Construction of density operator for a general mean-field Hamiltonian and its application to the models of correlated fermions

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Abstract
We analyze a class of mean-field (MF) lattice-fermion Hamiltonians and construct the corresponding grand-canonical density operator for such system. New terms are introduced, which may be interpreted as local fugacities, molecular fields, etc. The presence of such terms is an unavoidable consequence of a consistent statistical description. Although in some cases (e.g. in the Hartree or the Hartree-Fock-type approximation) the presented formalism is redundant, in general (e.g. for a renormalized t-J model) it leads to nontrivial modifications of the thermodynamic properties.

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1 Introduction
For most of realistic models of quantum many-particle systems an exact solution cannot be achieved. This is a typical situation condensed matter or nuclear physics. As a consequence, a number of approximate methods have been developed. Among them, widely used are various types of the mean-field approaches.

By mean-field (MF) description of the problem we understand making use of the Hamiltonian which depends on extra parameters, having the meaning of expectation values of well-defined operators. Values of those parameters are not a priori known and are to be determined. The Hartree-Fock method is a good example of such approach.

MF methods provide us with a valuable insight into the physical properties of a system under the consideration. They are capable of describing many interesting phenomena, especially those involving phase transitions, such as that from normal metal to superconductor transition (e.g. in the form of the Bardeen-Cooper-Schrieffer theory), or those from a paramagnet to either antiferro- or ferromagnet.
In implementing such a procedure, it is the physics of the problem, not
the mathematics, that tells us when the application of MF approach is jus-
tifiable. Nonetheless, we may also be faced with the problem of considering
the internal mathematical consistency of the method, as well as its underly-
ing general principles. The aim of this paper is to clarify this issue to some
extent, in a simple manner.

The paper is organized as follows. Sec. 2 contains formulation of theprob-
lem and invokes basic relevant notions from statistical mechanics. In Sec. 3,
by means of the maximum entropy principle we construct the statistical-
mechanical description of the system in the mean-field case. Explicitly, in
3.1 we derive the grand-canonical (GC) MF density operator, in 3.2 we com-
ment on the MF thermodynamics and its consistence with the MF statistical
mechanics, whereas in 3.3 we discuss the important case of the Hartree-
Fock (HF) type MF Hamiltonians. Finally, in 3.4 the connection of present
method with the variational principle based on the Bogoliubov inequality is
elaborated. In Sec. 4 two specific examples of mean-field Hamiltonians are
provided, for which our approach leads to significant corrections. Section 5
contains a summary.

2 Statement of the problem

We assume that the Hilbert-Fock state space is of finite dimension $D$. The
MF Hamiltonians are denoted as $\hat{H}$, whereas those which are not of MF type,
will be called exact and labelled with the subscript $'e'$.

As already mentioned in the Introduction, by mean-field approach we un-
derstand the situation in which Hamiltonian depends on certain parameters,
that are to be determined when solving the problem at hand. Such MF
Hamiltonian is usually derived from the exact Hamiltonian $\hat{H}_e$, by replacing
some of the operators, $\{\hat{A}_s\} = \hat{A}_1, \ldots, \hat{A}_M$, appearing in $\hat{H}_e$, by C-numbers
$\{A_s\} = A_1, A_2, \ldots, A_M (\equiv \vec{A})$. Those numbers have a natural interpretation
of expectation values of the corresponding operators $\{\hat{A}_s\}$. However, the
mean-field Hamiltonian $\hat{H}$ may be not be related in an obvious manner to
any exact Hamiltonian.

We assume that the system is in thermal equilibrium with the parti-

cle reservoir characterized by the temperature $T = \beta^{-1}$ and the chemical
potential $\mu$. The question then arises, how to determine the values of pa-
rameters $A_s$ appearing in $\hat{H}$. If the Hamiltonian of the system were exact,
i.e. not expectation-value dependent, then the treatment of such situation
is straightforward, in the sense, that the grand canonical (GC) ensemble is
well defined, and all information about the system is contained in the density
operator [1, 2] defined as
\[ \hat{\rho}_e = Z_e^{-1} \exp \left( -\beta(\hat{H}_e - \mu \hat{N}) \right), \] (1)
where \( Z_e = \text{Tr}\left[ \exp \left( -\beta(\hat{H}_e - \mu \hat{N}) \right) \right] \) is the grand-canonical partition function. The expectation value of any observable \( \hat{A} \) is then given by
\[ \langle \hat{A} \rangle_e \equiv \text{Tr}[\hat{A}\hat{\rho}_e]. \] (2)
Moreover, we assume, that in the mean-field case this basic definition still holds, i.e.
\[ \langle \hat{A} \rangle = \text{Tr}[\hat{A}\hat{\rho}(\vec{A})]. \] (3)
Regardless of the form of MF density operator \( \hat{\rho} \), we should be able to obtain any expectation value through (3). In particular, the last definition allows us to determine the values of \( A_1, A_2, \ldots, A_M \) appearing in \( \hat{\rho} \), by solving a system of \( M \) implicit equations for \( M \) variables (the so-called self-consistency equations), which take the form
\[ \langle \hat{A}_s \rangle = A_s = \text{Tr}[\hat{A}_s\hat{\rho}(A_1, A_2, \ldots, A_M)], \quad \forall s. \] (4)
We may hope that this system should have at least one solution.
One would expect, that MF grand-canonical density operator should be given by (1) with \( \hat{H}_e \) replaced with \( \hat{H} \), so
\[ \hat{\rho} = \tilde{Z}^{-1} \exp \left( -\beta(\hat{H} - \mu \hat{N}) \right), \quad \tilde{Z} = \text{Tr}\left[ \exp \left( -\beta(\hat{H} - \mu \hat{N}) \right) \right]. \] (5)
This is, however, not necessarily the case, as is discussed in detail below.
In order to find the correct mean-field GC density operator for a given MF Hamiltonian \( \hat{H} \), we proceed analogously to the exact (non-MF) case and derive the form of such density operator from the basic principles of statistical mechanics. Thus, before concentrating in the remaining part of the paper on the mean-field case, we first would like to summarize briefly the non-MF situation. Namely, for the exact Hamiltonian \( \hat{H}_e \), the GC density operator (1) may be derived from the requirement that it maximizes the von Neumann entropy, \( S \equiv -\text{Tr}\hat{\rho}_e \ln \hat{\rho}_e \), under the conditions that the expectation values of \( \hat{H}_e \) and of the particle number operator \( \hat{N} \), are fixed. This means, that we maximize the following functional (see [1, 2])
\[ S_e = \text{Tr}\left( -\hat{\rho}_e \ln \hat{\rho}_e - \beta \hat{\rho}_e \hat{H}_e + \beta \mu \hat{\rho}_e \hat{N} - \omega \hat{\rho}_e \right). \] (6)
The first two conditions are enforced with the help of the Lagrange multipliers \( \beta \) and \( \mu \), whereas the parameter \( \omega \) is introduced to ensure the normalization,
$\text{Tr}[\hat{\rho}_e] = 1$. Furthermore, $\hat{\rho}_e$ must be a constant of motion, so from the quantum Liouville equation \cite{1,2}

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_e(t) = [\hat{H}_e, \hat{\rho}_e(t)],$$

(7)

it follows, that $[\hat{H}_e, \hat{\rho}_e] = 0$. If, additionally, $[\hat{H}_e, \hat{N}] = 0$, which is usually the case in non-relativistic quantum mechanics, we may simultaneously diagonalize each of the operators appearing in \cite{6}.

