Site occupation constraints in mean-field approaches of quantum spin systems at finite temperature.

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Abstract

We study the effect of site occupation on the description of quantum spin systems at finite temperature and mean-field level. We impose each lattice site to be occupied by a single electron. This is realized by means of a specific prescription. The outcome of the prescription is compared to the result obtained by means of a projection procedure which fixes the site occupation to one particle per site on an average. The comparison is performed for different representations of the Hamiltonian in Fock space leading to different types of mean-field solutions. The behaviour of order parameters is analyzed for each choice of the mean-field and constraint which fixes the occupation rate at each site. Sizable quantitative differences between the outcomes obtained with the two different constraints are observed.

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1 Introduction

We consider ordered quantum spin systems at finite temperature in which each lattice site is occupied by one electron with a given spin. Such a configuration can be constructed by means of constraints imposed through a specific projection operation which fixes the occupation in a strict sense. The constraint can also be implemented on the average by means of a Lagrange multiplier procedure. It is the aim of the present work to confront these two approaches in the framework of Heisenberg-type models.

The description of strongly interacting quantum spin systems at finite temperature generally goes through a saddle point procedure which is a zeroth order approximation of the partition function. The so generated mean-field solution is aimed to provide a qualitatively realistic approximation of the exact solution.

However mean-field solutions are not unique. The implementation of a mean-field structure is for a large part subject to an educated guess which should rest on essential properties of the considered system, in particular its symmetries. This generates a major difficulty. A considerable amount of work on this point has been made and a huge litterature on the subject is available. In particular, systems which are described by Heisenberg-type models without frustration are seemingly well described by ferromagnetic or antiferromagnetic (AF) Néel states at temperature $T = 0$. It may however no longer be the case for many systems which are of low dimensionality ($d \leq 2$) and (or) frustrated. These systems show specific features. An extensive analysis and discussion in space dimension $d = 2$ has recently been presented by Wen. The competition between AF and chiral spin state order has been the object of very recent investigations in the framework of continuum quantum field approaches at $T = 0$ temperature, see.

The reason for the specific behaviour of low dimensional systems may qualitatively be related to the fact that low dimensionality induces strong quantum fluctuations, hence disorder which destroys the AF order. This motivates a transcription of the Hamiltonian in terms of composite operators which we call "diffusons" and "cooperons" below, with the hope that the actual symmetries different from those which are generated by AF order are better taken into account at the mean-field level.
In the present work we aim to work out a rigorous vs. average treatment of the half-filling occupation constraint on systems governed by Heisenberg-type Hamiltonians at the mean-field level, for different types of order.

The outline of the paper is the following. In section 2 we first recall the projection procedure which leads to a rigorous site occupation. Section 3 is devoted to the confrontation of the magnetization obtained through this procedure with the result obtained by means of an average projection procedure in the framework of the mean-field approach characterized by a Néel state. The same confrontation is done in section 4 for the order parameter which characterizes the system when its Hamiltonian is written in terms of so called Abrikosov fermions \[6, 2\] in \(d = 2\) space dimensions. In section 5 we show that the rigorous projection \[1\] is no longer applicable when the Hamiltonian is written in terms of composite ”cooperon” operators. Conclusions, further investigations and extensions are presented in section 6.

2 Site occupation constraint for quantum spin systems at finite temperature \(T\).

Heisenberg quantum spin Hamiltonians of the type

\[
H = \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j
\]  

with \(\{J_{ij}\} > 0\) can be projected onto Fock space by means of the transformation

\[
S_i^+ = a_i^{\dagger} a_i
\]

\[
S_i^- = a_i a_i^{\dagger}
\]

\[
S_i^z = \frac{1}{2}(a_i^{\dagger} a_i - a_i a_i^{\dagger})
\]
where \( \{a_{\uparrow i}, a_{\downarrow i}\} \) are anticommuting fermion operators.

