2), and in the absence of the long-range antiferromagnetic order, the mean-field Hamiltonian $\hat{H}$ may be taken in a form [4, 7, 8, 11, 12]

$$\hat{H} = \sum_{\langle ij \rangle \sigma} (t_{ij} g_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - \frac{3}{4} J_{ij} g_{ij} (\chi_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} - |\chi_{ij}|^2)$$

$$- \sum_{\langle ij \rangle \sigma} \frac{3}{4} J_{ij} g_{ij} (\Delta_{ij} c_{j\sigma}^\dagger c_{i\sigma} + \text{H.c.} - |\Delta_{ij}|^2). \quad (11)$$

In the above expression, $c_{i\sigma}^\dagger$ ($c_{j\sigma}$) are ordinary fermion creation (annihilation) operators, $\chi_{ij} = \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$, and $\Delta_{ij} = \langle c_{i-\sigma} c_{j\sigma} \rangle = \langle c_{j-\sigma} c_{i\sigma} \rangle$ are respectively, the hopping amplitude (bond-parameter) and the RVB gap parameter, both

\[\text{i.e. not proportional to the unit operator}\]
taken for nearest neighbors $\langle ij \rangle$. $\langle \hat{O} \rangle$ denotes the average value of the operator $\hat{O}$ evaluated with the help of a MF state\footnote{This corresponds to $\langle \hat{O} \rangle_0$ in notation of Ref. \cite{3}.}

In (11), the interaction term $(\mathbf{S}_i \cdot \mathbf{S}_j)$ of Hamiltonian (1) has been treated within the Hartree-Fock decoupling in both the particle-particle ($\Delta_{ij}$) and particle-hole ($\chi_{ij}$) channels. The renormalization factors $g^t_{ij}$ and $g^J_{ij}$ are given by (4), with $\hat{O} = \sum_{\langle ij \rangle_0}(g^t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.})$ and $\hat{O} = \mathbf{S}_i \cdot \mathbf{S}_j$, respectively. Their explicit form depends on the approximation used to obtain r.h.s. of (1).

As mentioned above, the non-Hartree-Fock character of RMFT Hamiltonians $\hat{H}$ is due to MF treatment of the Gutzwiller projection. Consequently, in order to obtain $\hat{H}_\lambda$, we must add to $\hat{H}$ the constraints corresponding to the mean fields appearing in $g^t$ and $g^J$.

The simplest renormalization factors \cite{2}-\cite{7} depend solely on local hole densities $x_i = 1 - n_i$, i.e.

\begin{equation}
    g^t_{ij} = \sqrt{\frac{4x_ix_j}{(x_i + 1)(x_j + 1)}} \quad \text{and} \quad g^J_{ij} = \frac{4}{(x_i + 1)(x_j + 1)}.
\end{equation}

In the framework of our method, in the homogeneous case $x = x_i$, the additional Lagrange multiplier coupled to the total particle number is introduced. For a non-homogeneous case, local chemical potentials should be introduced, which may be found in Refs. \cite{5, 6, 18}.

In the case of more complicated form of $g^t$, $g^J$ factors, depending apart from $x_i$ also on the inter-site mean-field variables (\cite{3, 8, 11, 12}), the MF Hamiltonian has to be modified further. The Lagrange multipliers related to the average hopping (bond order) and superconducting order parameters acquire non-zero values in the equilibrium situation.

As pointed out previously, the form of Gutzwiller approximation of Ref. \cite{3} does not reduce to multiplication by renormalization factors, (4). E.g., for the hopping amplitude, we have

\begin{equation}
    \langle c^\dagger_{i\uparrow}c_{j\uparrow} \rangle_G \approx \sqrt{\frac{1 - n_i}{1 - n_{i\uparrow}}} \sqrt{\frac{1 - n_j}{1 - n_{j\uparrow}}} \left( \chi_{ij\uparrow} - \chi_{ij\downarrow} \frac{\chi_{ij\uparrow} \chi_{ij\downarrow} + \Delta_{ij} \Delta^*_{ij}}{1 - n_i(1 - n_{i\uparrow})} \right),
\end{equation}

(Eqn. (15) of Ref. \cite{3}, but with different notation). This, in general, does not allow for identification of renormalization factor $g^t$. However, for completeness, we want to compare the variational approach with the non-variational treatment of RMFT based on Ref. \cite{3}. Hence, using (13) we may quite reasonably define those factors for a simple homogeneous non-magnetic states.
\( n_{i\uparrow} = n_{i\downarrow} = n_i / 2 \), \( \langle c^\dagger_{i\uparrow} c_{j\uparrow} \rangle = \chi_{ij\uparrow} = \chi_{ij\downarrow} = \chi_{ij} \) as

\[
(I) \quad g^I_{ij} = \sqrt{\frac{1 - n_i}{1 - \frac{n_i}{2}}} \sqrt{\frac{1 - n_j}{1 - \frac{n_j}{2}}} \left( 1 - \frac{\chi_{ij} \chi_j^* + \Delta_{ji} \Delta_j^*}{(1 - \frac{n_i}{2})(1 - \frac{n_j}{2})} \right). \tag{14}
\]

\[
g^J_{ij} = \frac{1}{(1 - \frac{n_i}{2})(1 - \frac{n_j}{2})}. \tag{15}
\]

