Journal of Physics: Conference Series

PAPER • **OPEN ACCESS**

Magnetic order of spin S = 1 antiferromagnetic quantum Heisenberg systems on a Bravais lattice: exact local constraint

To cite this article: Pham Thi Thanh Nga and Nguyen Toan Thang 2017 *J. Phys.: Conf. Ser.* **865** 012015

View the article online for updates and enhancements.

Related content

- Magnetic ordering of the quasi-two-dimensional system VOCl
A Wiedenmann, J P Venien, P Palvadeau et al.
- All-temperature magnon theory of ferromagnetism
Sambhu N Datta and Anirban Panda
- Zero-point fluctuation in quasi one-dimensional antiferromagnets: theory and experiment
D Welz

This content was downloaded from IP address 113.190.155.80 on 14/11/2017 at 02:10

IOP Conf. Series: Journal of Physics: Conf. Series **865** (2017) 012015 doi:10.1088/1742-6596/865/1/012015

Magnetic order of spin $S = 1$ antiferromagnetic quantum Heisenberg systems on a Bravais lattice: exact local constraint

Pham Thi Thanh Nga[1] **and Nguyen Toan Thang**[2]

[1] Thuyloi University, 175 Tay Son, Dong Da, Hanoi, Vietnam
[2] Institute of Physics, 10 Dao Tan, Ba Dinh, Hanoi, Vietnam

E-mail: nga_ptt@tlu.edu.vn

Abstract. We apply the Popov-Fedotov formalism for investigating magnetic properties of the spin $S = 1$ Heisenberg antiferomagnetic (HAF) on a Bravais lattice. Mapping spin-1 lattice systems on three-component auxiliary fermions with imaginary chemical potential and transforming to a local coordinate system allow us to express a sublattice magnetization, free energy and other thermodynamical quantities in unique forms for different lattice structures in various magnetically ordered phases. We compare them with the results obtained when the local constraint is disregarded. A comparison with the case of $S = 1/2$ is also discussed.

1. Introduction

The fact that spin operators satisfy the non-canonical commutation relations poses a great difficulty to study theoretically quantum spin systems, because it leads to the absence of Wick theorem [1], so it is impossible to apply a standard perturbation technique directly for spin operators. One of the ways to resolve this problem is to represent the spin operators in terms of the auxiliary Fermi or Bose-operators [1]. However, any representation of spin operators as a bilinear combination of auxiliary operators makes the Hilbert space for spin operators larger. As a result, one must remove the spurious unphysical states by imposing some constraint on the auxiliary operators for each lattice site. In general it is very difficult to treat the local constraint exactly. One simple common approximation is to replace the local constraint by a so-called global constraint, where the number of auxiliary particles is taken to be on average for the whole lattice system. Popov-Fedotov proposed a method for quantum spin systems with $S = 1/2$ and $S = 1$ free of the local constraint problem [2], introducing some proper imaginary chemical potential. They demonstrated that if the usual Fermionic Matsubara frequencies $\omega = \frac{2\pi}{\beta}\left(n + \frac{1}{2}\right)$ are replaced by $\omega = \frac{2\pi}{\beta}\left(n + \frac{1}{4}\right)$ for $S = 1/2$ and by $\omega = \frac{2\pi}{\beta}\left(n + \frac{1}{3}\right)$ for $S = 1$ then the contributions of the unphysical states cancel each other and give no contribution to the partition function. Later, the extention of the Popov-Fedotov formalism for arbitrary spin was done by Veits et al [3]. In fact, this paper is basically of a methodologically nature. The concret calculations then have been performed for various spin systems with $S = 1/2$: three dimensional ferromagnetic Heisenberg model [4], Heisenberg antiferromagnet on a d-dimensional hypercubical [5, 6] and a triangular [7] lattice. However, many real magnets have spin quantum number $S = 1$, in particular the well studied experimentally material $NiGaS_4$. Besides, the spin quantum number

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd

S can play a considerable role in the various magnetic phenomena. A well-known example of this kind is the Haldane phase for $S = 1/2$ one dimensional Heisenberg model, which is absent in his $S = 1/2$ counter parts [8]. It is thus of great interest to apply the Popov-Fedotov formalism to spin systems with $S = 1$. In this report, we derive the general expressions of a sublattice magnetization, free energy and other thermodynamical quantities in unique forms for a Bravais lattice in a magnetically ordered state. The plan of the report is the following. In section II we introduce the model and the formalism. The mean field approximation is considered in section III. The fluctuations around a mean-field state are investigated in section IV. The last section is devoted to conclusion and discussions.