This transformation is not bijective because the dimensionality of Fock space is larger than the dimensionality of the space in which the spin operators \( \{\vec{S}_i\} \) are acting. Indeed, in Fock space, each site \( i \) can be occupied by 0, 1 or 2 fermions corresponding to the states \(|0, 0>, |1, 0>, |0, 1>, |1, 1>\) where \(|0, 0>\) is the particle vacuum, \(|1, 0> = | + 1/2 >, |0, 1> = | - 1/2 >\) and \(|1, 1> = | + 1/2, -1/2 >\) in terms of spin 1/2 projections. Since one wants to keep states with one fermion per site only states \(|0, 0>\) and \(|1, 1>\) have to be eliminated. This can be performed on the partition function for a system at inverse temperature \( \beta \)

\[
Z = Tr e^{-\beta H}
\]

where the trace is taken over the whole Hilbert space by adding a projection term

\[
Z = Tr e^{-\beta (H - \mu N)}
\]

where \( N \) is the particle number operator and \( \mu = i \pi / 2 \beta \) an imaginary chemical potential \( \downarrow \). Indeed, the presence of the states \(|0, 0>_i\) and \(|1, 1>_i\) on site \( i \) leads in \( Z \) to phase contributions which eliminate each other

\[
e^{i\circ 0} + e^{i\circ \pi} = 0
\]

and hence the contributions of these spurious states are cancelled as a whole.

The common alternative approximate projection procedure would be to introduce a chemical potential in terms of real Lagrange multipliers \( \{\lambda_i\} \) and to fix this quantity by means of a saddle point procedure with respect to the \( \{\lambda_i\} \) s

\[
Z = Tr e^{-\beta H} \prod_i \int d\lambda_i e^{\lambda_i(n_i - 1)}
\]

where \( n_i \) is the particle number operator on site \( i \).

In the following we compare the outcome of these two projection procedures in the framework of different mean-field approximations of systems described by Heisenberg Hamiltonians.
3 Antiferromagnetic mean-field ansatz

3.1 Exact occupation procedure

Starting with the Hamiltonian defined in Eq. (1) the partition function $Z$ can be written in the form

$$Z = \int \prod_{i,\sigma} \mathcal{D}(\{\xi_{i,\sigma}^*, \xi_{i,\sigma}\}) e^{-A(\{\xi_{i,\sigma}^*, \xi_{i,\sigma}\})}$$

(5)

where the $\{\xi_{i,\sigma}^*, \xi_{i,\sigma}\}$ are Grassmann variables corresponding to the operators $\{a_{i\sigma}^\dagger, a_{i\sigma}\}$ defined above. They depend on the imaginary time $\tau$ in the interval $[0, \beta]$. The action $A$ is given by

$$A(\{\xi_{i,\sigma}^*, \xi_{i,\sigma}\}) = \int_0^\beta d\tau \sum_{i,\sigma} (\xi_{i,\sigma}^*(\tau) \partial_\tau \xi_{i,\sigma}(\tau) + \mathcal{H}(\{\xi_{i,\sigma}^*(\tau), \xi_{i,\sigma}(\tau)\}))$$

(6)

where

$$\mathcal{H}(\tau) = H(\tau) - \mu N(\tau)$$

(7)

and $N(\tau)$ is the particle number operator. A Hubbard - Stratonovich (HS) transformation which generates the vector fields $\{\vec{\varphi}_i\}$ leads to the partition function $Z$ which can be written in the form

$$Z = \int \prod_{i,\sigma} \mathcal{D}(\{\xi_{i,\sigma}^*, \xi_{i,\sigma}, \vec{\varphi}_i\}) e^{-\int_0^\beta d\tau \left[ \sum_{i,\sigma} \xi_{i,\sigma}^*(\tau) \partial_\tau \xi_{i,\sigma}(\tau) + \tilde{H}(\{\xi_{i,\sigma}^*, \xi_{i,\sigma}, \vec{\varphi}_i\}) \right]}$$

(8)