The prescription \( \text{(15)} \) will be referred to as a renormalization scheme (I). This will be confronted with \( g^I \)-factors taken from Ref. \[8\].

\[
(II) \quad g^J_{ij} = \sqrt{\frac{4x_i x_j (1 - x_i)(1 - x_j)}{(1 - x_i^2)(1 - x_j^2) + 8(1 - x_i x_j)|\chi_{ij}|^2 + 16|\chi_{ij}|^4}}, \tag{16}
\]

\[
g^J_{ij} = \frac{4(1 - x_i)(1 - x_j)}{(1 - x_i^2)(1 - x_j^2) + 8x_i x_j(|\Delta_{ij}|^2 - |\chi_{ij}|^2) + 16(|\Delta_{ij}|^4 + |\chi_{ij}|^4)}, \tag{17}
\]

referred to as renormalization scheme (II). Usually within the RMFT, the physical (renormalized) superconducting parameter is defined as \( g^I \Delta \) instead of bare \( \Delta \) itself, \[2\]. This is also the case for scheme (II). On the other hand, within the scheme (I), there appear a separate expression for renormalized value of \( \langle c_{i-\sigma} c_{j\sigma} \rangle_G = \langle c_{j-\sigma} c_{i\sigma} \rangle_G \), cf. Eqn. \( (18) \) of \[3\]. Again, for simple homogeneous, non-magnetic states, the corresponding \( g^I \Delta \) factor can be quite reasonably identified as

\[
(I) \quad g^I_{ij} = \sqrt{\frac{1 - n_i}{1 - \frac{n_i}{2}}} \sqrt{\frac{1 - n_j}{1 - \frac{n_j}{2}}} \left( 1 + \frac{\chi_{ij} \chi_j^* + \Delta_{ji} \Delta_j^*}{(1 - \frac{n_i}{2})(1 - \frac{n_j}{2})} \right). \tag{18}
\]

Note, that \( \text{(18)} \) differs from \( \text{(14)} \).

### 3 Results: d-wave superconducting and staggered flux phase

Below we present our numerical results, first for the plain d-wave superconducting state with no magnetic order (dRVB), and next for the staggered-flux (SF) normal solution. Even for those simplest MF states, the results obtained within various renormalization schemes and/or the solving methods differ remarkably.
3.1 d-wave superconducting (dRVB) solution at $x = \frac{1}{8}$

The solution analyzed here is constructed to possess full symmetry of the underlying square lattice, only the superconducting order parameter is assumed to have $d_{x^2-y^2}$ symmetry. Consequently, we are left with three independent mean fields $\mathcal{A} = (n, \chi, \Delta)$, where $\chi_x = \chi = \chi_y$, $\Delta_x = \Delta = -\Delta_y$, and the same number of the corresponding Lagrange multipliers, $\lambda = (\lambda, \lambda_x, \lambda^\Delta)$, where $\lambda^x = \lambda^y = \lambda^\Delta$, $\lambda^\Delta = -\lambda^\Delta$, and $n = n_i = \sum_\sigma \langle c^{\dagger}_i \sigma c_i \rangle$, $\chi_{ij} = \chi_{\tau}$, $\tau = x(y)$ for the bonds in $x(y)$ directions, respectively. Also, $\sqrt{2}\Delta_{ij} = \Delta_{\tau}$, and all the above quantities are taken as real. Diagonalization of (5) in the present case yields

$$\hat{H}_\lambda - \mu \hat{N} = \sum_k E_k (\hat{\gamma}_{k0}^1 \hat{\gamma}_{k0} + \hat{\gamma}_{k1}^1 \hat{\gamma}_{k1}) + \sum_k (\xi_k - E_k) + C,$$  \hspace{1cm} (19)

with

$$E_k = \sqrt{\xi_k^2 + D_k^2},$$  \hspace{1cm} (20)

$$D_k = \sqrt{2} \sum_\tau D_\tau \cos(k_\tau), \quad \xi_k = -2 \sum_\tau T_\tau \cos(k_\tau) - \mu - \lambda.$$  \hspace{1cm} (21)

Also,

$$T_\tau = -t_{1\tau} g_{1\tau}^J + \frac{3}{4} J_\tau g_{J\tau}^J \chi_\tau + \lambda_\tau^x, \quad D_\tau = \frac{3}{4} J_\tau g_{J\tau}^J \Delta_\tau + \lambda_\tau^\Delta,$$  \hspace{1cm} (22)

$$C_\lambda = \lambda n + \sum_\tau \left( \frac{3}{4} J_\tau g_{J\tau}^J (2\chi_\tau^2 + \Delta_\tau^2) + 4\chi_\tau \lambda_\tau^x + 2\Delta_\tau \lambda_\tau^\Delta \right).$$  \hspace{1cm} (23)