2. Formulation

We consider a general antiferromagnetic Heisenberg Hamiltonian on a Bravais lattice given by:

$$H_S = \sum_{ij} J_{ij} \vec{S}_i . \vec{S}_j \tag{1}$$

where $\vec{S}_i$ denotes the $S = 1$ spin vector operator. The interaction between the sites are antiferromagnetic ($J_{ij} > 0$). In the general frustrated lattice described by Hamiltionan (1) the classical ground states have long range order, which may be parametrized by some magnetic ordering vector $\vec{Q}$ [9]. We assume that the spins are planar in the plane Oxz and are described as follows [9]:

$$\vec{S}_i = S\left(\vec{u}\sin\vec{Q}\vec{r}_i + \vec{v}\cos\vec{Q}\vec{r}_i\right) \tag{2}$$

where $\vec{u}, \vec{v}$ are two orthonormal unit vectors in the plane Oxz. The vector $\vec{Q}$ defines the relative orientation of the spins on the lattice, namely an angle between the vectors $\vec{S}_i$ and $\vec{S}_j$ is given by:

$$\theta_{ij} = \theta_i - \theta_j = \vec{Q}\left(\vec{r}_i - \vec{r}_j\right) \tag{3}$$

Inserting $\vec{S}_i$ into Hamiltonian (1) we get the classical energy in terms of the ordering vector $\vec{Q}$ as folows:

$$E_{cl} = \frac{1}{2} N S^2 J\left(\vec{Q}\right) \tag{4}$$

where N is site number of the lattice and $J\left(\vec{Q}\right)$ is the Fourier transform of the exchange integral:

$$J\left(\vec{Q}\right) = \frac{1}{N}\sum_{ij} J_{ij} e^{-i\vec{Q}(\vec{r}_i - \vec{r}_j)} \tag{5}$$

The magnetic ordering vector $\vec{Q}$ can be obtained by minimizing (5) with respect to $\vec{Q}$, i.e by setting $\frac{\partial J(\vec{Q})}{\partial Q_\alpha} = 0, \alpha = \mathrm{x}, \mathrm{z}$.

In principle, there may exist several ordering vector $\vec{Q}$, minimizing the two-variable function $J\left(\vec{Q}\right)$. In order to incorporate the fluctuations in a unique way for all possible order phases, we folow Miyake [10], introducing a local coordinate system on each site i, where the local z axis is oriented along its classical direction. This transformation reads:

$$\begin{cases} S_i^z = S_i^{z'}\cos\theta_i - S_i^{x'}\sin\theta_i \\ S_i^x = S_i^{z'}\sin\theta_i - S_i^{x'}\cos\theta_i \\ S_i^y = S_i^{y'}. \end{cases} \tag{6}$$

Substituting (6) in (1), we get the following Hamiltonian, which is anisotropic on the spin space:

$$H_S = -\frac{1}{2}\sum_{\alpha\beta} J_{\mathrm{ij}}^{\alpha\beta} S_i^{\alpha} S_j^{\beta} \tag{7}$$

where:

$$\begin{cases} J_{ij}^{xx} = J_{ij}^{zz} \equiv X_{ij} = -J_{ij}\cos\theta_{ij} \\ J_{ij}^{yy} \equiv Y_{ij} = -J_{ij} \\ J_{ij}^{zx} = -J_{ij}^{xz} \equiv W_{ij} = -J_{ij}\sin\theta_{ij} \\ J_{ij}^{xy} = J_{ij}^{yx} = J_{ij}^{yz} = J_{ij}^{zy} = 0 \end{cases} \tag{8}$$

The tranformation (6) allows us to introduce only one type of auxiliary particles for all lattice sites rather than one type for each magnetic sublattice. Following Popov-Fedotov [2], the $S = 1$ spin vector operators are written in terms of Fermi operators $f_{i\alpha}^{+}, f_{i\alpha}\,(\alpha = 1, 2, 3)$

$$\vec{S}_i = f_{i\alpha}^{+}\tau_{\alpha\beta} f_{i\beta}\,(\alpha = 1, 2, 3) \tag{9}$$

where the $\vec{\tau}_{\alpha\beta}$ vector components are $S = 1$ $(3x3)$ matrices :

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ i & 0 & 1 \\ 0 & i & 0 \end{pmatrix}; S_y = \frac{1}{\sqrt{2}} = \begin{pmatrix} 0 & 1 & 0 \\ -i & 0 & 1 \\ 0 & -i & 0 \end{pmatrix}; S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{10}$$