In Eq. (8) the expression of $Z$ is quadratic in the Grassmann variables $\{\xi_{i,\sigma}^*, \xi_{i,\sigma}\}$ over which the expression can be integrated. The remaining expression depends on the fields $\{\vec{\varphi}_i(\tau)\}$. A saddle point procedure decomposes $\vec{\varphi}_i(\tau)$ into a mean-field contribution and a fluctuating term

$$\vec{\varphi}_i(\tau) = \vec{\varphi}_i^{(mf)} + \delta \vec{\varphi}_i(\tau)$$

(9)

where $\vec{\varphi}_i^{(mf)}$ are the constant solutions of the self-consistent equation

$$\vec{\varphi}_i^{(mf)} = \frac{1}{2} \sum_j J_{ij} \frac{\vec{\varphi}_j^{(mf)}}{||\vec{\varphi}_j^{(mf)}||} \text{th} \left( \frac{\beta ||\vec{\varphi}_j^{(mf)}||}{2} \right)$$

(10)
The partition function takes the form
\[ Z = Z_{mf} \int \mathcal{D}(\{\delta \vec{\varphi}_i\}) e^{-A(\delta \vec{\varphi})} \] (11)
where the first term on the r.h.s. corresponds to the mean-field contribution and the second term describes the contributions of the quantum fluctuations.

Considering the mean-field contribution the partition function \( Z_{mf} \) can be put in the form
\[ Z_{mf} = \text{Tr} e^{-\beta H_{mf}} \]
which reads
\[ Z_{mf} = i^{-N} e^{\frac{1}{2} \beta \sum_{ij} (J^{-1})_{ij} \vec{\varphi}_i^{(mf)} \cdot \vec{\varphi}_j^{(mf)}} \prod_i \left( 1 + e^{-\beta E^+_i} \right) \left( 1 + e^{-\beta E^-_i} \right) \] (12)
where \( N \) is the number of sites. The energies \( E^+_i \) and \( E^-_i \) are obtained through a diagonalization of the Hamiltonian by means of a Bogolioubov transformation in Fock space. Explicitly
\[ E^+_i = \mu + \frac{\| \vec{\varphi}_i^{(mf)} \|}{2} \]
\[ E^-_i = \mu - \frac{\| \vec{\varphi}_i^{(mf)} \|}{2} \]
Working out the expression of \( Z_{mf} \) leads to
\[ Z_{mf} = e^{\frac{1}{2} \beta \sum_{ij} (J^{-1})_{ij} \vec{\varphi}_i^{(mf)} \cdot \vec{\varphi}_j^{(mf)}} \prod_i \text{ch} \left( \frac{\beta \| \vec{\varphi}_i^{(mf)} \|}{2} \right) \] (13)
and the free energy is given by the expression
\[ \mathcal{F}_{mf} = -\frac{1}{2} \sum_{ij} (J^{-1})_{ij} \vec{\varphi}_i^{(mf)} \cdot \vec{\varphi}_j^{(mf)} - \frac{1}{\beta} \sum_i \log 2 \text{ch} \left( \frac{\beta \| \vec{\varphi}_i^{(mf)} \|}{2} \right) \] (14)
In order to obtain the expression of the local magnetization \( \{ \vec{m}_i \} \) one should add the term \( \sum_i \vec{B}_i \vec{S}_i \) to the Hamiltonian \( H \) in Eq. (1). Going through the same steps as above the local magnetization given by

\[
\vec{m}_i^{(mf)} = -\frac{\partial F_{mf}}{\partial \vec{B}_i} \bigg|_{\vec{B}_i=\vec{0}}
\]  

(15)

is related to the \( \{ \vec{\varphi}^{(mf)}_i \} \)'s by

\[
\vec{m}_i = \frac{1}{2} \vec{\varphi}_i \text{th} \left[ \frac{\beta \vec{\varphi}_i}{2} \right]
\]

which leads to the self-consistent equation for the \( \{ \vec{m}_i^{(mf)} \} \)'s

\[
\vec{m}_i^{(mf)} = \frac{2}{\beta} \sum_j (J^{-1})_{ij} \left( \text{th}^{-1}(2m_j) \frac{\vec{m}_j^{(mf)}}{m_j^{(mf)}} \right)
\]

