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# Magnetic orders of Heisenberg models with arbitrary spin in semi-fermionic representation

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**Abstract.** In 1988 Popov and Fedotov (PF) proposed a new method for spin Hamiltonians free of the local constraint problem for spin  $S = 1/2$  and  $S = 1$ . Later, this approach has been extended for arbitrary spin. PF formalism has been used to study magnetic orders in some spin  $S = 1/2$  and  $S = 1$  Heisenberg models. In this report we show how to study the low temperature phases of quantum Heisenberg models with arbitrary spin by means of PF method. We work out the analytical expressions needed for studying ordered phases of Heisenberg models in one-loop approximation.

## 1. Introduction

The study of quantum magnetic systems is a field of active both theoretical and experimental research in recent years. From the theoretical viewpoint, the quantum spins pose a serious problem connected with the fact that spin operators satisfy the commutation relations of the angular algebra so they are neither Fermi nor Bose operators [1]. This leads to the absence of a Wick theorem directly for spin operators, which is a basic of the powerful analytical methods such as Feynman diagrammatic expansions and functional integrations. In order to overcome this problem different representations of spins such as Fermi or Bose canonical operators have been proposed [1]. However, the representations of spin as a combination of canonical operators lead to the unphysical states because the dimensionality of Fock space for canonical operators always is higher than that of the spin space. For excluding the unphysical states from the consideration one introduces some constraint requirement which has to be satisfied on every site containing the spins. This local constraint cannot be exactly treated. For simplicity one relaxes the local constraint on each site by a so-called global one, where the constraint is fulfilled only in the average over all sites [2]. It is not sure that such an approximation is uncontrolled.

In 1988, Popov and Fedotov (PF) proposed a new method for spin systems with spin quantum number  $S = 1/2$  and  $S = 1$  by representing spin operators as a combination of Fermi operators with imaginary chemical potential (semi-fermionic representation) [3]. The PF formulation provides a rigorous treatment of the local constraint. Recently, the PF fermionization trick has been generalized for strongly correlated systems [4, 5]. The PF idea was also successfully developed in combination with bold diagrammatic Monte - Carlo simulation to investigate frustrated quantum systems [6]. For specific systems, the PF procedure has been effectively applied to the negative U Hubbard model [7], Kondo lattice Hamiltonian [8], spin glass systems [9]... The PF approach has also been used to investigate ordered phases of Heisenberg



Hamiltonians on various lattice structures for  $S = 1/2$  [10 -13] and for  $S = 1$  [14]. Later, the PF technique is extended for arbitrary spin quantum number  $s$  by Veits et al with introducing proper chemical potentials for spin fermions [15]. Nevertheless, the paper [15] is basically of a methodological nature. In this report we derive general expressions needed for studying ordered phases of Heisenberg models with arbitrary spins on the Bravais lattices. It is motivated by the progress in the synthesis of new magnetic materials with spin  $S = 1, 3/2, 5/2, \dots$ . On the theoretical side, although quantum fluctuations are larger for systems with lower values of the spin quantum number  $s$ , totally new physical effect can also sometimes appear [16].

The organization of the paper is as follows. We first set up a general formalism in Sec.2. In Sec. 3 we represent our main results. We summarize this paper in Sec.4.

## 2. Formalism

We apply the extended PF trick to the quantum Heisenberg model given by the following Hamiltonian:

$$H = \sum_{ij} J_{ij} S_i S_j, \quad (1)$$

where  $J_{ij}$  is exchange interaction between sites  $i$  and  $j$ ,  $S_i$  is spin operators satisfying the non-canonical commutation relations:

$$[S_i^\alpha, S_j^\beta] = i \epsilon_{\alpha\beta\gamma} \delta_{ij} S_j^\gamma. \quad (2)$$

### 2.1. The extended PF procedure

The spin- $S$  operators may be represented in terms of Fermi operators as follows [15]:

$$S_i^\alpha = \sum_{m, m'=-S}^S a_{i, m'}^+ (S^\alpha)_{m' m} a_{i, m'}, \quad (3)$$

where  $(S^\alpha)_{m' m}$  are the spin- $S$  matrices, given by:

$$\begin{aligned} (S^+)_{m' m} &= \sqrt{S(S+1) - m(m+1)} \delta_{m', m+1} \\ (S^-)_{m' m} &= \sqrt{S(S+1) - m(m-1)} \delta_{m', m-1} \\ (S^z)_{m' m} &= m \delta_{m', m} \end{aligned} \quad (4)$$

and  $S^\pm = S^x \pm iS^y$ .