Here and in the following we put $\hbar = 1$. The cost of the representation (9) is the extention of the Hilbert space into unphysical sectors, which have to be eliminated by imposing a constraint for each site i:

$$\sum_{\alpha} f_{i\alpha}^{\dagger} f_{i\alpha} = 1 \tag{11}$$

As it was shown by Popov-Fedotov [2], this can be done by means of introducing the projection operator $\hat{\mathrm{P}} = e^{i\mu\hat{N}_F}$ with $\hat{N}_F = \sum_{i\alpha} f_{i\alpha}^{+} f_{i\alpha}$ being number operator and $\mu = i\frac{\pi}{3\beta}, \beta = k_B T$ being the imaginary chemical potential. The partition of a spin system with Hamiltonian H_s can be expressed in term of Fermi operators as follows:

$$Z = \left(\frac{i}{\sqrt{3}}\right)^{N} Tr\left[e^{-\beta(\hat{H}_F - \mu\hat{N}_F}\right] \tag{12}$$

here $\hat{H}_F$ is Hamiltonian H_s in the fermionic representation (9). The appearence of the imaginary chemical potential in (12) results in that the corresponding Matsubara frequencies for Popov-Fedotov fermions read as:

$$\omega_n = \frac{2\pi}{\beta}\left(n + \frac{1}{3}\right) \tag{13}$$

The partition fuction Z in (12) can be treated following the standard fuctional integral formalism similar to the case of $S = 1/2$ [6, 7]. The main differences are that instead of Pauli (2x2) matrices and Matsubara frequencies $\mu = \frac{2\pi}{\beta}\left(n + \frac{1}{4}\right)$ we have to deal with the spin $S = 1$ (3x3) matrices (10) and Matsubara frequencies given by (13). The calculations are lenghthy but straightforward, so we only list here the main steps. Firstly, we express the partition fuction as path integral over Grassmann variables $\bar{\eta}_{i\alpha}, \eta_{i\alpha}$ and transform the Heisenberg Hamiltonian (7) into bilinear fermionic expression by introducing a Hubbard Stratonovich decoupling:

$$\begin{cases} Z = \frac{i}{(\sqrt{3})^N}\frac{1}{Z_0}\int\prod_i D\left[\vec{\varphi_i}\right]\int D\left[\bar{\eta}_{i\alpha}, \eta_{i\alpha}\right] e^{-S\left[\vec{\varphi_i}, \bar{\eta}_{i\alpha}, \eta_{i\alpha}\right]} \\ Z_0 = \int\prod_i D\left[\vec{\varphi_i}\right] e^{-S_o\left[\vec{\varphi_i}\right]} \end{cases} \tag{14}$$

$$\begin{cases} S\left[\overrightarrow{\varphi_i}, \bar{\eta}_{i\alpha}, \eta_{i\alpha}\right] = S_o\left[\overrightarrow{\varphi_i}\right] + S_1\left[\overrightarrow{\varphi_i}, \bar{\eta}_{i\alpha}, \eta_{i\alpha}\right] \\ S_o\left[\overrightarrow{\varphi_i}\right] = \int\limits_0^\beta d\tau \left\{ \sum\limits_{ij\lambda\gamma} \left(J^{-1}\right)_{ij}^{\lambda\gamma} \varphi_i^\lambda(\tau)\varphi_j^\gamma(\tau) \right\} \\ S_1\left[\overrightarrow{\varphi_i}, \bar{\eta}_{i\alpha}, \eta_{i\alpha}\right] = \int\limits_0^\beta d\tau \left\{ \sum\limits_{i\alpha} \bar{\eta}_{i\alpha}(\tau)\left(\partial_\tau - \mu\right)\eta_{i\alpha}(\tau) + \sum\limits_{i,\alpha,\lambda} \bar{\eta}_{i\alpha}(\tau)\tau_{\alpha\beta}^\lambda \eta_{i\beta}(\tau)\varphi_i^\lambda(\tau) \right\} \end{cases} \tag{15}$$

where τ is an imaginary time and $\vec{\varphi}_i$ stands for the auxiliary Bose field, which plays the role of the staggered magnetization. Then we perform integration over the Grassmann variables to get:

$$Z = \left(\frac{i}{\sqrt{3}}\right)^N \frac{1}{Z_0} \int D\left[\overrightarrow{\varphi_i}\right]\ e^{-S_{eff}[\vec{\varphi}_i]} \tag{16}$$

where the effective action $S_{eff}\left[\vec{\varphi}_i\right]$ is given by:

$$S_{eff}\left[\vec{\varphi}_i\right] = S_o\left[\vec{\varphi}_i\right] - \ln\det\hat{K}_i \tag{17}$$

The matrix K_i in the frequency representation reads:

$$\hat{K}_i\left(\omega_1, \omega_2\right) = \left(-i\omega_1 - \frac{i\pi}{3\beta}\right)\delta_{\omega_1,\omega_2}\hat{I} + \frac{1}{2}\vec{\tau}\vec{\varphi}_i\left(\omega_1 - \omega_2\right) \tag{18}$$

where $\hat{I}$ is (3x3) unit matrix.