(16)

If the local fields \( \{ \vec{B}_i \} \) are oriented along a fixed direction \( \vec{e}_z \), \( m_i^{(mf)} = m_i^{(mf)} \vec{e}_z \), the magnetizations are the solutions of the self-consistent equations

\[
m_i^{(mf)} = \frac{1}{2} \text{th} \left( \frac{\beta \sum_j J_{ij} m_j^{(mf)}}{2} \right)
\]

(17)

### 3.2 Lagrange multiplier approximation

Similarly to the preceding case one can introduce the one-particle site occupation by means of a Lagrange procedure added on the expression of the Hamiltonian

\[
H = \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \vec{S}_j + \lambda \sum_i (n_i - 1)
\]

where \( \lambda \) is a variational parameter and \( \{ n_i \} \) are particle number operators.
Following the same lines as above with the help of a HS transformation and staying in the ordinary space representation the mean-field partition function $Z_{mf}^\lambda$ can be worked out and reads

$$Z_{mf}^\lambda = e^{-\frac{1}{2}\sum_{ij}(J^{-1})_{ij}\varphi_i^{(mf)}\varphi_j^{(mf)} - N\lambda} \prod_i (1 + e^{-\beta E_i^+}) (1 + e^{-\beta E_i^-})$$

(18)

with

$$E_i^+ = \lambda + \frac{||\varphi_i^{(mf)}||}{2}$$

$$E_i^- = \lambda - \frac{||\varphi_i^{(mf)}||}{2}$$

The parameter $\lambda$ is fixed through a minimization of the corresponding free energy $\mathcal{F}_{mf}^{(\lambda)}$ with respect to this multiplier. The minimization shows that the extremum solution is obtained for $\lambda = 0$ and

$$\mathcal{F}_{mf}^{(\lambda)} = -\frac{1}{2} \sum_{ij} (J^{-1})_{ij} \varphi_i^{(mf)} \varphi_j^{(mf)} - \frac{2}{\beta} \sum_i \ln 2 \cosh \left( \frac{\beta ||\varphi_i^{(mf)}||}{4} \right)$$

(19)

which is different from the expression of Eq. (14).

The magnetization can be obtained in the same way as done above. One obtains

$$m_i^{(mf)} = \frac{1}{2} (\beta \sum_j J_{ij} m_j^{(mf)})$$

(20)

which is again different from the expression obtained in the case of a rigorous projection, see Eq. (17).

The uniform solutions $m_i^{(mf)} = (-1)^i m^{(mf)}$ and $m_{i,\lambda=0}^{(mf)} = (-1)^i m_{\lambda=0}^{(mf)}$ for $\{J_{ij}\} = J$ have been calculated by solving the selfconsistent equations (17) and (20).

The results are shown in Fig. 11. It is seen that the treatment of the site occupation affects sizably the quantitative behaviour of observables. In particular it shifts the location of the critical temperature $T_c$ by a factor 2. Such a
strong effect has already been observed on the behaviour of the specific heat, see refs. [15, 16].

4 Spin state mean-field ansatz in 2d

In 2d space the Heisenberg Hamiltonian given by Eq.(1) can be written in terms of composite non-local operators \( \{ \mathcal{D}_{ij} \} \) ("diffusons") defined as

\[
\mathcal{D}_{ij} = a_{i\uparrow}^\dagger a_{j\uparrow} + a_{i\downarrow}^\dagger a_{j\downarrow}
\]

Then the initial Hamiltonian Eq. (1) with \( J_{ij} = J \) takes the form

\[
H = -J \sum_{<ij>} \left( \frac{1}{2} \mathcal{D}_{ij}^\dagger \mathcal{D}_{ij} - \frac{n_i}{2} + \frac{n_i n_j}{4} \right)
\]

where \( i \) and \( j \) are nearest neighbour sites. The physical justification for such a transcription relies on the fact that systems with low space dimensionality at finite temperature show physical symmetry properties which are closer to a spin liquid than an ordered Néel state as already mentioned in the introduction.
The number operator products \( \{n_i n_j\} \) in Eq. (21) are quartic in terms of creation and annihilation operators in Fock space. In principle its existence necessitates the introduction of a further mean field. One can however show that its elimination has no influence on the results obtained from the partition function. As a consequence we leave it out from the beginning as well as the contribution corresponding to the \( \{n_i\} \) term.