The Gutzwiller renormalization factors read now, respectively

(I) \hspace{1cm} $g^J_\tau(n, \chi_\tau, \Delta_\tau) = \frac{2(1-n)}{2-n} \left( 1 - \frac{4\chi_\tau^2 + 2\Delta_\tau^2}{(2-n)^2} \right), \quad g^J_\tau(n) = \frac{4}{(2-n)^2},$

$$g_\tau^\Delta(n, \chi_\tau, \Delta_\tau) = \frac{2(1-n)}{2-n} \left( 1 + \frac{4\chi_\tau^2 + 2\Delta_\tau^2}{(2-n)^2} \right),$$  \hspace{1cm} (24)

(II) \hspace{1cm} $g^J_\tau(n, \chi_\tau) = \frac{2n(1-n)}{n(2-n) + 4\chi_\tau^2},$

$$g^J_\tau(n, \chi_\tau, \Delta_\tau) = \frac{4n^2}{n^2(2-n)^2 + (1-n)^2(4\Delta_\tau^2 - 8\chi_\tau^2) + 4\Delta_\tau^4 + 16\chi_\tau^4}. $$  \hspace{1cm} (25)

\footnote{Part of the results presented in this section may be found also in [13].}
Note, that for (II) \( g_r^\Delta = g_r^t \). The generalized Landau functional is given by

\[
F(\vec{A}, \vec{\lambda}) = C(\vec{A}, \vec{\lambda}) + \sum_k ((\xi_k - E_k) - \frac{2}{\beta} \ln (1 + e^{-\beta E_k})), \quad (26)
\]

from which the explicit form of Eqs. \( \text{(8)} \) can be easily obtained, but are not presented here in an explicit form.

**Numerical results.** We begin with the analysis of dRVB solution for the 'magic doping', \( x = \frac{1}{8} = 0.125 \). The equations \( \text{(8)} \) and \( \text{(9)} \) are solved for the lattice of \( \Lambda = \Lambda_x \Lambda_y \) sites, \( \Lambda_x = \Lambda_y = 256 \), with \( J_r = 1 \ t_r = -3J \) and for low temperature, \( \beta = 500 \). Both dRVB solution, as well as isotropic normal state (Fermi sea, (FS), not discussed explicitly here) are present. The staggered flux state, expected for lower doping, have not been found (\( \text{var} \)) or is not stable against FS (\( \text{s-c} \)) for \( x = 0.125 \).

In Tables I. and II. we give the values of the thermodynamic potentials, mean-fields and molecular fields for dRVB solutions obtained within both methods (var, s-c) and both renormalization schemes ((I), (II)).

**Table I.** Values of the thermodynamic potentials (per site) for dRVB solutions. \( \tilde{\Omega} (F) \) stands for \( \Omega - \lambda N \ (\Omega + \mu N) \) for var and \( \Omega_{s-c} \ (\Omega_{s-c} + \mu_{s-c} N) \) for s-c methods, respectively.

| Therm. Pot. | var (I) | var (II) | s-c (I) | s-c (II) |
|-------------|---------|----------|---------|----------|
| \( \Omega/\Lambda \) | -6.0444393 | -5.7586779 | - | - |
| \( \tilde{\Omega}/\Lambda \) | -1.0897421 | -1.0766359 | -1.01117344 | -1.03614582 |
| \( F/\Lambda \) | -1.343195431 | -1.366146003 | -1.339864247 | -1.364716747 |

For a fixed particle concentration \( n \), the relevant thermodynamical potential is the free energy \( F \). By construction of the solution the value of \( F \) obtained within each RS is always lower for the var method then for the s-c one. The free energy is also the quantity, that determines which solution of \( \text{(8)} \) or \( \text{(9)} \) corresponds to the stable equilibrium situation. However, by no means it may be used to favor one or another renormalization scheme. For example, if we compare the values of the \( F \) for var method in the present case, and also invoke its value \( F_{\text{var}}^0 \) corresponding to the simplest Gutzwiller factors (given by Eqn. \( \text{(12)} \), and not analyzed explicitly here, c.f. however Ref. \( \text{[12]} \)), we see that \( F_{\text{var}}^0 = -1.5070 < F_{\text{var}}^{\text{II}} < F_{\text{var}}^{\text{I}} \). Clearly, it does not mean that RS defined by \( \text{(12)} \) should be preferred over (I) or (II).

**Table II.** Values of the equilibrium chemical potentials and MF parameters \( (\vec{A}_0, \vec{\lambda}_0) \) for dRVB solutions. \( \tilde{\mu} \) stands for \( \lambda + \mu \) (var), and for \( \mu_{s-c} \) (s-c).