Parenthetically, the maximization procedure is most conveniently carried out in the basis, in which $\hat{\rho}_e$ is diagonal, i.e. $\hat{\rho}_e = \sum D p_i |i\rangle \langle i|$. The resulting $\hat{\rho}_e$ is then of the form given by \cite{1,2}. Density operators for the canonical and the micro-canonical ensembles may be obtained in a similar manner. The fact, that those density operators maximize the entropy functional \cite{3} or analogous expressions, may be considered as their basic property \cite{3}.

3 Maximum entropy principle in the mean-field case

3.1 Construction of the mean-field density operator

We turn now to the construction of the proper form of MF density operator. We concentrate on the case, for which the entire system description is based solely on MF Hamiltonian. In the previous Section it was stated, that maximum entropy condition is basic for canonical density operators. Moreover, the principle of maximum entropy is one of basic postulates of statistics, it ensures uniqueness and consistency of probability assignments, \cite{3}. Consequently, it should be applied also to the particular case of mean-field description. Now, the difference with the standard, i.e. non-MF situation above is that the Hamiltonian depends on $M$ additional variables $\{A_s\} \equiv \vec{A}$, interpreted as the expectation values of corresponding operators $\{\hat{A}_s\}$. Those $M$ expectation values, together with $D$ diagonal matrix elements of $\hat{\rho}$, are now the variational parameters, with respect to which the functional

$$S = \text{Tr}(-\hat{\rho} \ln \hat{\rho} - \beta \hat{\rho} \hat{H}(\vec{A}) + \beta \mu \hat{\rho} \hat{N} - \omega(\hat{\rho} - 1/D)),$$

(8)

is maximized. As earlier, $-\omega(\hat{\rho} - 1/D)$ term\footnote{Here taken in the form which slightly differs from that of \cite{6}, but this technical alteration is inessential.} is added to ensure normalization of the density operator. Next, if those $M + D$ parameters were treated as
independent, there is no certainty that \( \{A_s\} \) obtained in that manner coincide with those resulting form the self-consistency conditions (4). In principle, one may use (4) to eliminate the \( A_s \) variables from \( \hat{H} \). Nonetheless, the resulting dependence of \( S \) on \( D \) diagonal elements of \( \hat{\rho} \) is usually very complicated, and the MF density operator cannot be obtained in an explicit form.

To resolve the situation, we use the Lagrange-multiplier method. Explicitly, the \( M \) conditions (4) are enforced with the help of \( M \) Lagrange multipliers \( \{\lambda_s\} \equiv \vec{\lambda} \). To account for that, the terms of the form \( \lambda_s(\text{Tr}[\hat{\rho}\hat{A}_s] - A_s) \) must be added to the functional (8). Under these circumstances, we have in total \( D + 2M \) variables, \( \{p_1, \ldots, p_D, A_1, \ldots, A_M, \lambda_1, \ldots, \lambda_M\} \), treated as independent (apart from the normalization condition). In effect, the constrained entropy functional reads

\[
S_{\lambda} = \text{Tr} \left[ -\hat{\rho}_\lambda \ln \hat{\rho}_\lambda - \beta (\hat{\rho}_\lambda \hat{H} - \mu \hat{\rho}_\lambda \hat{N} - \sum_{s=1}^{M} \lambda_s \hat{\rho}_\lambda (\hat{A}_s - A_s)) - \omega(\hat{\rho}_\lambda - \frac{1}{D}) \right]. \quad (9)
\]

The incorporation of the self-consistency constraints may be regarded as a redefinition of the MF Hamiltonian

\[
\hat{H} \rightarrow \hat{H}_\lambda = \hat{H} - \sum_{s=1}^{M} \lambda_s (\hat{A}_s - A_s). \quad (10)
\]

The last step is the basic novel ingredient of our method and is discussed in detail in the remaining part of this paper.

Few remarks are in place here. First, we are mainly interested in a situation when each operator \( \hat{A}_s \) is bilinear in creation and/or annihilation operators \( \hat{a}^{\dagger} \) as then \( \hat{H}_\lambda \) is easily tractable. Second, some combination of the operators \( \{\hat{A}_s\} \) appearing in (10) may be proportional to the number operator \( \hat{N} \). Nonetheless, the presence of the chemical potential \( \mu \) fixes the average number of particles \( N \).

Third, the operators \( \hat{H} \) and \( \hat{N} \) in (9) have a different status than the operators \( \{\hat{A}_s\} \). The expectation values of the former are assumed to be fixed \textit{a priori}, enforced by the values of temperature and chemical potential. In contrast, the expectation values of the latter are obtained from a variational procedure, and are not \textit{a priori} given. Consequently, the same distinction holds for parameters \( \beta, \mu \) from one side and \( \{\lambda_s\} \) from the other, even though all of them play the role of Lagrange multipliers. Nonetheless, some of \( \{\lambda_s\} \) may have a physical interpretation. Depending on the corresponding operator \( \hat{A}_s \), they may be termed as local fugacities, molecular fields, etc. Note,
that for $\hat{A}_s = \hat{A}_s^\dag$, $\lambda_s$ is real, but for non-Hermitian $\hat{A}_s$, it is a complex number in general.

Apart from $\hat{H}$ and $\hat{N}$, there may be more observables with expectation values fixed \textit{a priori}. In such a situation the terms $(-\xi_s\hat{A}_s)$, analogous to $-\mu \hat{N}$ term, should be also added, to ensure that the quantity $\langle \hat{A}_s \rangle$ is consistent with the prior information about the system. If we ignore some available information about the physical system under consideration, we obtain a broader probability distribution.

Fourth, the operators appearing in (10) do not necessarily commute with each other, and thus cannot be, in general, simultaneously diagonalized. However, in analogy to the canonical case, we require that $\hat{\rho}_\lambda$ thus obtained is stationary, i.e. $\frac{\partial \hat{\rho}_\lambda(t)}{\partial t} = 0$, from which, using the quantum Liouville equation (7) for the MF case the condition $[\hat{H}_\lambda, \hat{\rho}_\lambda] = 0$ follows. In particular, in the case $[\hat{N}, \hat{H}_\lambda] \neq 0$ (e.g. in the BCS theory of superconductivity), we can also redefine the Hamiltonian according to $\hat{H}_\lambda \rightarrow \hat{K}_\lambda = \hat{H}_\lambda - \mu \hat{N}$, and then demand, that the corresponding grand Hamiltonian commutes with the density operator, $[\hat{K}_\lambda, \hat{\rho}_\lambda] = 0$. In result, diagonalization of $\hat{K}_\lambda$ provides us again with the set of $\vec{A}$ and $\vec{\lambda}$- dependent eigenvectors $\{|i(\vec{A}, \vec{\lambda})\rangle\}^D_{i=1}$ and corresponding eigenvalues of the density operator $\hat{\rho}_\lambda$.

Fifth, the present formalism may be easily modified and applied to the case of canonical ensemble or discrete classical models (e.g. lattice gas, or spin systems).