### 4.1 Exact occupation procedure

Starting with the Hamiltonian

\[
H = -\frac{J}{2} \sum_{<ij>} D_{ij}^\dagger D_{ij} - \mu N
\]  

one performs an HS transformation on the corresponding functional integral partition function in which the action contains the occupation number operator as written out in Eq. (7). The Hamiltonian takes the form

\[
H = \frac{2}{|J|} \sum_{<ij>} \bar{\Delta}_{ij} \Delta_{ij} + \sum_{<ij>} \left[ \bar{\Delta}_{ij} D_{ij} + \Delta_{ij} D_{ij}^\dagger \right] - \mu N
\]  

The fields \( \Delta_{ij} \) and their conjugates \( \bar{\Delta}_{ij} \) can be decomposed into a mean-field contribution and a fluctuation term

\[
\Delta_{ij} = \Delta_{ij}^{mf} + \delta \Delta_{ij}
\]  

The field \( \Delta_{ij}^{mf} \) can be chosen as a complex quantity \( \Delta_{ij}^{mf} = |\Delta_{ij}^{mf}| e^{i\phi_{ij}^{mf}} \). Consider a square plaquette \( (\vec{i}, \vec{i} + \vec{e}_x, \vec{i} + \vec{e}_y, \vec{i} + \vec{e}_x + \vec{e}_y) \) where \( \vec{e}_x \) and \( \vec{e}_y \) are the unit vectors along the directions \( \vec{O}x \) and \( \vec{O}y \) starting from site \( \vec{i} \) on the lattice. On this plaquette

\[
\phi = \prod_{(ij) \in pl} \phi_{ij}^{mf}
\]

is taken to be constant. If the gauge phase \( \phi_{ij}^{mf} \) fluctuates in such a way that \( \phi \) keeps constant the average of \( \Delta_{ij}^{mf} \) will be equal to zero in agreement
with Elitzur’s theorem [17]. In order to guarantee $SU(2)$ invariance of the mean-field Hamiltonian along the Wilson loop on the plaquette we follow [10] [11] [12] [13] [14] and introduce

$$\phi_{ij} = \begin{cases} e^{i \frac{\pi}{4} (-1)^i}, & \text{if } \vec{r}_j = \vec{r}_i + \vec{e}_x \\ e^{-i \frac{\pi}{4} (-1)^i}, & \text{if } \vec{r}_j = \vec{r}_i + \vec{e}_y \end{cases}$$

(25)

Then the total flux through the plaquette

$$\phi = \pi$$

In the mean-field approximation the corresponding partition function reads

$$Z_{mf} = e^{-\beta(H_{mf} - \mu N)}$$

(26)

where

$$H_{mf} = \frac{2}{|J|} \sum_{<ij>} \Delta_{ij}^m \Delta_{ij}^m + \sum_{<ij>} \left[ \Delta_{ij}^m D_{ij} + \Delta_{ij}^m D_{ij}^\dagger \right] - \mu N$$

(27)

Performing a Bogoliubov transformation which diagonalizes the remaining expression in Fourier space leads to

$$H_{mf} = \frac{Nz \Delta^2}{|J|} + \sum_{\mathbf{k}, \sigma} \left[ E_{\mathbf{k}, \sigma}^{\uparrow} \beta_{\mathbf{k}, \sigma}^{\dagger} \beta_{\mathbf{k}, \sigma} + E_{\mathbf{k}, \sigma}^{\downarrow} \beta_{\mathbf{k}, \sigma}^{\dagger} \beta_{\mathbf{k}, \sigma} \right]$$