Decomposing the matrix $\hat{K}$ into nonperturbation and perturbation parts:

$$\hat{K} = \hat{K}_o + \hat{M} \tag{19}$$

and expanding $Tr\left(\ln\hat{K}\right)$ in a Taylor series:

$$Tr\left(\ln\hat{K}\right) = Tr\left(\ln\hat{K}_o\right) + Tr\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\hat{K}_o^{-1}\hat{M}\right)^n \tag{20}$$

We can calculate the partition function in a given order of $\hat{M}$. The explicit forms of $\hat{K}_o$ and $\hat{M}$ depend on the way of decomposing the Hubbard Stratonovich auxilary field $\vec{\varphi}_i$. In the following we set:

$$\vec{\varphi}_i\left(\Omega\right) = \vec{\varphi}_{io}\left(\Omega = 0\right) + \delta\vec{\varphi}\left(\Omega\right) \tag{21}$$

where $\vec{\varphi}_{io}$ is the mean field part and $\delta\vec{\varphi}\left(\Omega\right)$ is the fluctuation part of the auxilary field $\vec{\varphi}_i\left(\Omega\right)$.

Substituting (21) in (18), the expression (19) gives:

$$\begin{aligned} \hat{K}_o &= \left(i\omega_1\hat{I} + \vec{\tau}\vec{\varphi}_{io}\right)\delta_{\omega_1\omega_2}\delta_{\mathrm{ij}} \\ \hat{M} &= \vec{\tau}\delta\vec{\varphi}_i\left(\omega_1 - \omega_2\right)\delta_{\mathrm{ij}} = \vec{\tau}\delta\vec{\varphi}_i\left(\Omega\right)\delta_{\mathrm{ij}} \end{aligned} \tag{22}$$

In order to calculate the sublattice magnetization we add a local magnetic field $\vec{B}_i$ to Hamiltonian (7) and let $\vec{B}_i = 0$ at the end of final calculations. Then at the one-loop approximation one derives the effective action as follows:

$$S_{eff} = S_{eff}^{(0)} + S_{eff}^{(1)} + S_{eff}^{(2)} \tag{23}$$

$$S_{eff}^{(0)} = \frac{1}{2}\sum_{ij\lambda\nu}\left(\varphi_{io}^\lambda + B_i^\lambda\right)\left(J^{-1}\right)_{ij}^{\lambda\nu}\left(\varphi_{jo}^\gamma + B_j^\nu\right) - \ln\det\hat{K}_o \tag{24}$$

$$S_{eff}^{(1)} = \frac{1}{2}\sum_{ij\lambda\nu}\left[\left(J^{-1}\right)_{ij}^{\lambda\nu}\left(\varphi_{io}^{\lambda}+B_i^{\lambda}\right)\delta\varphi_j^{\nu}(0)+\delta\varphi_i^{\lambda}(0)\left(\varphi_{jo}^{\nu}+B_j^{\nu}\right)\left(J^{-1}\right)_{ij}^{\lambda\nu}\right] - Tr\left(\hat{K}_o^{-1}\hat{M}\right) \tag{25}$$

$$S_{eff}^{(2)} = \frac{1}{2}\sum_{ij\lambda\gamma,\Omega}\left(J^{-1}\right)_{ij}^{\gamma\lambda}\delta\varphi_i^{\lambda}(-\Omega)\,\delta\varphi_j^{\gamma}(-\Omega)+\frac{1}{2}Tr\left(\hat{K}_o^{-1}\hat{M}\right)^2 \tag{26}$$

The mean field φ_{io}^{α} is chosen by minimizing the effective action in the application of the least action principle.

Setting $\delta\varphi_j^{\pm}(\omega) = \delta\varphi_j^{x}(\omega)\pm\delta\varphi_j^{y}(\omega)$, the partition function can be decomposed into a product of three terms:

$$Z = Z_{MF}.Z_{zz}.Z_{+-} \tag{27}$$

where Z_{MF} is the mean field contribution, Z_{zz} and Z_{+-} are the fluctuation contributions for the longitudinal part $\delta\varphi^{z}(\omega)$ and the transverse parts $\delta\varphi^{+}(\omega), \delta\varphi^{-}(\omega)$. Consequently, the free energy may be written in the following way:

$$F = F_{MF} + \delta F_{zz} + \delta F_{+-} \tag{28}$$

3. Mean field approximation

Minimizing the efective action according the least action principle, we derive the mean field equations for the auxiliary fields φ_{io}^{α} :

$$\left.\frac{\delta S_{\mathrm{eff}}}{\delta\varphi_i^{\alpha}}\right|_{\delta\varphi_i^{\alpha}=0} = 0 \tag{29}$$