Finally, even if, strictly speaking, the $T = 0$ situation cannot be investigated directly within the framework of the present formalism, (must be analyzed separately), it is fully legitimate as well as convenient to analyze the situation in question as the $T \rightarrow 0$ limit, e.g. for finite, but sufficiently low temperature. A more detailed analysis of this point will be presented elsewhere [5].

Let us go back to the problem of finding the maximum of the entropy subject to the constraints. The functional (11), written in the common eigenbasis of $\hat{K}_\lambda$ and $\hat{\rho}_\lambda$ reads

$$S_\lambda = \sum_{i=1}^D \left\{-q_i \ln q_i - \beta q_i \left((\hat{H})_{ii} - \mu (\hat{N})_{ii} - \sum_{s=1}^M \lambda_s ((\hat{A}_s)_{ii} - A_s)\right) - \omega (q_i - \frac{1}{D})\right\},$$

(11)

(with $(\hat{N})_{ii} = \langle i | \hat{N} | i \rangle$ etc.) We assume, that the maximum of (11) corresponds to stationary point. Then, the necessary conditions for an extremum of $S_\lambda$ with the normalization preserved, are

$$\frac{\partial S_\lambda}{\partial \omega} = 1 - \sum_{j=1}^D q_j = 0,$$

(12)
\[
\forall j : \frac{\partial S_\lambda}{\partial q_j} = -(1+\omega) - \ln q_j - \beta(\hat{H})_{jj} + \beta \mu(\hat{N})_{jj} + \sum_{s=1}^{M} \beta \lambda_s ((\hat{A}_s)_{jj} - A_s) = 0,
\]

(13)

\[
\forall w : \frac{\partial S_\lambda}{\partial A_w} = -\beta \sum_{i=1}^{D} q_i \left( \frac{\partial \hat{H}_{ii}}{\partial A_w} + \lambda_w \right) = 0,
\]

(14)

and

\[
\forall w : \frac{\partial S_\lambda}{\partial \lambda_w} = \beta \sum_{i=1}^{D} q_i \left( (\hat{A}_w)_{ii} - A_w \right) = 0.
\]

(15)

In (14) and (15), we ignored the possible explicit \(\vec{A}\)- and \(\vec{\lambda}\)- dependence of the (normalized) eigenvectors \(|i\rangle\). This is justified due to the Hellmann-Feynman theorem, [4]. Using (12) and (13) we obtain the explicit, basis-independent form of density operator \(\hat{\rho}_\lambda\),

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

(16)

We see that (16) differs from (5) by the presence of additional terms in the Hamiltonian, in accordance with (10). Additionally, Eqs. (14) and (15) may be rewritten respectively as

\[
-\frac{1}{\beta} \frac{\partial S_\lambda}{\partial A_w} = \text{Tr}[\hat{\rho}_\lambda \left( \frac{\partial \hat{H}}{\partial A_w} + \lambda_w \right)] = \left\langle \frac{\partial \hat{H}}{\partial A_w} \right\rangle_\lambda + \lambda_w = \left\langle \frac{\partial \hat{H}_\lambda}{\partial A_w} \right\rangle_\lambda = 0,
\]

(17)

and

\[
\frac{1}{\beta} \frac{\partial S_\lambda}{\partial \lambda_w} = \text{Tr}[\hat{\rho}_\lambda (\hat{A}_w - A_w)] = \left\langle \hat{A}_w \right\rangle_\lambda - A_w = \left\langle \frac{\partial \hat{H}_\lambda}{\partial \lambda_w} \right\rangle_\lambda = 0.
\]

(18)

Next, we define the generalized grand-canonical Landau functional

\[
\mathcal{F}(\vec{A}, \vec{\lambda}) \equiv -\beta^{-1} \ln \mathcal{Z}_\lambda = -\beta^{-1} S_\lambda(\hat{\rho}_\lambda(\vec{A}, \vec{\lambda}), \vec{A}, \vec{\lambda}),
\]

(19)

with \(\mathcal{Z}_\lambda\) given by (16). That last relation may be easily verified by inserting \(\hat{\rho}_\lambda\) given by (16) into (9). Thus, the constrained minimum of \(\mathcal{F}(\vec{A}, \vec{\lambda})\) corresponds to the constrained maximum of \(S_\lambda(\hat{\rho}_\lambda(\vec{A}, \vec{\lambda}), \vec{A}, \vec{\lambda})\), here understood as a function of \(\vec{A}\) and \(\vec{\lambda}\) only, once Eqs. (12) and (13) are solved. From now on we will use \(\mathcal{F}\) instead of \(S_\lambda\). With the help of (19), the Eqs. (17) and (18) are equivalent to

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

(20)
where $\nabla_A \equiv \left( \frac{\partial}{\partial A_1}, \frac{\partial}{\partial A_2}, \ldots, \frac{\partial}{\partial A_M} \right)$, and analogously for $\nabla_\lambda$. When deriving the last condition we made use of the identity (c.f. [2])

$$\frac{\partial}{\partial x} e^{C(x)} = \int_0^1 d\tau e^{\tau C(x)} \left( \frac{\partial}{\partial x} C(x) \right) e^{(1-\tau)C(x)}, \quad (21)$$

in combination with the linearity of the trace operation, as well as its invariance with respect to cyclic permutation of the operators.

For each solution of (12)-(15) or, equivalently, of (20), it should be verified separately if also the sufficient conditions for the existence of the constrained minimum of $F$ are fulfilled. In practice, this will be most conveniently carried out through numerical analysis.

We may expect that one of the solutions of (20), labeled $(\vec{A}_0, \vec{\lambda}_0)$, yields such desired global minimum of $F$ subject to constraints, and this defines the equilibrium state. If more than one solution with the minimal value of $F$ exist, we select one of them, breaking the remaining symmetry.

However, $F$ is well defined also for the values of $\vec{A}$ which differ from $\vec{A}_0$, and may possess physical interpretation provided that the consistency conditions (18) are met. Namely, $F(\vec{A}, \vec{\lambda}(\vec{A}))$ may be interpreted as a Landau functional corresponding to the given MF model. The explicit analytical form of $F(\vec{A}, \vec{\lambda}(\vec{A}))$ or its series expansion in the powers of order parameter(s) may be difficult to obtain, and then again we have to resort to the numerical analysis. Nonetheless, the concepts of Landau theory of phase transitions may be utilized. E.g., the quantity $\mathcal{N}^{-1} \exp \left( -\beta F(\vec{A}, \vec{\lambda}(\vec{A})) \right)$, where $\mathcal{N}$ is normalization constant, may be interpreted as the probability distribution of $\vec{A}$. Also, plots of $F(\vec{A}, \vec{\lambda}(\vec{A}))$ may be used for qualitative analysis of the character of the emerging phase transition.