Here and in the following we take  $\hbar = 1$ .

For the case  $S = 1/2$ ,  $2(S^\alpha)_{m' m}$  are the Pauli matrices. The representation (3) satisfies the commutation relation (2). The Fock space of the fermions  $a_{i\sigma}$  is spanned by  $2S + 2$  states including the vacuum. Thus every site in the Fock space may be occupied by  $N$  fermions of spin  $S$  where  $0 < N < 2S + 1$ . Among them only two states with  $N = 1$  or  $N = 2S$  are physical. (Due to electron-hole symmetry the state with  $N = 2S$  is equivalent to the state with  $N = 1$ ). The unphysical states with  $N = 0$  (empty sites),  $N = 2S + 1$  (fully occupied sites),  $0 < N < 2S + 1$  have to be removed by imposing a constraint. For spin  $S = 1/2$ , the unphysical states  $|0\rangle, |2\rangle = a_{i\uparrow}^+ a_{i\downarrow}^+ |0\rangle$  are excluded by adding a term  $-\mu \sum_{i, \sigma} a_{i\sigma}^+ a_{i\sigma}$  to the Hamiltonian with

an imaginary chemical potential  $\mu = -\frac{i\pi}{2\beta}$ , with  $\beta = \frac{1}{k_B T}$  [3]. For general  $S > 1$ , as proved by Veits et al [15] it may be done with introducing a discrete set of  $2S + 1$  different imaginary chemical potentials on every site. The partition function of the spin system in the fermionic

representation (3) can be written in the following form:

$$Z = Tr_{spin} e^{-(\beta H_{spin})} = \prod_{i=1} \int P(\mu_i) d\mu_i Tr_{Fock} e^{-\beta \left( H_{Fock} - \sum_i \mu_i \hat{N}_i \right)} \quad (5)$$

where  $H_{Fock}$  means that all operators  $S_i$  are replaced by (3) and  $\hat{N}_i$  are the number operators of site  $i$ ,  $\hat{N}_i = \sum_{m=-S}^S a_{i,m}^+ a_{i,m}$ . The distribution  $P(\mu_i)$  reads as:

$$P(\mu_i) = \sum_{l=0}^{2S} \gamma_l \delta(\mu_i - \mu_l), \quad (6)$$

where the imaginary potentials are given by:

$$\mu_l = \frac{i\pi}{\beta} \frac{2l+1}{2S+1}, \quad (7)$$

and the coefficients  $\gamma_l$  take the following values:

$$\gamma_l = \frac{e^{-\beta\mu_l}}{2S+1}. \quad (8)$$

The eqs. (5) – (8) will be used for considering the ordered phases of the Heisenberg model (1).

## 2.2. Classical ground state and local reference frame

For taking into account the fluctuations around the classical it is convenient to parameterize in the classical limit the spin on site  $i$  as:

$$\vec{S}_i = S \left( \vec{u} \sin \vec{Q} \vec{r}_i + \vec{v} \cos \vec{Q} \vec{r}_i \right), \quad (9)$$

with  $\vec{u}$  and  $\vec{v}$  are two orthonormal unit vectors. The classical ground state is assumed to have coplanar magnetic structure, which may be shown for Hamiltonian (1) with the isotropic exchange interactions. The magnetic ordering vector  $\vec{Q}$  can be derived by minimizing the classical energy. Depending on the exchange interactions  $J_{ij}$  and on the lattice structure of the model there may exist different sets of vectors  $\vec{Q}$  corresponding to different ordered phases, so by parameterizing the classical ground state one could consider all ordered phases of the system in one common scheme [14]. Next, following Myiake [17] we transform the spin components from the laboratory reference frame to the local reference frame with the spin quantization axis on each site being along its classical direction. This transformation gives us the possibility of introducing only one type of the fermion (3) in term of the ordering vector  $\vec{Q}$  for each spin for all possible ordered phases such as Neel, spiral, canted state...