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Let us now analyze Table II. First, within RS (II), \(|\lambda^2_\tau|\) is significantly larger than \(|\lambda^\Delta_\tau|\). This indicates that the Hamiltonian (19) deviates from the Hartree-Fock form more with respect to \(\chi_\tau\) then with respect to \(\Delta_\tau\). This is due to the particular form of \(\chi_\tau\)-dependent, \(\Delta_\tau\)-independent renormalized hopping term. Similar conclusions are valid for RS (I), but then the \(\chi_\tau\)- and \(\Delta_\tau\)-dependence of \(\langle \hat{H} \rangle\) is more symmetric (c.f. Eqs. 14 and 15, or 24) and thus the difference between \(|\lambda^2_\tau|\) and \(|\lambda^\Delta_\tau|\) is smaller then for RS (II).

![Dispersion relations along the main symmetry lines in the Brillouin zone for the dRVB solutions for a square lattice, of the size \(L_x = L_y = 256\), and for the filling \(n = 0.875\). Triangles - self-consistent, non-variational results for (I) and (II), red squares (I) and green circles (II)-the present variational method.](image)

Figure 1: (Color online) Dispersion relations along the main symmetry lines in the Brillouin zone for the dRVB solutions for a square lattice, of the size \(L_x = L_y = 256\), and for the filling \(n = 0.875\). Triangles - self-consistent, non-variational results for (I) and (II), red squares (I) and green circles (II)-the present variational method.

Large values of \(|\lambda^2_\tau|\) significantly affect (through \(T_\tau\) and \(D_\tau\), Eqn. (22)) the
quasi-particle spectra, $E_k$, cf. Fig. 1. Namely, the excitation energies within our method are always lower than those of BdG self-consistent approach. This is due to relative minus sign between equilibrium values of $\lambda^\tau_\chi$ and $\chi_\tau$ ($\lambda^\Delta_\chi$ and $\Delta_\chi$), cf. also Ref. [13]. Although for RS (II) the differences between the methods ($\text{var}$, $s$-$c$) are pronounced mainly in the regions of the Brillouin zone which are far from the Fermi surface, the difference of the tangent at the cone near point $S$ may be of some significance. However, what is more important, RS (I) $\text{var}$ gives different excitation energies than other cases also along the $X$-$Y$ direction, i.e. close to the Fermi surface ($\xi_k = 0$). The reason for such behavior is obvious from the analysis of Tab. II; along $X$-$Y$ direction $\xi_k = \text{const}$ and the main contribution to $E_k$ comes from $D_k$, determined in turn by $D_\tau$, which is exceptionally low for (I) $\text{var}$.

### 3.2 Doping dependence of the mean-field quantities: critical hole concentrations

![Figure 2](image.png)

Figure 2: (Color online). Renormalization scheme (I): Doping dependence of the bond-order parameters $\chi_x = \chi_y$, the superconducting order parameters $\Delta_x = -\Delta_y$, and their renormalized correspondents $g^\Delta_\chi_x = g^\Delta_\chi_y$ and $g^\Delta_\Delta_x = -g^\Delta_\Delta_y$, both for the $s$-$c$ (triangles) and the $\text{var}$ (squares) methods.

Next, we are going to discuss the changes appearing as the function of doping. Those are the most interesting results obtained in the present paper.

The $(1 - n)$-dependences of mean-fields $\chi_\tau$ and $\Delta_x$, as well as the physical (renormalized) gap parameter $g^\Delta_\Delta_x$ and renormalized hopping $g^\Delta_\chi_\tau$ for scheme (I) are analyzed in Fig. 2 (The analogous picture for RS (II) is
Figure 3: (Color online). Doping dependence of renormalized superconducting order parameter $g^x \Delta_x$ for the paired (dRVB) state within various schemes described in the text. For $x = 0.2$, from the top to the bottom: (I) s-c (blue triangles), (II) var (green circles), (II) s-c (violet triangles), (I) var (red squares). Only the latter choice yields the (right value of the) critical doping $x_c \approx 0.27$, above which the gap disappears.

given in [13]). Note, that for (I) var, $\Delta_x$ vanishes at the critical concentration $x_c \approx 0.27$. This is in much better agreement with the experimental results then the predictions of the other cases, for which $x_c > 0.35$. The situation is illustrated explicitly in Fig. 3 where the $x$-dependence of the $g^x \Delta_x$ is shown also for the scheme (II), for both methods. Also, the right value of the optimal hole concentration ($x \approx 0.125$) is obtained for (I) var, in contrast to either non-variational treatment or to RS (II).

3.3 Staggered flux solution at $x \approx \frac{1}{8}$

As a next example we analyze the staggered-flux (SF) phase. This MF state has a long history, first being proposed by Affleck and Marston [22], as a variational trial MF state for the Heisenberg model. It was intensively investigated later, due to its possible connection with the pseudo-gap state in cuprates, cf. e.g. [23].