### 3.2 Mean-field equilibrium thermodynamics

The equilibrium description is justified, provided that at the point $\vec{A} = \vec{A}_0$ the function $\mathcal{N}^{-1} \exp \left( -\beta F(\vec{A}, \vec{\lambda}(\vec{A})) \right)$ possesses a sharp peak, and consequently, the fluctuations of order parameter can be neglected. This condition is expected to hold for a wide class of MF Hamiltonians defined on lattice, in the $\Lambda \to \infty$ limit, where $\Lambda$ is the number of lattice sites. Obviously, for such models, this condition is equivalent to the thermodynamic limit $V \to \infty$, $N \to \infty$ with finite $N/V = n$. Then we can define the thermodynamic grand potential

$$\Omega(T, V, \mu) = F(T, V, \mu; \vec{A}_0(T, V, \mu), \vec{\lambda}_0(T, V, \mu)). \quad (22)$$

With this definition, the MF thermodynamics can be constructed, but we still have to demonstrate its consistency with MF statistical mechanical de-
description based on (16), cf. [6]. Such consistency is certainly present for an exact description, making use of non-mean-field Hamiltonians [1, 2, 3, 6]; in that case we have for example

\[ S = -\left[ \frac{\partial \Omega}{\partial T} \right]_{V,\mu}, \quad p = -\left[ \frac{\partial \Omega}{\partial V} \right]_{T,\mu}, \quad N = -\left[ \frac{\partial \Omega}{\partial \mu} \right]_{T,V}. \]  

(23)

One may ask if in the MF case the r.h.s. of (23) correspond to their statistical-mechanical definitions, as the equilibrium MF Hamiltonian \( \hat{H}_\lambda \) obviously depends on temperature and chemical potential through its dependence on the equilibrium values of mean fields and Lagrange multipliers \((\vec{A}_0, \vec{\lambda}_0)\). It can be shown, that (23) indeed holds, due to the underlying variational principle. Explicitly,

\[
\left( \frac{\partial \Omega}{\partial T} \right)_{V,\mu} = \beta^2 \partial_\beta \left( \beta^{-1} \ln Z_\lambda \right) = \beta Z_\lambda^{-1} \partial_\beta Z_\lambda - \ln Z_\lambda \\
= -\beta Z_\lambda^{-1} \text{Tr}[(\beta \partial_\beta \hat{K}_\lambda + \hat{K}_\lambda) e^{-\beta \hat{K}_\lambda}] - \ln Z_\lambda \\
= -\beta^2 \langle \partial_\beta \hat{K}_\lambda \rangle_\lambda - \beta \langle \hat{K}_\lambda \rangle_\lambda - \ln Z_\lambda \\
= -\beta^2 \langle \partial_\beta \hat{K}_\lambda \rangle_\lambda + \langle \ln \rho_\lambda \rangle_\lambda = -\beta^2 \langle \partial_\beta \hat{K}_\lambda \rangle_\lambda - S, 
\]

(24)

where \( \hat{K}_\lambda = \hat{H}_\lambda - \mu \hat{N} \) and \( Z_\lambda \) are evaluated for \( \vec{A} = \vec{A}_0, \vec{\lambda} = \vec{\lambda}_0 \). Also, \( \ln Z_\lambda(\vec{A}_0, \vec{\lambda}_0) = -\beta \Omega \), and \( \langle \hat{K}_\lambda \rangle_\lambda = U - \mu N \). In effect, we obtain the desired result (23), provided that the term \( \langle \partial_\beta \hat{K}_\lambda \rangle_\lambda \) vanishes. Indeed, in equilibrium we have

\[
\langle \partial_\beta \hat{K}_\lambda \rangle_\lambda = \left\langle \sum_{s=1}^{M} \left( \frac{\partial \hat{K}_\lambda}{\partial A_s} \frac{\partial A_{s0}}{\partial \beta} + \frac{\partial \hat{K}_\lambda}{\partial \lambda_s} \frac{\partial \lambda_{s0}}{\partial \beta} \right) \right\rangle_\lambda \\
= \sum_{s=1}^{M} \left( \left\langle \frac{\partial \hat{H}_\lambda}{\partial A_s} \right\rangle_\lambda \frac{\partial A_{s0}}{\partial \beta} + \left\langle \frac{\partial \hat{H}_\lambda}{\partial \lambda_s} \right\rangle_\lambda \frac{\partial \lambda_{s0}}{\partial \beta} \right) = 0, 
\]

(25)

due to relations (17) and (18). The same reasoning applies to the derivatives of \( \Omega \) with respect to \( \mu \) and \( V \). In the latter case, Hamiltonian depends explicitly on \( V \) (e.g. through the volume dependence of its parameters). In effect, we recover proper expressions for average number of particles \( N \) and pressure \( p \). Other thermodynamic potentials may be constructed in the standard manner, e.g. \( F = \Omega + \mu N \).

Note that as the \( \beta \)- and \( \mu \)- dependences of equilibrium values of mean-fields \( \vec{A}_0 \) obtained through self-consistent Eqs. (11) are nontrivial in general, \footnote{We exclude the possibility of explicit dependence of \( \hat{H}_\lambda \) on \( \beta = 1/T \) or \( \mu \).}
and also because \( (17) \) with \( \lambda = 0 \) usually does not hold in such case, there is no reason for \( \langle \partial_\beta \hat{K} \rangle \) (as well as for analogous expressions for the derivatives with respect to \( \mu, V \) etc.) to vanish. This feature results in the lack of consistency between MF thermodynamics and MF statistical mechanics even on the level of the first-order derivatives of the corresponding thermodynamic potential and constitutes an obvious and serious drawback of non-variational self-consistent approach\(^4\). The problem of such consistency is also analyzed in Ref. [6], however, from a slightly different perspective. The analysis of the second-order derivatives of \( \Omega \) is slightly more complicated and is carried out in [5].

### 3.3 Redundancy conditions

The natural question is, when the presence of Lagrange multipliers in the Hamiltonian (10) is unnecessary. We will not provide the general answer, but instead present an important example. Suppose we have the exact Hamiltonian of the following form

\[
\hat{H}_e = \hat{H}_{0e} + \sum_{\{\kappa,\gamma\}} V_{\kappa\gamma} \hat{O}_\kappa \hat{O}_\gamma, \tag{26}
\]

where each \( \hat{O}_\kappa \) is assumed to be bilinear in the creation and/or annihilation operators, and the summation is taken over all pairs \( \{\kappa, \gamma\} \) of multi indices. If the interaction term in (26) is decoupled (i.e. replaced by its MF counterpart) according to

\[
\hat{O}_\kappa \hat{O}_\gamma \rightarrow \hat{A}_s \hat{A}_t + A_s \hat{A}_t - A_s A_t, \tag{27}
\]

with \( A_s, A_t \) given by (4) for the appropriate density matrix, then the standard Hartree or the Hartree-Fock (HF) type mean-field Hamiltonian is obtained. With the constraint terms it reads

\[
\hat{H}_\lambda = \hat{H}_{0e} + \sum_{\{s,t\}} \tilde{V}_{st} (\hat{A}_s \hat{A}_t + A_s \hat{A}_t - A_s A_t) - \sum_s \lambda_s (\hat{A}_s - A_s) \\
\equiv \hat{H} - \sum_s \lambda_s (\hat{A}_s - A_s). \tag{28}
\]

\(^4\)A notable exception, the case of pure Hartree or Hartree-Fock type of MF Hamiltonians, is discussed in the next paragraph.