From Eqs. (23) - (26) and (29) we get:

$$\sum_{\beta,j}\left(J^{-1}\right)_{ij}^{\alpha\beta}\left(\varphi_{jo}^{\beta}+B_j^{\beta}\right)\delta_{\Omega,0}+K_{1i}^{\alpha}(\Omega) = 0 \tag{30}$$

Where $K_{1i}^{\alpha}(\Omega)$ is defined as follows:

$$\sum_{i,\alpha,\Omega}K_{1i}^{\alpha}(\Omega)\,\delta\varphi_i^{\alpha}(\Omega) = -Tr\left(\hat{K}_0^{-1}\hat{M}\right) \tag{31}$$

From the definition of a magnetization per site i:

$$m_i^{\alpha} = -\frac{\partial F}{\partial B_i^{\alpha}} = -\frac{1}{\beta}\frac{\partial}{\partial B_i^{\alpha}}Z \tag{32}$$

one can find the relation between the local magnetization m_i^{α} and the auxiliary field φ_i^{α} . In particular, from (25) and (32), the mean field magnetization m_{io}^{α} related to the auxiliary field φ_{io} as follows:

$$\varphi_{io}^{\alpha}+B_i^{\alpha} = -\sum_{j\beta}m_{jo}^{\beta}J_{ji}^{\beta\alpha} \tag{33}$$

From (30) and (33), we obtain:

$$m_{io}^{\alpha} = K_{1i}^{\alpha} \tag{34}$$

Because we are working in the local coordinates with the classical magnetization pointing along the z-axis, thus, in the mean field approximation:

$$\begin{cases} m_{io}^{\alpha} = m_{io}\delta_{\alpha,z} \\ \varphi_{io}^{\alpha} = \varphi_{io}\delta_{\alpha,z} \end{cases} \tag{35}$$

Taking into account Eqs. (35), from (31) we get:

$$K_{1i}^{\alpha}(\Omega) = 2\sum_{i,\omega} \frac{\varphi_{io}}{(i\omega)^2 - \varphi_{io}^2}\delta_{\alpha,z}\delta_{\Omega,0} \tag{36}$$

For a Bravais lattice, all the sites are equivalent, so: $\varphi_{io} = \varphi_o; m_{io} = m_o$. The sum over the modified Matsubara frequencies can be carried out by the contour integration trick and gives:

$$K_{1i}^{\alpha}(\Omega) = \Delta(\varphi_o)\,\delta_{\alpha,z}\delta_{\Omega,0} \tag{37}$$

with $\Delta(\varphi_o)$ being:

$$\Delta(\varphi_o) = -\frac{2sh\beta\varphi_o}{1 + 2cosh\beta\varphi_o} \tag{38}$$

Together with Eqs. (33) and (34), it leads to the following equation for the mean-field magnetization:

$$m_o = \Delta(\lambda m_o) \tag{39}$$

where:

$$\lambda = -J\left(\vec{Q}\right) \tag{40}$$

Note that in the case of everage projection $(\mu = 0)$, the sum over the fermionic Matsubara frequencies in (36) gives:

$$K_{1i}^{\alpha}(\Omega) = -th\frac{\beta\varphi_o}{2} \tag{41}$$

Then instead of Eq. (39) one has:

$$\tilde{m}_o = -th\left(\frac{\beta\lambda\tilde{m}_o}{2}\right) \tag{42}$$

Accordingly the equations (39) and (42) result in different critical temperature:

$$\begin{array}{l} \text{exact-constraint} : T_C = \frac{2\lambda}{3} \\ \text{average-constraint} : \tilde{T}_C = \frac{\lambda}{2} \end{array} \tag{43}$$

From (43) we obtains: $\frac{T_C}{\tilde{T}_C} = \frac{4}{3}$ for $S = 1$, while for the case of $S = 1/2$ one has $\frac{T_C}{\tilde{T}_C} = 2$ [5-7]. In both cases of $S = 1/2$ and $S = 1$ the critical temperature for the case of exact constraint is higher than for average one. This is due to thermal fluctuations into unphysical spinless states in the case of global constraint, which reduce the magnetic moment. In the case of spin $S = 1/2$ the number of physical states in the Fock space of the auxiliary fermion $N_{ph} = 2$ (one particle states), while two states are unphysical (the vacuum and the two-particle states): $N_{un} = 2$. Assuming $T_C \sim \frac{1}{N_{ph}}; \tilde{T}_C \sim \frac{1}{N_{ph}+N_{un}}$, it results in the ratio $\frac{T_C}{\tilde{T}_C} = 2$ for $S = 1/2$. For the case of spin $S = 1$, two states are unphysical (the vacuum and the three-particle states): $N_{un} = 2$. Due to the particle-hole symmetry of the spin Hamiltonian the three one-particle and three two-particle states are physical: $N_{ph} = 6$. Thus, one has for the $S = 1$ case: $\frac{T_C}{\tilde{T}_C} = \frac{4}{3}$. However, at zero temperature both constraint methods give the same result:

$$\lim_{T\to 0K} m_o = \lim_{T\to 0K} \tilde{m}_o = 1 \tag{44}$$

Free energy in mean-field approximation can be expressed in terms of the magnetization in the following way, letting the fictive magnetic field $B = 0$:

For exact constraint $(\mu = i\pi/3\beta)$:

$$F_{MF} = \frac{N\lambda m_o^2}{2} - \frac{2}{\beta}\ln\left(2\cosh\beta\lambda \mathrm{m}_o + 1\right) \tag{45}$$

For global constraint $(\mu = 0)$:

$$F_{MF} = \frac{N\lambda \tilde{m}_o^2}{2} - \frac{2}{\beta}\ln\left(2\cosh\frac{\beta\lambda\tilde{\mathrm{m}}_o}{2}\right) \tag{46}$$

4. Fluctuation contributions

Due to the Eq. (30), the first order fluctuation contributions vanish: $S^{(1)}{}_{\mathrm{ef}f} = 0$. The effective action in the second order of fluctuation (26) may be rewriten in the form:

$$S^{(2)}_{\mathrm{ef}f} = \frac{1}{2}\sum_{\mathrm{ij}\alpha\beta} D^{\alpha\beta}_{ij}(\Omega)\delta\varphi^{\alpha}_{i}(-\Omega)\,\delta\varphi^{\beta}_{j}(\Omega) \tag{47}$$

where:

$$D^{\alpha\beta}_{ij}(\Omega) = \left(J^{-1}\right)^{\alpha\beta}_{ij}(\Omega) + K^{\alpha\beta}_{2ij}(\Omega) \tag{48}$$

In the local coordinates in the mean field approximation we have $\varphi^{\pm}_{io} = 0, \varphi^{z}_{io} = \varphi_o$ for every site i, therefore the kernel $K^{\alpha\beta}_{2ij}(\Omega)$ has only three nonzero components:

$$K^{zz}_{2ij}(\Omega) = \sum_{\omega}\sum_{k=-1}^{1}\frac{k^2}{(i\omega + k\varphi_o)(i\omega + \Omega + k\varphi_o)}\delta_{ij} \tag{49}$$

$$K^{+-}_{2ij}(\Omega) = \frac{1}{4}\sum_{\omega}\sum_{k=-1}^{0}\frac{2 - k(k+1)}{(i\omega + k\varphi_o)(i\omega + \Omega + (k+1)\varphi_o)}\delta_{ij} \tag{50}$$

$$K^{+-}_{2ij}(\Omega) = \frac{1}{4}\sum_{\omega}\sum_{k=0}^{1}\frac{2 - k(k-1)}{(i\omega + k\varphi_o)(i\omega + \Omega + (k-1)\varphi_o)}\delta_{ij} \tag{51}$$

Summing over the modified Matsubara frequencies, by mean of contour integration method,the above eqs give:

$$K^{zz}_{2ij}(\Omega) = -\frac{1}{3}\left(4 - 3\Delta^2(\varphi_o) - \sqrt{4 - 3\Delta^2(\varphi_o)}\right)\delta_{\Omega,0}\delta_{ij} \tag{52}$$

$$K^{+-}_{2ij}(\Omega) = \left(K^{+-}_{2ij}\right)^{*}(\Omega) = \frac{\beta}{2}\frac{\Delta(\varphi_o)}{\varphi_o + i\Omega}\delta_{ij} \tag{53}$$

The fluctuation corrections to the partition function Zfl are quadratic in the field variable $\delta\varphi^{+}_{i}, \delta\varphi^{-}_{i}, \delta\varphi^{z}_{i}$ and can be carried out:

$$Z_{fl} = \int D\left[\delta\vec{\varphi}\right]e^{-S_{\mathrm{ef}f}[\delta\vec{\varphi}]} = \left[\det\hat{D}_{ij}\right]^{-1/2} = Z_o\left[\det\left(\hat{I} + \hat{J}_{ij}\hat{K}_{2\mathrm{ij}}\right)\right]^{-1/2} \tag{54}$$