(28)

where $z = 4$ is the coordination and $N$ the number of sites. The momenta $\{\mathbf{k}\}$ act in the first half Brillouin zone (spin Brillouin zone) and the operators $\{\beta^\dagger, \beta\}$ are the transformed of the $\{a^\dagger, a\}$’s through the rotation which leads to the diagonal expression Eq. (28). The eigenenergies $E_{\mathbf{k}, \sigma}^{\uparrow}$ and $E_{\mathbf{k}, \sigma}^{\downarrow}$ are given by

$$E_{\mathbf{k}, \sigma}^{\uparrow} = -\mu + 2\Delta [\cos^2(k_x) + \cos^2(k_y)]^{1/2}$$

(29)

and similarly

$$E_{\mathbf{k}, \sigma}^{\downarrow} = -\mu - 2\Delta [\cos^2(k_x) + \cos^2(k_y)]^{1/2}$$

(30)
The partition function $Z_{mf}$ has the same structure as the corresponding partition function in Eq. (18) and the free energy is given by

$$F_{mf} = \frac{Nz\Delta^2}{|J|} - \frac{1}{\beta} \sum_{\vec{k},\sigma} \ln 2 (\chi h \Delta \epsilon_{\vec{k}})$$

(31)

with

$$\epsilon_{\vec{k}} = 2[\cos^2(k_x) + \cos^2(k_y)]^{1/2}$$

(32)

Finally the variation of $F_{mf}$ with respect to $\Delta$ leads to the self-consistent mean-field equation

$$\tilde{\Delta} = \frac{1}{2N} \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} th \left( \frac{\beta |J| \epsilon_{\vec{k}} \tilde{\Delta}}{z} \right)$$

(33)

with $\tilde{\Delta} = z\Delta/|J|$.

### 4.2 Lagrange multiplier approximation

Similarly to Eq. (23) one may introduce a Lagrange constraint and write

$$H^{(\lambda)} = \frac{2}{|J|} \sum_{<ij>} \bar{\Delta}_{ij} \Delta_{ij} + \sum_{<ij>} \left( \bar{\Delta}_{ij} D_{ij} + \Delta_{ij} D_{ij}^\dagger \right) + \sum_i \lambda_i (n_i - 1)$$

(34)

Then for $\lambda_i = \lambda$

$$H^{(\lambda)}_{mf} = \frac{Nz\Delta^2}{|J|} + \sum_{\vec{k},\sigma} \left( E_{\vec{k},\sigma}^+ \beta_{(+)}^\dagger \beta_{(+)}^\sigma + E_{\vec{k},\sigma}^- \beta_{(-)}^\dagger \beta_{(-)}^\sigma \right)$$

(35)

with the eigenenergies

$$E_{\vec{k},\sigma}^+ = \lambda + 2\Delta[\cos^2(k_x) + \cos^2(k_y)]^{1/2}$$

(36)

and similarly

$$E_{\vec{k},\sigma}^- = \lambda - 2\Delta[\cos^2(k_x) + \cos^2(k_y)]^{1/2}$$

(37)
The expression of the free energy is now given by

\[
\mathcal{F}_{mf}^{(\lambda)} = -N \lambda + \frac{N z \Delta^2}{|J|} - \frac{1}{\beta} \sum_{\vec{k},\sigma} \ln[1 + e^{-\beta E_{\vec{k},\sigma}^+}][1 + e^{-\beta E_{\vec{k},\sigma}^-}] - 1 \beta \sum_{\vec{k},\sigma} \ln[1 + e^{-\beta E_{\vec{k},\sigma}^+}][1 + e^{-\beta E_{\vec{k},\sigma}^-}] (38)
\]