\(^5\)Usually, the \( \hat{O}_\kappa \hat{O}_\gamma \) term may be decoupled in more then one way, but this does not change the arguments presented.
In the above, $\hat{H}_0$ does not depend on $\vec{A}$, and $\tilde{V}_{st}$ are the combinations of matrix elements $V_{\kappa \gamma}$. Then, one can find that

$$\langle \frac{\partial \hat{H}}{\partial A_t} \rangle_{\lambda} = \langle \sum_s \tilde{V}_{st}(\hat{A}_s - A_s) \rangle_{\lambda} = 0,$$

(29)

which together with (17) implies that $\lambda_t = 0$, for any $t$. Also, for Hamiltonian of such form, the solution of $M$ self-consistent equations (11) coincide with those of $M$ equations $\nabla_A F = 0$ of unconstrained variational approach. A related discussion of this problem may be found in [7].

Summarizing, for any MF Hamiltonian of the Hartree-Fock type, application of our method is not necessary. However, there are important examples of the MF Hamiltonians not being of HF form, in Section 4 we present two such examples.

3.4 Relation of the present method to the variational principle of Bogoliubov and Feynman

In the previous Sections we considered the situation, when the description of the system has been based solely on the MF Hamiltonian $\hat{H}$. In other words, we made no use of any exact Hamiltonian $\hat{H}_e$ present in a problem at hand, from which $\hat{H}$ may be derived and for which it may play the role of a simplified counterpart.

However, frequently the MF density operators are used as a trial variational states in order to determine the bounds on the grand potential $\Omega_e$ or free energy $F_e$ of the system described by $\hat{H}_e$. Such bounds are provided by the well-known inequality due to Bogoliubov and Feynman [8, 9]

$$\Omega_e \leq \langle \hat{K}_e - \hat{K}_0 \rangle_0 + \tilde{\Omega} = \text{Tr}[\hat{\rho}_0(\hat{K}_e - \hat{K}_0)] + \tilde{\Omega},$$

(30)

In the above, $\hat{H}_0$ is a trial Hamiltonian, $\tilde{\Omega} = -\beta^{-1} \ln \text{Tr}[\exp (-\beta(\hat{H}_0 - \mu_0 \hat{N}))], \text{and} \ \Omega_e = -\beta^{-1} \ln \text{Tr}[\exp (-\beta(\hat{H}_e - \mu_e \hat{N}))].$ Also, $\hat{K}_e = \hat{H}_e - \mu_e \hat{N}$ and analogously for $\hat{K}_0$, with $\mu_e$ ($\mu_0$) being respective chemical potentials. There are several ways to prove (30), probably the shortest of them is that of making use of the Klein inequality, [10]

$$\text{Tr}[\hat{\rho} \ln \hat{\rho}] \geq \text{Tr}[\hat{\rho} \ln \hat{\sigma}],$$

(31)

which holds for any normalized density operators $\hat{\rho}$ and $\hat{\sigma}$. Inserting

$$\hat{\rho} = \hat{\rho}_0 = Z_0^{-1} \exp(-\beta(\hat{H}_0 - \mu_0 \hat{N})), \quad \hat{\sigma} = \hat{\rho}_e = Z_e^{-1} \exp(-\beta(\hat{H}_e - \mu_e \hat{N})), \quad \text{and} \quad \text{Tr}[\hat{\rho} \ln \hat{\rho}] = \text{Tr}[\hat{\rho} \ln \hat{\sigma}],$$

(32)
(with $Z_0 = \text{Tr}[\exp(-\beta(\hat{H}_0 - \mu_0 \hat{N}))]$ and $Z_e = \text{Tr}[\exp(-\beta(\hat{H}_e - \mu \hat{N}))]$ into (31), we obtain (30). If one wants to work with the chemical potential as an independent variable, then $\mu_e = \mu_0 \equiv \mu$ and (30) reduces to

$$\Omega_e \leq \langle \hat{H}_e - \hat{H}_0 \rangle_0 + \tilde{\Omega} = \text{Tr}[\hat{\rho}_0(\hat{H}_e - \hat{H}_0)] + \tilde{\Omega}.$$  \hspace{1cm} (33)

However, usually it is more convenient to have particle number $N$ as an independent variable. In such a case $\mu_0$ and (unknown) $\mu_e$ are not equal in general, as they are determined from different conditions, i.e. $\langle \hat{N} \rangle_0 = N$ and $\langle \hat{N} \rangle_e = N$, respectively. However, (30) may be then given the form

$$F_e = \Omega_e + \mu_e N \leq \langle \hat{H}_e - \hat{H}_0 \rangle_0 + \tilde{\Omega} + \mu_0 N.$$  \hspace{1cm} (34)

Bogoliubov inequality is the basis of the variational principle, the best trial state $\hat{\rho}_0$ is the one minimizing r.h.s. of (33), or (34), depending on the choice of independent variables, $\mu$ or $N$, respectively.

If one wants to use the Bogoliubov inequality in order to determine upper bounds for $\Omega_e$ or $F_e$ of some $\hat{H}_e$, but with the self-consistency of the approach being preserved, then the density operators (5) are not good candidates for the trial states. Clearly, they have no free variational parameters if only the values of mean-fields, $\vec{A} = \vec{A}_0$, are obtained in a self-consistent fashion through (4). On the other hand, if $\vec{A}_0$ were obtained from unwary minimization of the r.h.s. of (33), (34) with $\hat{\rho}$ given by (5), then the self-consistency of the approach would be violated in general (again with the notable exception of the Hartree-Fock MF Hamiltonians).

In contrast, consider the trial state chosen in the form (16), with the trial Hamiltonian $\hat{H}_0 = \hat{H}_\lambda$, yet unrelated to the $\hat{H}_e$ in question. Then the r.h.s. of (33) reads

$$\text{Tr}[\hat{\rho}_\lambda(\hat{H}_e - \hat{H}_\lambda)] + \mathcal{F}(\vec{A}, \vec{\lambda}) \equiv \mathcal{B}(\vec{A}, \vec{\lambda}),$$  \hspace{1cm} (35)

whereas that of (34), respectively (with $\mu_0 \equiv \mu$)

$$\text{Tr}[\hat{\rho}_\lambda(\hat{H}_e - \hat{H}_\lambda)] + \mathcal{F}(\vec{A}, \vec{\lambda}) + \mu N = \mathcal{B}(\vec{A}, \vec{\lambda}) + \mu N \equiv \mathcal{B}_N(\vec{A}, \vec{\lambda}).$$  \hspace{1cm} (36)

Depending on the choice of independent variable, the necessary $2M$ conditions for r.h.s of the Bogoliubov inequality, i.e $\mathcal{B}$ or $\mathcal{B}_N$, to have a minimum subject to constrains of self-consistency acquire slightly different form. For (35) we have

$$\nabla_A \mathcal{B}(\vec{A}, \vec{\lambda}) = 0, \quad \nabla_{\lambda} \mathcal{F}(\vec{A}, \vec{\lambda}) = 0.$$  \hspace{1cm} (37)

\footnote{We neglect the situation, in which there appear some extra variational parameters, not being expectation values of operators present in a problem, and thus not requiring the corresponding Lagrange multipliers.}

\footnote{Similarly as previously, here we assume, that the desired minimum corresponds to a stationary point.}
On the other hand, for \((36)\) we have

\[
\nabla'_{A} B_N(\vec{A}, \vec{\lambda}) = 0, \quad \nabla_{\lambda}(\mathcal{F}(\vec{A}, \vec{\lambda}) + \mu N) = 0, \quad \frac{\partial}{\partial N}(\mathcal{F}(\vec{A}, \vec{\lambda}) + \mu N) = \mu.
\]