The SF differs from a normal Fermi sea (FS) solution by the presence of complex hopping amplitude $\chi_{ij} = |\chi| \exp((-1)^{(i+k+j)} i \varphi) \equiv \xi_1 \pm i \xi_2$. Such $\chi_{ij}$ implies existence of circulating currents, which direction changes from plaquette to plaquette in an alternating fashion (orbital antiferromagnet), [23]. Consequently, a two-sublattice structure emerges, with the unit cell of
the size $\sqrt{2}a \times \sqrt{2}a$ in direct space and new (folded) Brillouin zone (NBZ).

Within the framework of our method we add appropriate constraints. This introduces, apart from $\lambda$ ascribed to $n$, also the complex Lagrange multiplier $\eta_{ij} = \eta + i\eta_2$, tailored to $\chi_{ij}$ (our sign convention for $\eta_{ij}$ for each bond is opposite to that for $\chi_{ij}$). Thus, we have three independent real mean fields $\vec{A} = (n, \xi_1, \xi_2)$, and the same number of the corresponding real Lagrange multipliers, $\vec{\lambda} = (\lambda, \eta_1, \eta_2)$. In the present case the renormalization factors (15) and (17) read, respectively

$$g^J(n, \xi_1, \xi_2) = 2(1-n) \left(1 - \frac{4(\xi_1^2 + \xi_2^2)}{(2-n)^2}\right), \quad g^J(n) = \frac{4}{(2-n)^2}. \quad (27)$$

$$g^J(n, \xi_1, \xi_2) = \frac{2n(1-n)}{n(2-n) + 4(\xi_1^2 + \xi_2^2)}, \quad g^J(n) = \frac{4n^2}{n^2(2-n)^2 - 8(1-n)^2(\xi_1^2 + \xi_2^2) + 16(\xi_1^2 + \xi_2^2)^2}. \quad (28)$$

Instead of Eqs. (19) - (7) we have now

$$\hat{H}_\lambda - \mu \hat{N} = C(\vec{A}, \vec{\lambda}) + \sum_{k\sigma} E_{k\sigma} \hat{a}^\dagger_{k\sigma} \hat{a}_{k\sigma}, \quad (29)$$

where $E_{k\sigma} = -\tilde{\mu} + s\sqrt{\epsilon_k^2 + \chi_k^2}, \epsilon_k = T_1 \gamma_+(k)$, and $\chi_k = T_2 \gamma_-(k)$. Also, $\gamma_{\pm}(k) \equiv 2\cos(k_x) \pm \cos(k_y)$ and

$$T_1 = tg' + \frac{3}{4} Jg' \xi_1 + \eta_1, \quad T_2 = \frac{3}{4} Jg' \xi_2 + \eta_2. \quad (30)$$

$$C = \Lambda \left(\lambda n + 3g(J(\xi_1^2 + \xi_2^2) + 8(\xi_1 \eta_1 + \xi_2 \eta_2))\right). \quad (31)$$

The generalized Landau functional (7) takes now the following form

$$F(\vec{A}, \vec{\lambda}) = C(\vec{A}, \vec{\lambda}) - \frac{1}{\beta} \sum_{k\sigma} \ln \left(1 + e^{-\beta E_{k\sigma}}\right). \quad (32)$$

Numerical results. As mentioned in Sec. ??, at $x = 1/8$ the existence of SF solution of Eqs. (8) has not been numerically confirmed (for var method), whereas for the s-c method the SF solutions of of Eqn. (9) have been found unstable against Fermi sea (FS) with $\xi_2 = 0$. In all four cases the SF→FS transition is located at the critical concentrations $0.11 < x_c < 0.12$. However, our numerical procedures for var method turned out to be unstable in the vicinity of the $x_c$. For that reason, we chose doping $x = 13/128$
(n ≈ 0.898), which is in a safe distance from each of \( x_c \), but for which the differences between the methods are pronounced (as they generally increase with increasing doping).

The parameters of the Hamiltonian are the same as for the RVB case, except sign convention for \( t \), now \( t = 3 \) (\( t = -3 \) in the RVB case), also \( \Lambda_x = \Lambda_y = 512 \). Again, we work with low \( T = 1/500 \). The thermodynamic potentials and mean-field variables are listed in Tabs. III and IV.