In result, the Hamiltonian (1) is rewritten in the form [14]:

$$H = -\frac{1}{2} \left( \sum_{i,j,\alpha,\beta=x,y,z} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta \right) \quad (10)$$

where:

$$\begin{aligned} J_{ij}^{xx} &= J_{ij}^{zz} = X_{ij} = -J_{ij} \cos \vec{Q} (\vec{r}_j - \vec{r}_i) \\ J_{ij}^{yy} &= Y_{ij} = -J_{ij} \\ J_{ij}^{zx} &= -J_{ij}^{xz} = W_{ij} = J_{ij} \sin \vec{Q} (\vec{r}_j - \vec{r}_i) \\ J_{ij}^{xy} &= J_{ij}^{yx} = J_{ij}^{yz} = J_{ij}^{zy} = 0 \end{aligned} \quad (11)$$

### 2.3. Perturbation technique

Now we apply the extended PF trick given in subsection 2.1 to the Hamiltonian (10).

We represent the partition function (5) with the Hamiltonian (10), where the spin operators are replaced by the fermion ones according to (3). Then we replace the fermion operators by Grassmann variables and eliminate the 4 fermions in the partition function by a Hubbard - Stratonovich transformation, introducing the Bose auxiliary field  $\vec{\varphi}_i$ , which plays the role of magnetization. After integration over the Grassmann variables we get:

$$Z = \prod_i^N \int d\mu_i P(\mu_i) Z(\mu_i), \quad (12)$$

where

$$Z(\mu_i) = \frac{1}{Z_o} \int D\vec{\varphi} e^{-S^{eff}[\vec{\varphi}_i, \mu_i]}, \quad (13)$$

with

$$Z_o = \left[ \det \hat{J}^{-1} \right]^{-1/2} \quad (14)$$

Here  $\hat{J}^{-1}$  is the inverse matrix of the exchange interaction  $\hat{J}_{ij}$ . Reasoning similarly as in Refs. 18, 19, after decomposing the Hubbard - Stratonovich auxiliary fields into the mean field values  $\vec{\varphi}_{io}$  and the fluctuations  $\delta\vec{\varphi}_i(\Omega)$  ( $\Omega$  being boson Matsubara frequencies) and introducing a fictive magnetic field into the Hamiltonian we get in one-loop approximation:

$$S_{eff}[\vec{\varphi}_i, \mu_i] = S_{eff}^{(0)}[\vec{\varphi}_{io}, \mu_i] + S_{eff}^{(1)}[\delta\vec{\varphi}_i, \mu_i] + S_{eff}^{(2)}[\delta\vec{\varphi}_i, \mu_i], \quad (15)$$

where

$$S_{eff}^{(0)}[\vec{\varphi}_{io}, \mu_i] = \frac{1}{2} \sum_{ij\alpha\beta} (\varphi_{io}^\alpha + B_i^\alpha) (J^{-1})_{ij}^{\alpha\beta} (\varphi_{jo}^\beta + B_j^\beta) - \sum_i A(\mu_i) \quad (16)$$

$$S_{eff}^{(1)}[\delta\vec{\varphi}_i, \mu_i] = \frac{1}{2} \sum_{ij\alpha\beta} \left[ (J^{-1})_{ij}^{\alpha\beta} (\varphi_{io}^\alpha + B_i^\alpha) \delta\varphi_j^\beta(0) + \delta\varphi_i^\alpha(0) (\varphi_{jo}^\beta + B_j^\beta) (J^{-1})_{ij}^{\alpha\beta} \right] \\ + \sum_{i\alpha\Omega} K_{1i}^\alpha(\Omega, \mu_i) \delta\varphi_i^\alpha(\Omega) \quad (17)$$

$$S_{eff}^{(2)}[\delta\vec{\varphi}_i, \mu_i] = \frac{1}{2} \sum_{ij\alpha\beta} \left[ (J^{-1})_{ij}^{\alpha\beta} + K_{2ij}^{\alpha\beta}(\Omega, \mu_i) \right] \delta\varphi_i^\alpha(-\Omega) \delta\varphi_j^\beta(\Omega). \quad (18)$$