(38)

In the above, \(\nabla'_{A}\) labels the gradient taken with respect to all mean-fields except \(A_1 = N\). Also

\[
\nabla'_{A} B_N(\vec{A}, \vec{\lambda}) = \nabla'_{A} B(\vec{A}, \vec{\lambda}), \quad \nabla_{\lambda}(\mathcal{F}(\vec{A}, \vec{\lambda}) + \mu N) = \nabla_{\lambda}\mathcal{F}(\vec{A}, \vec{\lambda}).
\]

(39)

If \(B(\vec{A}, \vec{\lambda}) \neq \mathcal{F}(\vec{A}, \vec{\lambda})\), the solution of \((37)\) or \((38)\) leads to different values of \(\tilde{A}_0\) and \(\tilde{\lambda}_0\), than those obtained from \((20)\). Then, \(\hat{\rho}_{\lambda}\) is no longer a true grand-canonical MF density operator for \(\hat{H}_{\lambda}\). The above remarks hold for other inequalities (i.e. various generalizations of \((30)\)), and the corresponding variational principles built on them. \([9]\). One may use the \(\hat{\rho}_{\lambda}\) \((16)\) as useful ansätze in such cases as well. Nonetheless, the entropy functional \((9)\) with the corresponding variational principle plays a special role, and it determines the form \((16)\) of GC MF density operator. Also, the self-consistency conditions may be conveniently formulated with the help of \(\mathcal{F}(\vec{A}, \vec{\lambda})\), as in \((37)\) and \((38)\).

However, clearly, for any pair of \(\hat{H}_e, \hat{H}_{\lambda}\), for which the condition

\[
\langle \hat{H}_e - \hat{H}_{\lambda} \rangle_{\lambda} = 0
\]

holds, so consequently also \(\hat{\Omega}(\vec{A}, \vec{\lambda}) = \mathcal{F}(\vec{A}, \vec{\lambda}) = B(\vec{A}, \vec{\lambda})\), the Bogoliubov - Feynman and Maximum Entropy variational principles coincide. In such case the optimal, from the point of view of maximum entropy inference, i.e. the most uninformative MF density operator \(\hat{\rho}_{\lambda}\) provides us also with the upper bound for exact grand potential \(\Omega_e\) or free energy \(F_e\) of \(\hat{H}_e\). For \((37)\) this is obvious. For \((38)\), this may be shown using \(\partial \mathcal{F}/\partial \mu = -N\) and replacing \(B \rightarrow \mathcal{F}\), then we obtain the identity

\[
\mu = \frac{\partial}{\partial N}(\mathcal{F}(\vec{A}, \vec{\lambda}) + \mu N) = \frac{\partial \mathcal{F}}{\partial N} + \frac{\partial \mathcal{F}}{\partial \mu} \frac{\partial \mu}{\partial N} + N \frac{\partial \mu}{\partial N} = \frac{\partial \mathcal{F}}{\partial N} + \mu.
\]

(41)

Consequently, \(\partial \mathcal{F}/\partial N = 0\) for the solutions of Eqs. \((38)\). From Eqs. \((39)\) and \((41)\), it follows that any solution of \((38)\), i.e. \((\tilde{A}_0, \tilde{\lambda}_0, \mu)\) is also a solution of \((37)\), if \(N\) and \(\mu\) related by the condition \(\langle \tilde{N} \rangle = N = -\partial \mathcal{F}/\partial \mu\). Also, conversely, Eqs. \((39)\), \((41)\) imply that the solutions of \((37)\) are also solutions of \((38)\), thus both schemes are equivalent.

4 Two nontrivial examples

We now discuss briefly two MF models, for which the proposed method leads to nontrivial corrections. To show this, we make use of Eq. \((17)\), and argue, that the condition \(\vec{\lambda} = \vec{0}\) cannot be, in general, satisfied.
4.1 Renormalized t-J model

The first example we analyze is the MF Hamiltonian of the so-called renormalized t-J model \[11\]-[16]. It originates from the standard t-J model [17], believed to describe correctly the essential physics of the cuprate high-temperature superconductors, that is expressed by the Hamiltonian

\[
\hat{H}_e = \sum_{i,j(i),\sigma} t_{ij} \hat{c}_{i\sigma} \hat{c}_{j\sigma} + J \sum_{\langle ij \rangle} \langle S_i \cdot S_j - \frac{1}{4} \hat{\nu}_i \hat{\nu}_j \rangle - \mu \sum_{i,\sigma} \hat{\nu}_{i\sigma}.
\]

Here \(\hat{c}_{i\sigma} = (1 - n_{i\sigma}) c_{i\sigma}\) and \(\hat{\nu}_i = \sum_{\sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}\) are the operators with double occupancies on site \(i\) projected out. The corresponding renormalized MF Hamiltonian may be taken in the form [13, 15]

\[
\hat{H} = \sum_{\langle ij \rangle \sigma} \left( (t_{ij} g_{ij}^t c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) - \frac{3}{4} J g_{ij}^J (\chi_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.} - |\chi_{ij}|^2) \right. \\
+ \left. \frac{3}{4} J g_{ij}^J (\Delta_{ij} c_{j\sigma}^{\dagger} c_{i\sigma}^{\dagger} + \text{H.c.} - |\Delta_{ij}|^2) \right) - \mu \sum_{i,\sigma} c_{i\sigma}^{\dagger} c_{i\sigma},
\]

with \(n_i = \sum_{\sigma} \langle c_{i\sigma}^{\dagger} c_{i\sigma} \rangle\), \(\chi_{ij} = \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle\), and \(\Delta_{ij} = \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle = \langle c_{j\sigma} c_{i\sigma} \rangle\). In this form the projections have been abolished at the price of introducing the expectation-value dependent renormalization factors \(g_{ij}^t\) and \(g_{ij}^J\) resulting from the Gutzwiller approximation [18]. At first, we consider the renormalization factors depending solely on \(x_i = 1 - n_{i\sigma}\), i.e.

\[
g_{ij}^t = \sqrt{\frac{4x_i x_j}{(x_i + 1)(x_j + 1)}}, \quad \text{and} \quad g_{ij}^J = \frac{4}{(x_i + 1)(x_j + 1)}. \tag{44}
\]

The task is to determine the values of the mean-field parameters \(\chi_{ij}, \Delta_{ij}\) and \(x_i\). This could be achieved with the help of self-consistent Eqs. (4) for \(\hat{H}\) given by (43) (cf. [11]-[15]).