The minimization of this expression in terms of \( \lambda \) delivers the solution \( \lambda = 0 \) and

\[
\mathcal{F}_{mf}^{(\lambda)} = -N \lambda + \frac{N z \Delta^2}{|J|} - \frac{1}{\beta} \sum_{\vec{k},\sigma} 2 \ln \left( 2 \sqrt{\beta \Delta \epsilon_{\vec{k}}^2} \right) - 1 \beta \sum_{\vec{k},\sigma} \ln[1 + e^{-\beta E_{\vec{k},\sigma}^+}][1 + e^{-\beta E_{\vec{k},\sigma}^-}] (39)
\]

The variation of \( \mathcal{F}_{mf}^{(\lambda)} \) with respect to \( \Delta \) leads to the self-consistent mean-field equation equation

\[
\tilde{\Delta}^{(\lambda)} = \frac{1}{N} \sum_{\vec{k},\sigma} \epsilon_{\vec{k}}^2 h \left( \frac{\beta |J| \epsilon_{\vec{k}} \tilde{\Delta}^{(\lambda)}}{2z} \right) (40)
\]

with \( \tilde{\Delta}^{(\lambda)} = z \Delta / |J| \).

Expressions in Eq. (39) and Eq. (40) should be compared to the expressions obtained in Eq. (31) and Eq. (33). Fig. 2 shows the behaviour of \( \Delta \) for the two different treatments of site occupation on the lattice.

### 4.3 Magnetization

We calculate the magnetization in the case of a rigorous one-particle site occupation. Starting with the Hamiltonian \( H \) given by Eq. (22) and adding the staggered interaction \( h \sum_i (-1)^i S_i^z \) of the spins with an homogeneous external field \( h \) one obtains the mean field expression

\[
H_{mf} = \frac{N z \Delta^2}{|J|} + \sum_{\vec{k},\sigma} [E_{h,\vec{k},\sigma}^+ \beta_{\vec{k},\sigma}^+ \beta_{\vec{k},\sigma} + E_{h,\vec{k},\sigma}^- \beta_{\vec{k},\sigma}^+ \beta_{\vec{k},\sigma}^-] (41)
\]
Figure 2: $\tilde{\Delta}$ vs. reduced temperature $\tilde{t} = zT/|J|$. Full line: exact site occupation. Dashed line: average site occupation.

where

$$E_{h,\bar{k},\sigma}^+ = -\mu + \tilde{E}_{h,\bar{k},\sigma}$$ (42)

and similarly

$$E_{h,\bar{k},\sigma}^- = -\mu - \tilde{E}_{h,\bar{k},\sigma}$$ (43)

with

$$\tilde{E}_{h,\bar{k},\sigma} = \left(\frac{\hbar^2}{4} + \Delta^2 \epsilon_{\bar{k}}^2\right)^{1/2}$$

The free energy can now be written

$$F_{h,mf} = \frac{N z \Delta^2}{|J|} - \frac{1}{\beta} \sum_{\bar{k},\sigma} \ln \left(2\hbar \beta \tilde{E}_{h,\bar{k},\sigma}\right)$$ (44)

and the magnetization

$$m^{(mf)} = -\frac{\partial F_{mf}}{\partial h} \bigg|_{h=0}$$

reads

$$m^{(mf)} = \frac{\partial \Delta}{\partial h} \bigg|_{h=0} \left(\frac{2N z \Delta}{|J|} - \sum_{\bar{k},\sigma} \epsilon_{\bar{k}} \theta(\beta \epsilon_{\bar{k}})\right)$$ (45)
The sum over $\vec{k}$ runs over half the Brillouin zone. Going back to Eq. (33) one sees that $m^{(mf)}$ is equal to zero.

The same result holds in the case of the average Lagrange multiplier procedure.

### 5 Cooperon mean-field ansatz

Starting from the Hamiltonian

$$H = -|J| \sum_{<i,j>} \vec{S}_i \vec{S}_j$$

(46)

one can introduce a further set of non-local composite operators ("cooperons")

$$C_{ij} = a_{i\uparrow} a_{j\downarrow} - a_{i\downarrow} a_{j\uparrow}$$

(47)

This leads to the expression

$$H = \frac{|J|}{2} \sum_{<i,j>} \left( C_{ij}^\dagger C_{ij} + \frac{n_i n_j}{2} \right)$$

(48)

where $n_i = \sum_\sigma n_{i\sigma}$.