The components of the exchange matrix $\hat{J}_{ij}$ may be given in the terms of X_{ij}, Y_{ij}, W_{ij} as follows:

$$\begin{cases} J_{ij}^{++} = J_{ij}^{--} = X_{ij} - Y_{ij} \\ J_{ij}^{+-} = J_{ij}^{-+} = X_{ij} + Y_{ij} \\ J_{ij}^{zz} = X_{ij} \\ J_{ij}^{+z} = J_{ij}^{-z} = -J_{ij}^{z+} = -J_{ij}^{z-} = -W_{ij} \end{cases} \tag{55}$$

After Fourier the components of the exchange interaction in (55) read:

$$\begin{cases} X(\vec{p}) = -\frac{1}{2}\left(J\left(\vec{p}-\vec{Q}\right) + J\left(\vec{p}+\vec{Q}\right)\right) \\ Y(\vec{p}) = -J(\vec{p}) \\ W(\vec{p}) = -\frac{1}{2}\left(J\left(\vec{p}+\vec{Q}\right) - J\left(\vec{p}-\vec{Q}\right)\right) \end{cases} \tag{56}$$

From the Eqs. (52) (54) and (56) we obtain the fluctuation contributions to the free energy:

$$\delta F_{zz} = \frac{1}{2\beta} \sum_{\vec{p}\in BZ} \ln A(\vec{p}) \tag{57}$$

$$\delta F_{+-} = \frac{1}{\beta} \sum_{\vec{p}\in BZ} \ln \frac{\mathrm{sh}\frac{\beta E(\vec{p})}{2}}{\mathrm{sh}\frac{\beta|\varphi_0|}{2}} \tag{58}$$

where:

$$A(\vec{p}) = 1 + X(\vec{p}) K_2^{zz} + \frac{m_o K_2^{zz} W^2(\vec{p})}{\varphi_o + m_o X(\vec{p})} \tag{59}$$

$$E(\vec{p}) = \sqrt{(\varphi_o + m_o X(\vec{p}))(\varphi_o + m_o Y(\vec{p}))} \tag{60}$$

In the Eqs. (59) (60), the mean field auxiliary field φ_o in the presence of the fictive magnetic field B is related to the magnetization mo as follows:

$$\varphi_o = -B - \lambda(m_o + B\Delta m_o) \tag{61}$$

where:

$$\Delta m_o = -\frac{\beta K_2^{zz}(-\lambda m_o)}{1 + \beta\lambda K_2^{zz}(-\lambda m_o)} \tag{62}$$

Taking the derivative of the free energy (57) (58) with respect to the fictive magnetic field, we obtain the fluctuation contributions to the longitudinal δm_{zz} and transerve δm_{+-} parts for the magnetization as follows:

$$\delta m^{zz} = -\frac{1}{2N} \sum_{\vec{p}\in BZ} \frac{B_o(\vec{p})}{A_o(\vec{p})} \tag{63}$$

$$\delta m^{zz} = -\frac{1}{2N} \sum_{\vec{p}\in BZ} \frac{B_o(\vec{p})}{A_o(\vec{p})} \tag{64}$$

where:

$$A_o(\vec{p}) = 1 + \beta C_o \left(X(\vec{p}) + \frac{W^2(\vec{p})}{X(\vec{p}) - \lambda}\right) \tag{65}$$

$$B_o(\vec{p}) = \beta \left(X(\vec{p}) + \frac{W^2(\vec{p})}{X(\vec{p}) - \lambda}\right) D_o + \beta \frac{W^2(\vec{p}) C_o}{m_o(\lambda - X(\vec{p}))^2} \tag{66}$$

C_o and D_o is given by:

$$C_o = -\frac{1}{3}\left(4 - 3m_o^2 - \sqrt{4 - 3m_o^2}\right) \tag{67}$$

$$D_o = m_o \Delta m_o \left(2 - \frac{1}{\sqrt{4 - 3m_o^2}}\right) \tag{68}$$

The magnon energy reads:

$$\begin{cases} E(\vec{p}) = \lambda m_0 \omega(\vec{p}) \\ \omega^2(\vec{p}) = \left(1 - \frac{X(\vec{p})}{\lambda}\right)\left(1 - \frac{Y(\vec{p})}{\lambda}\right) \end{cases} \tag{69}$$

When the single occupancy condition is disregarded the following replacement should be done on the equations from (57) to (69):

$$\begin{cases} m_o \to \tilde{m}_o \\ K_2^{zz} \to \tilde{K}_2^{zz} = -\frac{1}{2}\left(1 - \tilde{m}_o^2\right) \end{cases} \tag{70}$$

Using the following relations:

$$U = \left(\frac{\partial \beta F}{\partial \beta}\right) \tag{71}$$

$$C_v = -\beta^2 \left(2\frac{\partial F}{\partial \beta} + \beta \frac{\partial^2 F}{\partial \beta^2}\right) \tag{72}$$

it is straightforward to derive explicit expressions for internal energy U and specific heat C_v from the Eqs. (45), (57), (58), putting the fictive magnetic field $B = 0$.