On the other hand, we may proceed in the framework of our method, and redefine the Hamiltonian (43) according to

\[
\hat{H}_\lambda = \hat{H} - \sum_{i} \lambda_i^n (\sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} - n_i) - \sum_{\langle ij \rangle \sigma} (\lambda_{ij}^x (c_{i\sigma}^{\dagger} c_{j\sigma} - \chi_{ij}) + \text{H.c.}) \\
- \sum_{\langle ij \rangle \sigma} (\lambda_{ij}^\Delta (c_{i\sigma}^{\dagger} c_{j\sigma} - \Delta_{ij}) + \text{H.c.}). \tag{45}
\]

Assuming no additional symmetries, using \(\partial / \partial n_i = - \partial / \partial x_i\), converting the sums over bonds to that over sites in (43) according to \(2 \sum_{\langle i,j \rangle} = \sum_{i,j(i)}\) and finally taking \(A_w \equiv n_i\) in Eqs. (17) we obtain
$$2\lambda_i^n = \left\langle \sum_{j(i), \sigma} t_{ij} \frac{\partial g_{ij}^t}{\partial x_i} (c_{i\sigma}^c c_{j\sigma} + \text{H.c.}) \right\rangle_{\lambda}$$

$$- \left\langle \frac{3}{4} J \sum_{j(i), \sigma} \frac{\partial g_{ij}^t}{\partial x_i} (\chi_{ij}^t c_{i\sigma}^c c_{j\sigma} + \text{H.c.} - |\chi_{ij}|^2) \right\rangle_{\lambda}$$

$$- \left\langle \frac{3}{4} J \sum_{j(i), \sigma} \frac{\partial g_{ij}^t}{\partial x_i} (\Delta_{ij}^t c_{i\sigma}^c c_{j\sigma} + \text{H.c.} - |\Delta_{ij}|^2) \right\rangle_{\lambda}$$

$$= \sum_{j(i)} \left( 4t_{ij} \frac{\partial g_{ij}^t}{\partial x_i} \text{Re} \chi_{ij} - \frac{3}{2} J \frac{\partial g_{ij}^t}{\partial x_i} \left( |\chi_{ij}|^2 + |\Delta_{ij}|^2 \right) \right). \quad (46)$$

Below it will be shown that in this particular case, $\lambda_{ij}^x = \lambda_{ij}^\Delta = 0$, for each bond $\langle ij \rangle$. Consequently, if for all $i$, we put $\lambda_i^n = 0$, then the density operator, and all averages coincide with those of the standard self-consistent MF treatment. However, in such situation equations (46) and the self-consistent equations (4) for $\hat{H}$ given by (43) cannot in general be simultaneous satisfied. For example, if one sets $J = 0$ and $x_i \in (0, 1)$, then from (46) it follows that

$$\left\langle \sum_{j(i), \sigma} \frac{\partial g_{ij}^t}{\partial x_i} (c_{i\sigma}^c c_{j\sigma} + \text{H.c.}) \right\rangle_{\lambda} = 0. \quad (47)$$

This is a senseless result, as in such case our Hamiltonian reduces essentially to that of free fermions, at least for the case of homogeneous solution, $x_i \equiv x$. Similarly, for $t_{ij} = 0$, one obtains $|\chi_{ij}|^2 = 0, |\Delta_{ij}|^2 = 0$ for each bond $ij$, provided that each $t_{ij}$ is of the same sign, as $\partial g_{ij}^t / \partial x_i > 0$, for any $x_i$ and $\langle ij \rangle$. This is in contradiction with the numerical results of Raczkowski et al., [14]. In other words, in this particular case, we can infer about the predictions of our method using the previous, non-variational results. Consequently, it follows that $\lambda_i^n \neq 0$, for every $i$.

From the point of view of our findings, a related situation can be found in Ref. [16]. Namely, the inhomogeneous solutions of the model (13) (with slightly different definitions of $\chi_{ij}$ and $\Delta_{ij}$), and with the renormalization factors given by (44) are analyzed. However, the additional terms of the form $\sum_i \epsilon_i (\sum_{j(i), \sigma} c_{i\sigma}^c c_{i\sigma} + x_i - 1)$, are included, where $\epsilon_i$ is the local fugacity. The quantity $\epsilon_i$ plays a role analogous to $\lambda_i^n$ in our method. Inclusion of that additional constraint allows to treat each $x_i$ as a variational parameter, and leads to the equations analogous to (46). This should be clear in the light of the discussion in the preceding Sections.
Next, we pose the question of redundancy of the Lagrange multipliers $\lambda^{\chi}_{ij}$ and $\lambda^{\Delta}_{ij}$. We may expect, according to discussion carried out in Section 3.3, that these quantities vanish, as the Hamiltonian \[ \text{(13)} \] with $g^{t}_{ij}$ and $g^{J}_{ij}$ given by \[ \text{(14)} \] is of the Hartree-Fock type with respect to both $\chi_{ij}$ and $\Delta_{ij}$. This is indeed the case, we may use once more Eq. \[ \text{(17)} \] with $A_{w} = \chi_{ij}$ or $A_{w} = \Delta_{ij}$, respectively, to obtain

\[
\lambda^{\chi}_{ij} = \left< \frac{3}{4} J \sum_{\sigma} g^{J}_{ij}(c_{j\sigma}^{\dag}c_{i\sigma} - \chi_{ij}^{*}) \right>_{\lambda} = 0, \quad (48)
\]

\[
\lambda^{\Delta}_{ij} = \left< \frac{3}{4} J \sum_{\sigma} g^{J}_{ij}(c_{j\sigma}^{\dag}c_{i\sigma}^{\dag} - \Delta_{ij}^{*}) \right>_{\lambda} = 0. \quad (49)
\]

Obviously, those self-consistency equations must be fulfilled both in the previous treatments ($\vec{\lambda} = \vec{0}$) as well as in the present method.

Next, we consider the renormalization factors of the form \[ \text{(15)} \],

\[
g^{t}_{ij} = \sqrt{\frac{4x_{i}x_{j}(1-x_{i})(1-x_{j})}{(1-x_{i}^{2})(1-x_{j}^{2}) + 8(1-x_{i}x_{j})|\chi_{ij}|^{2} + 16|\chi_{ij}|^{4}}}, \quad (50)
\]

\[
g^{J}_{ij} = \frac{4(1-x_{i})(1-x_{j})}{(1-x_{i}^{2})(1-x_{j}^{2}) + 8x_{i}x_{j}(|\Delta_{ij}|^{2} - |\chi_{ij}|^{2}) + 16(|\Delta_{ij}|^{2} + |\chi_{ij}|^{4})}. \quad (51)
\]

In such more general situation, the equation \[ \text{(46)} \] is still valid, and Eqs. \[ \text{(48)} \] and \[ \text{(49)} \] acquire the form, respectively

\[
\lambda^{\chi}_{ij} = - \sum_{\sigma} \left< t_{ij} \frac{\partial g^{t}_{ij}}{\partial \chi_{ij}} (c_{i\sigma}^{\dag}c_{j\sigma} + \text{H.c.}) - \frac{3}{4} J \frac{\partial g^{J}_{ij}}{\partial \chi_{ij}} (\chi_{ij}c_{i\sigma}^{\dag}c_{j\sigma} + \text{H.c.} - |\chi_{ij}|^{2}) \right>_{\lambda} + \frac{3}{4} J \frac{\partial g^{J}_{ij}}{\partial \chi_{ij}} (\chi_{ij}c_{i\sigma}^{\dag}c_{j\sigma}^{\dag} + \text{H.c.} - |\Delta_{ij}|^{2}) \right>_{\lambda} + \frac{3}{2} J \frac{\partial g^{J}_{ij}}{\partial \Delta_{ij}} (|\Delta_{ij}|^{2} + |\chi_{ij}|^{2}) \right>_{\lambda} = -4t_{ij} \frac{\partial g^{t}_{ij}}{\partial \chi_{ij}} \text{Re} \chi_{ij} + \frac{3}{2} J \frac{\partial g^{J}_{ij}}{\partial \chi_{ij}} (|\Delta_{ij}|^{2} + |\chi_{ij}|^{2}), \quad (52)
\]