#### 5.1 Exact occupation procedure

As in the preceding cases it is possible to implement a HS procedure on the $\{C_{ij}\}$ and $\{n_i\}$ in such a way that the expression of the corresponding partition function gets quadratic in the fields $\{a_{i\uparrow}, a_{i\downarrow}\}$. The corresponding HS fields are $\{\Gamma_{ij}\}$, $\{\nu_i\}$ and

$$H - \mu N = \frac{2}{|J|} \sum_{<i,j>} \Gamma_{ij} \Gamma_{ij} + \sum_{<i,j>} \left( \Gamma_{ij} C_{ij} + \Gamma_{ij} C_{ij}^\dagger + \frac{2}{|J|} \nu_i \nu_j \right) + \sum_i \nu_i n_i$$

(49)

Introducing the homogeneous fields $\{\Gamma = \Gamma_{ij}\}$, $\{\nu = \nu_i\}$ and integrating over
the cooperon fields \( \{C_{ij}\} \) one gets in Fourier space

\[
H = \frac{N z |\Gamma|^2}{|J|} + \frac{2 N |\nu|^2}{z |J|} + \sum_{\vec{k}, \sigma} (\nu - \mu) a_{\vec{k}, \sigma}^\dagger a_{\vec{k}, \sigma} + \sum_{\vec{k}, \sigma} \sigma z \gamma_{\vec{k}} \left( \bar{\Gamma} a_{\vec{k}, \sigma} a_{-\vec{k}, -\sigma} - \Gamma a_{\vec{k}, \sigma}^\dagger a_{-\vec{k}, -\sigma} \right)
\]

with

\[
\gamma_{\vec{k}} = \frac{1}{2} (\cos k_x + \cos k_y)
\]

The third term in this expression is complex since \( \mu = i \pi / 2 \beta \). In this representation it is not possible to find a unitary Bogolioubov transformation which diagonalizes \( H \). Hence a rigorous implementation of the constraint on the particle number per site is not possible.

Reasons for this situation may be the fact that the Hamiltonian contains terms with two particles with opposite spin created or annihilated on the same site which is incompatible with the fact that such configurations are not allowed in the present scheme. Terms of this type are typical in mean-field pairing Hamiltonians which lead to a non-conservation of the number of particles of the system.

5.2 Lagrange multiplier approximation

If the sites are occupied by one electron in the average the Lagrange procedure works. We do not develop the derivation of the mean-field here since it has been done elsewhere \[2\].

6 Conclusions.

In summary we have shown that a strict constraint on the site occupation of a lattice quantum spin system described by Heisenberg-type models shows a sizable quantitative different localization of the critical temperature when
compared with the outcome of an average occupation constraint. Consequently it generates sizable effects on the behaviour of order parameters and other physical observables. This is true both in the case of antiferromagnetic (Néel) and spin state symmetry.

Due to the complexity of quantum spin systems the choice of a physically meaningful mean field may depend on the coupling strengths of the model which describes the systems [19]. A specific mean-field solution may even be a naive way to fix the "classical" contribution to the partition function which may in fact contain a mixture of different types of states. As already mentioned many efforts have been and are done in order to analyze and overcome these problems, see f.i. [8, 9, 10]. It is our aim to repeat the analysis we did above in the framework of a description which is able to implement more appropriate descriptions at the mean-field level.

In a more realistic analysis one should of course take care of the contributions of quantum fluctuations which may be of overwhelming importance particularly in the vicinity of critical points. We expect to work out the first order contributions in a loop expansion for both types of constraints and symmetries considered in the present work in order to analyze and compare their relative importance as a function of temperature. Such an analysis may provide some view on the relative contribution of quantum corrections to order parameters and other observables for the different chosen mean-field ansätze.

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