5. Conclusions and Discussions

In this paper we have obtained the explicit expressions for the free energy of antiferromagnetic Heisenberg model with $S = 1$ on a Bravais lattice by means of Popov-Fedotov formalism. Working in a local coordinates and parametrizing a magnetically ordered phase by a magnetic ordering vector $\vec{Q}$, we have derived the general equations of a sublattice magnetization and free energy in unique forms for any Bravais lattice and any magnetically ordered state. For a particular model, one need to find the ordering vectors $\vec{Q}$, the quantities $X(\vec{p}), Y(\vec{p}), W(\vec{p})$ and then one can apply directly the Eqs.(45), (57), (58). It is easy to check that at zero temperature limit it does not matter whether the constraint is treated exactly or average. The magnetization and the free energy are the same, as for the case $S = 1/2$. However, at finite temperature the exact local constraint gives a significant effect. As an example we consider the antiferromagnetic Heisenberg model on D-dimensional hypercubic and triangular lattice with nearest - neighbour bonds.

The Fourier transform of the exchange interactions are given respectively as follows:

$$J_{HC}(\vec{p}) = 2J \sum_{k=1}^{D} \cos \vec{p}_x \tag{73}$$

$$J_{TRL}(\vec{p}) = 2J \left(\cos \vec{p}_x + 2\cos\frac{\vec{p}_x}{2}\cos\frac{\sqrt{3}}{2}\vec{p}_y\right) \tag{74}$$

Minimizing $J_{HC}(\vec{p})$ and $J_{TRL}(\vec{p})$ with respect to $\vec{p}$, we find that the classical state is described by ordering vectors $Q_{HC} = (\pi, \pi)$ for the D-dimensional hypercubic lattice and $Q_{TRL} = 2\pi\left(\frac{1}{3}, \frac{1}{\sqrt{3}}\right)$ for the triangular lattice. According to the Eqs. (40) and (56), we obtain:

For the hypercubic lattice:

$$\begin{cases} \lambda_{HC} = 2JD \\ X_{HC}(\vec{p}) = -Y_{HC}(\vec{p}) = J_{HC}(\vec{p}) \end{cases} \tag{75}$$

For the triangular lattice:

$$\begin{cases} \lambda_{TRL} = 3J \\ X_{TRL}(\vec{p}) = -\frac{1}{2}Y_{TRL}(\vec{p}) = \frac{3}{2}J(\vec{p}) \end{cases} \tag{76}$$

Subtituting Eqs. (75) and (76) in the Eqs. in Section III, we obtain the magnetization and the free energy for Neel state in the hypercubic lattice and for 120° spin structure in the triangular lattice, taking into account the local constraint condition in one loop approximation. The obtained expressions have a similar structure as for the case $S = 1/2$ [5-7]. Taking limit of zero temperature $T \to 0K$ for the obtained equations, we get the same ground state energy and sublattice magnetization derived in linear spin wave approximation by means of Holstein Primakov representation [7].

The results of this report could be applied for investigating anisotropic Heisenberg models beyond a nearest-neighbour bonds. It would be also interesting to extend the above results for the case of arbitrary quantum spin number S and for a non-Bravais lattice. It is left for a future.

Acknowledgment
This work was financially supported by the National Foundation for Science and Technology Development (NAFOSTED) of Vietnam under Grant No 103.01- 2014.23.

References

[1] Auerbach 1994, *"Interacting electrons and quantum magnetism",* Springer Verlag
[2] Popov N and Fedotov S A 1988, *Sov. Phys. JETP* **67** 535
[3] Veits O et al 1994, *J. France* **4** 493
[4] Tejima S and Oguchi A 1995, *J. Phys. Soc. Jpn.* **64** 4923
[5] Azakov S, Dilaver M and Oztas 2000, *Int. J. Mod. Phys.* B **14** 13
[6] Dillenschneider R and Richert J 2006, *Eur. Phys. J.* B **49** 187
[7] Pham Thi Thanh Nga and Nguyen Toan Thang 2012, *Comm. in Phys.* **22** 33 (2012),*Comm. in Phys.* **22** 383 (2012) Erratum
[8] Haldane F D 1983, *Phys. Rev. Lett.* **50** 1153
[9] Misguich G and Lhuillier C 2015, in *"Frustrated Spin Systems"*, Ed. by H. T. Diep, World Scientific Singapore, p.299
[10] Miyake S J 1992, *J. Phys. Soc. Jpn.* **91** 938