\[
\lambda^{\Delta}_{ij} = \frac{\sum_{\sigma} \left< J \frac{\partial g^{J}_{ij}}{\partial \Delta_{ij}} (\chi_{ij}c_{i\sigma}^{\dag}c_{j\sigma} + \text{H.c.} - |\chi_{ij}|^{2}) + \frac{3}{4} J g^{J}_{ij}(c_{i\sigma}^{\dag}c_{j\sigma}^{\dag} - \Delta_{ij}^{*}) + \frac{3}{4} J g^{J}_{ij}(\Delta_{ij}c_{j\sigma}^{\dag}c_{i\sigma} + \text{H.c.} - |\Delta_{ij}|^{2}) \right>_{\lambda} + \frac{3}{2} J \frac{\partial g^{J}_{ij}}{\partial \Delta_{ij}} (|\Delta_{ij}|^{2} + |\chi_{ij}|^{2}) \right>_{\lambda} = \frac{3}{2} J \frac{\partial g^{J}_{ij}}{\partial \Delta_{ij}} (|\Delta_{ij}|^{2} + |\chi_{ij}|^{2}). \quad (53)
\]
Again, if we put $\vec{\lambda} = \vec{0}$ in order to reduce our approach to the standard treatment, that Eqs. (52) and (53) cannot be satisfied. For Eq. (52) this can be easily shown for the case $t_{ij} = -t$ by adding it to its complex conjugate part. Then, at least for the class of solutions with for $\text{Re} \chi_{ij} > 0$, one can convince oneself by explicitly computing respective derivatives of $g^I_{ij}$ and $g^J_{ij}$, that the resulting expression should have nonzero value, for a wide range of values $x_i$. For Eq. (53) or (52) in the case of $t_{ij} = 0$, no additional explanation is required.

Similar arguments apply if, instead of $\vec{\lambda} = \vec{0}$, a weaker conditions, $\lambda \chi_{ij} = 0$ or $\lambda \Delta_{ij} = 0$, are imposed. In such situation we can no longer make use of the numerical or analytical results of the purely self-consistent approach. Nonetheless, it is unlikely that such conditions do not lead to contradictions. E.g. from Eqs. (52) with $t_{ij} = 0$ or from (53) in a general case, we infer, that $\chi_{ij} = \Delta_{ij} = 0$.

In that slightly hand-waving manner we tried to argue, that for the Hamiltonian (43) our variational approach does not reduce to that based solely on the self-consistency equations.

This model has been recently analyzed and solved numerically in a separate publication [19].

4.2 Electrons with spin-dependent effective masses

In Ref. [20], an approximate one-particle description of a strongly-correlated electron system was introduced, based on the observation, that the effective masses of quasiparticles may be spin-dependent. The MF Hamiltonian of this model depends on $A_1 = N$ and $A_2 = M$, where

$$\hat{N} = \hat{A}_1 = \sum_k \sum_\sigma c_{k\sigma}^\dagger c_{k\sigma}, \quad \hat{M} = \hat{A}_2 = \sum_k \sum_\sigma \sigma c_{k\sigma}^\dagger c_{k\sigma}. \quad (54)$$

With additional constraint terms, the Hamiltonian reads

$$\hat{H}_\lambda^{SDM} = \left( \sum_k \sum_{\sigma} (\Phi_\sigma(N, M) \epsilon_{k\sigma} - \sigma h_a - \mu) \hat{n}_{k\sigma} \right) - \lambda_1 (\hat{N} - N) - \lambda_2 (\hat{M} - M), \quad (55)$$

where $(-\sum_k \sigma h_a \hat{n}_{k\sigma})$ is the Zeeman term, and $h_a$ is the reduced applied magnetic field. The present case is, in fact, quite similar to the previous one, the band-narrowing factors $\Phi_\sigma(N, M)$ are also derived using the Gutzwiller approach. Then analogously, by making use of Eq. (17), either with $A_w = N$ or $A_w = M$, we obtain respectively

$$\lambda_1 = -\left\langle \sum_k \sum_{\sigma} \frac{\partial \Phi_\sigma(N, M)}{\partial N} \epsilon_{k\sigma} \hat{n}_{k\sigma} \right\rangle_{\lambda}, \quad (56)$$
\[ \lambda_2 = - \left\langle \sum_k \sum_\sigma \frac{\partial \Phi_\sigma(N, M)}{\partial M} \epsilon_{k\sigma} \hat{n}_{k\sigma} \right\rangle_\lambda. \]  

(57)

Regardless of the detailed analytical form of \( \Phi_\sigma(N, M) \), we multiply (57) by

\[ - \frac{\partial}{\partial N} \Phi_\downarrow(N, M) \left( \frac{\partial}{\partial M} \Phi_\downarrow(N, M) \right)^{-1} \]

and add it to (56). The resulting r.h.s is then proportional to \( \langle E_{\text{kin},\uparrow} \rangle_\lambda = \langle \sum_k \epsilon_{k\uparrow} \hat{n}_{k\uparrow} \rangle_\lambda \), the average band energy of particles with \( z \)-spin component \( \sigma = \uparrow \). If we put \( \lambda_1 = \lambda_2 = 0 \), all the averages become identical to those of the standard treatment. Consequently, for (56) and (57) to hold in such a case we have to require that \( \langle E_{\text{kin},\uparrow} \rangle = 0 \), for any admissible value of \( N, M \), and functional dependence of \( \Phi_\sigma(N, M) \) on its variables, which is a trivial and inconsistent result. Obviously, the same holds for \( \sigma = \downarrow \).

The numerical studies of this model and its extensions are carried out recently, [21].

5 Summary and conclusions

In this paper we have presented the method, based on the maximum entropy principle, of constructing the grand-canonical density operator for a wide class of mean-field Hamiltonians. We have shown, that such a density operator is not, in general, obtained by replacing the exact Hamiltonian by its mean-field counterpart in the grand canonical density operator. Usually, some extra terms, which may be interpreted as a kind of source terms or molecular fields, must be added to the mean-field Hamiltonian. This modification also ensures consistency of basic thermodynamic relations, which is not guaranteed for self-consistent methods which are not based on the variational principle.

It is also shown, that although for the Hartree-Fock type of mean-field Hamiltonians application of our method is not necessary, there are also some important examples, for which it does not reduce to the standard approach. The renormalized mean-field t-J Hamiltonian is such case.

If there is \( M \) expectation values appearing in a mean-field Hamiltonian that are to be determined, the method presented here results in a system of \( 2M \) equations. This is in contrast to the standard treatment, where only \( M \) such equations appear.

The problem of the application of maximum entropy inference in the mean-field case was studied also in a series of the papers [22]. However, the presented point of view and the results obtained differ essentially from ours.
Also, the problem partly related to that discussed in the present paper, namely the construction of variational principles suited for optimization of physical quantities of interest, is examined in an interesting article [23]. This paper contains a detailed analysis of the problem, as well as covers a large area of the subject (for example the authors discuss time-dependent formalism).

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