Table III. Equilibrium values of the thermodynamic potentials (per site) for SF solutions, for \( n ≈ 0.898, \Lambda = 512 \). \( \Omega \) (\( F \)) stands for \( \Omega - \lambda N (\Omega + \mu N) \) for var and \( \Omega_{s-c} (\Omega_{s-c} + \mu_{s-c} N) \) for s-c methods, respectively.

| Therm. Pot. | var (I) | var (II) | s-c (I) | s-c (II) |
|-------------|---------|----------|---------|----------|
| \( \Omega/\Lambda \) | -5.90103948 | -5.75555848 | - | - |
| \( \hat{\Omega}/\Lambda \) | -0.69003640 | -0.71583672 | -0.49006797 | -0.49344983 |
| \( F/\Lambda \) | -1.18762800 | -1.16898668 | -1.18536044 | -1.16599431 |

Table IV. Values of chemical potentials and MF parameters for SF solutions for \( n ≈ 0.898, \Lambda = 512 \). \( \hat{\mu} \) stands for \( \lambda + \mu \) (var), and for \( \mu_{s-c} \) (s-c).

| Variable | var (I) | var (II) | s-c (I) | s-c (II) |
|----------|---------|----------|---------|----------|
| \( \mu \) | 5.24623 | 5.10505 | - | - |
| \( \lambda \) | -5.80007 | -5.60943 | - | - |
| \( \hat{\mu} \) | -0.55384 | -0.50438 | -0.77389 | -0.74857 |
| \( \xi_1 \) | 0.19222 | 0.19321 | 0.18805 | 0.18844 |
| \( \xi_2 \) | 0.10298 | 0.09840 | 0.11856 | 0.11731 |
| \( \eta_1 \) | -0.13476 | -0.14848 | - | - |
| \( \eta_2 \) | -0.07220 | -0.07562 | - | - |
| \( S_{AF} \) | -0.23514 | -0.22522 | -0.24436 | -0.23527 |
| \( \Phi_{\square} \) | 0.31311 | 0.29987 | 0.35811 | 0.35449 |
| \( T_1 \) | 0.80695 | 0.77919 | 0.92799 | 0.91123 |
| \( T_2 \) | 0.18241 | 0.16008 | 0.29312 | 0.28009 |

Within the standard mean-field approach (e.g. [12]) the (fictitious) flux is defined as \( \Phi_{\square} = \frac{1}{2\pi} \sum_{(ij)\in\square} \text{Arg}(\chi_{ij}) \), and \( \square \) denotes plaquette composed from four bonds. Also, for s-c method, i.e. for \( \eta_1 = \eta_2 = 0 \), we have

\[
\text{Arg}(\chi_{ij}) = \arctan \left( \frac{\xi_2}{\xi_1} \right) = \arctan \left( \frac{T_2}{T_1 - tg^t} \right),
\]

the last equality follows from (30). Interestingly, this equality holds also for the variational approach with \( \eta_1 \neq 0, \eta_2 \neq 0 \). It can be shown analytically, that \( \xi_1/\xi_2 = \eta_1/\eta_2 \), which together with (30) yields (33). Thus the two
possible and *a priori* different definitions of $\Phi_{\square}$ within *var* method turn out to be equivalent. Antiferromagnetic correlations are defined on the MF level as $S_{AF} = -\frac{3}{2}gJ(\xi_1^2 + \xi_2^2)$, [1, 12].

![Figure 4](image)

Figure 4: (Color online) Dispersion relations for both upper ($E_{k+}$) and lower ($E_{k-}$) subbands for the SF solutions along the main symmetry lines in the Brillouin zone of the square lattice, of the size $\Lambda_x = \Lambda_y = 512$, and for the filling $n \approx 0.898$. Triangles - self-consistent, non-variational results for (I) and (II), red squares (I) and green circles (II)- the present variational method. Explicitly, for ($E_{k+}$) near the maximum at point M, from the bottom to the top: (II) *var*, (I) *var*, (II) *s-c* (violet triangles), (I) *s-c* (dark blue triangles).

In contrast to the dRVB case, now the differences between renormalization schemes ((I) vs (II)) within each (*var*, *s-c*) method are small. This is because in the absence of $\Delta_{ij}$, the $\chi_{ij}$ -dependences of $g_{(I)}^I$ and $g_{(II)}^I$ are quite similar, and the $\chi_{ij}$ -dependence of $g_{(II)}^I$ is weak for doping $x \approx 0.1$, thus causing no qualitative and only minor quantitative differences between the renormalization schemes. On the other hand, the generic modifications introduced by the variational approach within each RS are more significant.

Namely, from Tab. IV we see, that *s-c* method favors SF more strongly than *var* method, which is indicated by the values of $\Phi_{\square}$ and $\xi_2$. Also, $T_1$ and $T_2$, determining quasi-particle spectra, are smaller within *var* method, and so are the quasi-particle energies, c.f. Fig. 4.
4 Concluding remarks

In summary, in this work we have compared, within two methods of approach, the two Gutzwiller renormalization schemes for the renormalized mean-field theory (RMFT) of t-J model in its simplest form. We emphasize the advantages of the combination of the renormalization scheme of Ref. [3] with the variational method proposed in Ref. [14]. First, a number of theoretical arguments strongly favor this choice. Moreover, in contrast to the other cases investigated by us (e.g. either non-variational method or renormalization scheme of Ref. [8]), the former approach quite correctly predicts the upper critical doping $x_c \approx 0.27$ for a disappearance of the SC order. Also, the value of the optimal doping $x \approx 0.125$ is quite correctly predicted. In our opinion, the formalism of Ref. [3] augmented with the self-consistent variational treatment, gives a chance for the complete and consistent one-particle description (in the form of RMFT) for a t-J model. Such description, however, must encompass the t-J model in its complete form [1], and include also more complicated symmetry breaking patterns. This is the subject of our current investigation.