Analogously to Refs. 18, 19, one can get explicit expression of free energy and thermodynamic quantities in one loop approximation for any Bravais lattice and some Bravais lattice if one knows analytical results for the expression of  $A(\mu_i)$ ,  $K_{1i}^\alpha(\Omega, \mu_i)$ ,  $K_{2ij}^{\alpha\beta}(\Omega, \mu_i)$  in the above equations.

For spin-1/2, spin-1 it may be done by manipulating directly with Pauli or spin-1 matrices. For arbitrary spin- $S$ , it is essential to use angular momentum algebra of spin operators.

### 3. Results

In order to derive explicit expressions of  $A(\mu_i)$ ,  $K_{1i}^\alpha(\Omega, \mu_i)$ ,  $K_{2ij}^{\alpha\beta}(\Omega, \mu_i)$ , we use the relations (4) and perform summation over fermion Matsubara frequencies. The calculation is lengthy but straightforward and will be published elsewhere. The results read:

$$A(\mu_i) = \sum_{k=-S}^S \ln \left( 1 + e^{-\beta k \varphi_{io} - \beta \mu_i} \right), \quad (19)$$

$$K_{1i}^{\alpha}(\Omega, \mu_i) = \sum_{k_{\min}}^S k \Delta(k\varphi_{i0}, \mu_i) \delta_{\alpha,z} \delta_{\Omega,0}, \quad (20)$$

$$K_{2ij}^{zz}(\Omega, \mu_i) = - \sum_{k_{\min}}^S \frac{k^2}{\sinh^2 \beta |\mu_i|} \left[ 1 - \sinh^2 \beta |\mu_i| \Delta^2(k\varphi_{i0}, \mu_i) - \sqrt{1 - \sinh^2 \beta |\mu_i| \Delta^2(k\varphi_{i0}, \mu_i)} \right] \delta_{ij}, \quad (21)$$

$$K_{2ij}^{+-}(\Omega, \mu_i) = \left( K_{2ij}^{-+}(\Omega, \mu_i) \right)^* = \frac{\delta_{ij}}{(i\Omega + \varphi_{i0})} B(S, \mu_i). \quad (22)$$

In the above expressions  $k_{\min} = 1/2$  for half integer spin and  $k_{\min} = 0$  for integer spin. The following notations are used:

$$\Delta(\varepsilon, \mu_i) = - \frac{\text{Sinh} \beta \varepsilon}{\text{Cosh} \beta \mu_i + \text{Cosh} \beta \varepsilon}, \quad \varepsilon = k\varphi_{i0}. \quad (23)$$

$$B(S, \mu_i) = \frac{1}{4} \sum_{k=0}^{S-1} (S(S+1) - k(k+1)) [\Delta((k+1)\varphi_{i0}, \mu_i) - \Delta(k\varphi_{i0}, \mu_i)], \quad (24)$$

for integer spin, and

$$B(S, \mu_i) = \left( S(S+1) + \frac{1}{4} \right) \Delta\left(\frac{\varphi_{i0}}{2}, \mu_i\right) + \frac{1}{4} \sum_{k=1/2}^{S-1} (S(S+1) - k(k+1)) [\Delta((k+1)\varphi_{i0}, \mu_i) - \Delta(k\varphi_{i0}, \mu_i)]. \quad (25)$$

for half integer spin.