Appendix A: Equivalence relation for mean-field Hamiltonians

Below we present some details of our formalism, which are necessary for the present discussion. We also comment on the relationship between our method and the formalisms of Ref. [10]. We start from the MF Hamiltonian of the form

$$\hat{H}(\vec{A}) = \hat{H}_{e0} + C_0(\vec{A}) \cdot \mathbf{1}_D + \sum_{s=1}^{M} C_s(\vec{A}) \hat{A}_s + \sum_{w=1}^{M'} G_w(\vec{A}) \hat{B}_w.$$  

In the above, $\hat{H}_{e0}$ is an $\vec{A}$-independent part, $C_0(\vec{A})$, $C_s(\vec{A})$ and $G_w(\vec{A})$ are some complex-valued functions of mean-fields $\vec{A}$. Operators $\hat{B}_w$ are those, which average values are not present in $\hat{H}(\vec{A})$. We also assume that all the operators appearing above are bilinear in creation and/or annihilation operators. From (34) we have

$$\hat{H}_\lambda(\vec{A}) = \hat{H}(\vec{A}) - \sum_{s=1}^{M} \lambda_s (\hat{A}_s - A_s)$$

$$= \hat{H}_{e0} + C_0(\vec{A}) \cdot \mathbf{1}_D + \sum_{s=1}^{M} C_s^\lambda(\vec{A}) \hat{A}_s + \sum_{w=1}^{M'} G_w(\vec{A}) \hat{B}_w.$$  

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with $C_0^\lambda = C_0 + \sum_{s=1}^M \lambda_s A_s$, $C_s^\lambda = C_s - \lambda_s$. For a given value of $\vec{A}$, the self-consistency equations (second half of the $2M$ equations (37)) may be written as

$$A_t \equiv \langle \hat{A}_t \rangle_{\lambda} = \text{Tr}[\hat{A}_t \hat{\rho}_\lambda] = \frac{\text{Tr}[\hat{A}_t \exp (-\beta(\hat{K}_{e0} + \sum_{s=1}^M C_s^\lambda(\vec{A}) \hat{A}_s + \sum_{w=1}^{M'} G_w(\vec{A}) \hat{B}_w))] - \text{Tr}[\exp (-\beta(\hat{K}_{e0} + \sum_{s=1}^M C_s^\lambda(\vec{A}) \hat{A}_s + \sum_{w=1}^{M'} G_w(\vec{A}) \hat{B}_w))] }{\text{Tr}[\exp (-\beta(\hat{K}_{e0} + \sum_{s=1}^M C_s^\lambda(\vec{A}) \hat{A}_s + \sum_{w=1}^{M'} G_w(\vec{A}) \hat{B}_w))]}, \quad (36)$$

In above, the $C_0^\lambda(\vec{A})$ term canceled, and $\hat{K}_{e0} = \hat{H}_{e0} - \mu \hat{N}$. Eqs. (36) may be formally solved (which usually cannot be achieved in an analytic fashion) for $\vec{\lambda}$, and then $\vec{\lambda} = \vec{\lambda}(\vec{A})$, thus for a given $\vec{A}$, Eqs. (36) determine $C_s^\lambda(\vec{A})$. As a result, the $\vec{A}$-dependence of the coefficients $C_s^\lambda(\vec{A})$ is determined by the choice of operators $\hat{H}_{e0}$, $\{\hat{A}_s\}_{s=1}^M$ and $\{\hat{B}_w\}_{w=1}^{M'}$. If we change the original form of the coupling of $\{A_s\}_{s=1}^M$ operators to the mean fields, according to

$$C_s(\vec{A}) \rightarrow \tilde{C}_s(\vec{A}) = \varphi_s(C_s(\vec{A})), \quad (37)$$

but without changing $G_w(\vec{A})$ functions, then the Lagrange multipliers change in a way that $C_s^\lambda(\vec{A})$ is unchanged, in order to fulfill (36). The only $\vec{A}$-dependent part which may be non-trivially modified by (37) is $C_0(\vec{A}) = \vec{1}_D$. Obviously, $S_{\lambda}$, defined as (c.f. (14))

$$S_{\lambda} = \text{Tr}[-\hat{\rho}_\lambda \ln \hat{\rho}_\lambda - \beta(\hat{\rho}_\lambda \hat{H} - \mu \hat{\rho}_\lambda \hat{N} - \sum_{s=1}^M \lambda_s \hat{\rho}_\lambda (\hat{A}_s - A_s)) - \omega(\hat{\rho}_\lambda - \frac{1}{D})], \quad (38)$$

and $F(\vec{A}, \vec{\lambda}) = -\beta^{-1} S_{\lambda}(\hat{\rho}_\lambda(\vec{A}, \vec{\lambda}), \vec{A}, \vec{\lambda})$ may be also modified. However, the density operator $\hat{\rho}_\lambda$ is invariant under (37), so are, for given $\vec{A}$, all the averages, also those of $\hat{H}_{e0}$ and $\hat{B}_w$ operators. Moreover, if the transformations (37) are such that $\langle \hat{H}_{\lambda} \rangle_{\lambda} = \langle \hat{H} \rangle_{\lambda}$ remains unchanged, the value of $F(\vec{A}, \vec{\lambda}(\vec{A}))$ is not modified. Consequently, in such a situation, the equilibrium values of mean fields, as well as of the quantities $C_s^\lambda(\vec{A})$ (e.g. $T_r, D_r$ of Eqn. (22) or $T_1, T_2$ of Eqn. (31)) are also invariants of (37). Summarizing, all MF Hamiltonians constructed from the same set of operators $\hat{H}_{e0}$, $\{\hat{A}_s\}_{s=1}^M$ and $\{\hat{B}_w\}_{w=1}^{M'}$ and having the same $\vec{A}$-dependence of the expectation value, are equivalent, and belong to the same equivalence class. The transformations (37) may be viewed in analogy to gauge transformations, not changing the physical content of the model.

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5We assume that the solution exists and is unique, or there exist a finite number of the solutions, but one of them may be unambiguously selected.
Suppose, that the MF Hamiltonian (34) is such that
\[ \hat{H}_{e0} = 0, \quad \forall w : \quad G_w = 0. \] (39)
Then the equilibrium values of \( \lambda_s \) may be easily obtained in an analytic fashion, using Eqn. (17) of Ref. \[14\], i.e.
\[ \lambda_w = -\left\langle \frac{\partial \hat{H}}{\partial A_w} \right\rangle_{\lambda}. \] (40)
Now, we choose a transformation (37) of a specific form,
\[ C_s(\vec{A}) \rightarrow \tilde{C}_s(\vec{A}) = 0, \quad s \neq 0 \]
\[ C_0(\vec{A}) \rightarrow \tilde{C}_0(\vec{A}) = C_0(\vec{A}) + \sum_s C_s(\vec{A}) A_s. \] (41)
This yields
\[ \hat{H}_\lambda(\vec{A}) = -\sum_{s=1}^{M} \lambda_s (\hat{A}_s - A_s) + W(\vec{A}), \] (42)
with \( \hat{H}(\vec{A}) = W(\vec{A}) \hat{1}_D, \ W(\vec{A}) = \langle \hat{H}(\vec{A}) \rangle = \tilde{C}_0(\vec{A}) \). Using (40) we may rewrite (42) as
\[ \hat{H}_\lambda(\vec{A}) = \sum_{s=1}^{M} \frac{\partial W(\vec{A})}{\partial A_s} (\hat{A}_s - A_s) + W(\vec{A}), \] (43)
because \( \frac{\partial W(\vec{A})}{\partial A_s} = \frac{\partial \langle \hat{H}(\vec{A}) \rangle}{\partial A_s} = \frac{\partial \langle \hat{H}(\vec{A}) \rangle}{\partial A_s} \). The form (43) is the most convenient, as half of the variables (\( \vec{\lambda} \)) are eliminated, which reduces the number of equations to be solved numerically.

Also, in the limit (\( \beta \rightarrow \infty \)) the results of finite-temperature formalism are essentially identical to those the true \( T = 0 \) analysis, and we may compare them with those of Ref. \[10\]. Hamiltonian of that Reference reads in our notation
\[ \hat{H}_\lambda^{(K)}(\vec{A}) = -\sum_{s=1}^{M} \lambda_s (\hat{A}_s - A_s) = \sum_{s=1}^{M} \frac{\partial W(\vec{A})}{\partial A_s} \hat{A}_s, \] (44)
and differs from (42) only by the constant term \( \sum_{s=1}^{M} \lambda_s A_s + \langle \hat{H}(\vec{A}) \rangle \). Consequently, both (42) and (44) have the same eigenvalues and eigenvectors (the presence of \( -\mu \hat{N} \) obviously does not change the above arguments). Please note, that the analytical evaluation of Lagrange multipliers through (40), and hence the application of the method of Ref. \[10\] is possible only if the conditions (39) are fulfilled, but not for the general form (34) of the MF Hamiltonian.
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∗ e-mail: jedrak@th.if.uj.edu.pl
† e-mail: ufspalek@if.uj.edu.pl

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