We note that due to the least action principle  $\left. \frac{\delta S_{eff}}{\delta \varphi_i} \right|_{\delta \varphi_i=0}$  the linear term in the fluctuations of the effective action  $S_{eff}^{(1)}[\delta \vec{\varphi}_i, \mu_i] = 0$ . Therefore the functional integral over the auxiliary boson field  $\vec{\varphi}_i$  in eq. (13) has a Gaussian form and may be performed explicitly. In the result, it is ready to derive the analytical expression for the partition function (12) of the generic Hamiltonian (10). Once given the partition function, it is straightforward to calculate  $F = -\frac{1}{\beta} \ln Z$  and related thermodynamical quantities such as magnetization in a site  $m_i^{\alpha} = -\frac{\partial}{\partial B_i^{\alpha}} F$ ; susceptibility  $\chi_{\alpha\beta} = -\frac{\partial^2 F}{\partial B_i^{\alpha} \partial B_i^{\beta}}$ , specific heat  $C_v = -\beta^2 \left( \alpha \frac{\partial F}{\partial \beta} + \beta \frac{\partial^2 F}{\partial \beta^2} \right) \dots$

For checking we consider the case of the quantum spin number  $S = 1/2$  and  $S = 1$ . For  $S = 1/2$  the eq. (7) and (27) yield:

$$\mu = \frac{i\pi}{2\beta}, \quad \Delta(\varepsilon, \mu) = -\text{Tanh} \beta \varepsilon. \quad (26)$$

And Eqs.(19) – (23) give:

$$A(\mu) = \sum_i 2 \ln 2 \text{Cosh} \frac{\beta \varphi_{i0}}{4} \quad (27)$$

$$K_{1i}^{\alpha}(\Omega, \mu) = -\frac{1}{2} \text{Tanh} \left( \frac{\beta \varphi_{i0}}{2} \right) \delta_{\Omega,0} \delta_{\alpha,z} \quad (28)$$

$$K_{2ij}^{zz}(\Omega, \mu) = -\frac{1}{4} \left[ 1 - \Delta^2 \left( \frac{\varphi_{i0}}{2} \right) \right] \delta_{\Omega,0} \delta_{\alpha,z}, \quad (29)$$

$$K_{2ij}^{+-}(\Omega, \mu) = \frac{\beta \Delta(\frac{\varphi_{io}}{2}, \mu)}{4 \varphi_{io} + i\Omega} \delta_{ij}, \quad (30)$$

Thus we recover the results of the Refs.12, 18. Analogously we get for  $S = 1$ :

$$\mu = \frac{i\pi}{3\beta}, \quad \Delta(\varepsilon, \mu) = -\frac{2\text{Sinh}\beta\varepsilon}{1 + 2\text{Cosh}\beta\varepsilon}. \quad (31)$$

$$K_{1i}^{\alpha}(\Omega, \mu) = \Delta(\varepsilon, \mu) \delta_{\Omega,0} \delta_{z,0} \quad (32)$$

$$K_{2ij}^{zz}(\Omega, \mu) = -\frac{1}{3} \left[ 4 - 3\Delta^2(\varphi_{io}, \mu) - \sqrt{4 - 3\Delta^2(\varphi_{io}, \mu)} \right] \quad (33)$$

$$K_{2ij}^{+-}(\Omega, \mu) = \frac{\beta \Delta(\varphi_{io}, \mu)}{2 \varphi_{io} + i\Omega} \delta_{ij}, \quad (34)$$

The Eqs.(31) – (34) are the same as obtained in Ref.19.

#### 4. Summary

In this report we have shown how to apply the extended PF formalism for studying the ordered phases of the Heisenberg model with arbitrary quantum spin numbers  $S$ . By parameterizing a classical phase by an ordering vector and transforming to local coordinates one can investigate the ordered phases of the Heisenberg model with different lattice structures and different exchange interactions  $J_{ij}$  in a unified procedure. The fluctuation contributions may be taken into account by means of Hubbard - Stratonovich transformation and keeping up to second order of the auxiliary Hubbard - Stratonovich fields. We have derived the general analytical expressions for the kernels  $K_{1i}^z(\Omega, \mu)$  and  $K_{2ij}^{\alpha\beta}(\Omega, \mu)$  presented in the functional integral over auxiliary fields of the partition function. Given the above kernels it is straightforward to derive the partition function and the other related quantities such as the magnetization, the entropy, the internal energy..., as it have been shown in Refs.12, 18.

The results of the present paper can be applied to study specific cases with quantum spin number  $S = 3/2, 5/2...$  on different lattices, including non Bravais one.

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