

NÉEL STATE IN THE FERMIONIZED SPIN $\frac{1}{2}$ HEISENBERG ANTIFERROMAGNET ON HYPERCUBIC AND TRIANGULAR LATTICES

PHAM THI THANH NGA

Water Resources University, 175 Tay Son, Hanoi

NGUYEN TOAN THANG

Institute of Physics, VAST

Abstract. *We study the Néel state of the spin $\frac{1}{2}$ Heisenberg antiferromagnet model on hypercubic and triangular lattices, employing an auxiliary fermion representation for spin operators with Popov-Fedotov trick. The unphysical states are eliminated on each site by introducing an imaginary chemical potential. Working in local coordinate systems we obtain the free energy and the sublattice magnetization for both lattices in an unified manner. We show that exact treatment of the single occupancy constraint gives a significant effect at finite temperatures.*

I. INTRODUCTION

The fundamental problem in the theoretical investigation of spin systems is that spin operators satisfy neither Bose nor Fermi commutation relations, so one cannot use Wick's theorem to construct a standard many body techniques. In order to avoid this difficulty various approaches to the study of spin systems have been suggested. One of the approaches is based upon representing operators in term of Bose or Fermi spin operators [1-2]. However, introduction of the auxiliary Bose or Fermi operators enlarges the Hilbert space in which these operators are acting. As a result, the unphysical states appear and should be excluded. In order to exclude these states one has to impose the constraint on bilinear combinations of Fermi or Bose operators. For example, for spin $S = \frac{1}{2}$ the fermi operators introduce the spurious double occupied and empty states which must be freed out. Unfortunately in general it is very difficult to take the constraint exactly into account and usually the local constraint is replaced with the global one, where the number of states is fixed only on an average for the whole system instead of being fixed on each site. It is not clear whether such an approximation is a good starting point for the investigation of the spin systems. In 1988, Popov and Fedotov [4] proposed an alternative approach for spin $\frac{1}{2}$ and spin equal 1 Hamiltonian free from local constraint difficulty. Based on the exact fermionic representation for spin operators, the Popov-Fedotov approach enables one to enforce the auxiliary-particle constraint on each site independently by introducing purely imaginary chemical potential. The auxiliary-particle representation used by Popov-Fedotov is neither fermionic nor bosonic and is called semionic representation. The Popov-Fedotov trick has been developed for arbitrary values of spin S [5] and for the systems out of the equilibrium [6]. The semionic representation of spin operators

has been applied successfully to various problems: ferromagnetic [7] and antiferromagnetic [8-10] Heisenberg model in hypercubic lattice; negative $-U$ Hubbard model [11]; antiferromagnetic Kondo lattices [12]; spin glass model [13]; nanostructure [14]... In this work, we consider the Néel state in the spin $\frac{1}{2}$ Heisenberg antiferromagnet model on hypercubic and triangular lattices in an unified manner using the Popov-Fedotov approach. Spin $\frac{1}{2}$ triangular lattice Heisenberg antiferromagnets (TLHAF) give rise to many interesting phenomena originating from the low dimensionality and geometric frustration. Experimentally, Cs_2CuBr_4 [15], Cs_2CuCl_4 [16] and $K - (BEDT - TTF)_2Cu_2(CN)_3$ [17] have been actively studied as spin $\frac{1}{2}$ TLHAFs. Recently, Y. Shirata et al reported the results of magnetization and specific heat measurement on $Ba_3CoSb_2O_9$ and demonstrated that spin $\frac{1}{2}$ TLHAF has been realized in $Ba_3CoSb_2O_9$ [18]. Many theories are applied to investigate the physics of spin $\frac{1}{2}$ TLHAF: spin wave theory [19-21]; coupled cluster method [22] and exact diagonalization [23]. However, experimental verification of the theoretical results has not been conducted at quantitative level because the above substances are not regular but distorted, so the exchange interaction is spatially anisotropic. The outline of the paper is as follows. In Sec. II we describe the model Hamiltonian and the Popov-Fedotov method. In Sec. III we consider mean field approximation. Quantum fluctuations around a classical ground state are treated in Sec. IV. The conclusions are presented in Sec. V.

II. MODEL HAMILTONIAN AND FORMALISM

An isotropic Heisenberg antiferromagnetic on hypercubic and triangular lattices considered in the following is given by the Hamiltonian:

$$H = \frac{J}{2} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (1)$$

The sum covers all nearest neighbor pairs $\langle ij \rangle$. The starting point for evaluating the fluctuations is a classical ground state of (1). For a hypercubic lattice antiferromagnet consists two sublattice called A and B , one spin-up and the other spin-down. For a triangular lattice, the classical ground state is three sublattice Néel state with an angle of 120° between the spins of different sublattice called A, B and C . In order to introduce only one type of auxiliary particle we perform a transformation to change the Néel configuration into a ferromagnetic state in each sublattice. We define the local spatially varying coordinates $Ox'y'z'$ with Oz' pointing along the local classical Néel direction, the direction of y' -axis is invariable. Accordingly, the Hamiltonian (1) in the new local coordinates is expressed in a form:

$$H = \frac{J}{2} \sum_{\langle ij \rangle} \left\{ S_i^y S_j^y + \cos(\theta_i - \theta_j) (S_i^x S_j^x + S_i^z S_j^z) + \sin(\theta_i - \theta_j) (S_i^z S_j^x + S_i^x S_j^z) \right\} \quad (2)$$

The Hamiltonian (2) can be written in the following form, which is convenient for the

Popov-Fedotov method:

$$H = -\frac{1}{2} \sum_{ij;\alpha\beta} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta \quad (3)$$

where:

$$\begin{cases} J_{ij}^{xy} = J_{ij}^{yx} = J_{ij}^{yz} = J_{ij}^{zy} = 0 \\ J_{ij}^{xz} = -J_{ij}^{zx} = J \sin(\theta_i - \theta_j) \\ J_{ij}^{xx} = J_{ij}^{zz} = J \cos(\theta_i - \theta_j) \\ J_{ij}^{yy} = -J \end{cases} \quad (4)$$

For a hypercubic lattice $\cos(\theta_i - \theta_j) = 1$, $\sin(\theta_i - \theta_j) = 0$ while for a triangular lattice $\cos(\theta_i - \theta_j) = 1/2$, $\sin(\theta_i - \theta_j) = \pm\frac{\sqrt{3}}{2}$. Therefore we can express the coupling matrix $J_{ij}^{\alpha\beta}$ in an unified way for both hypercubic and triangular lattice: $\cos(\theta_i - \theta_j) = \alpha$, $\sin(\theta_i - \theta_j) = \pm\sqrt{1-\alpha^2}$ with $\alpha = 1$ for the hypercubic lattice and $\alpha = 1/2$ for the triangular lattice. The non-canonical commutation relations of spin operator \mathbf{S} poses a great difficulty for an analytical approach to the Hamiltonian (3) because the Wick's theorem and standard perturbation techniques cannot be applied. Following Popov-Fedotov [4] we represent the spin $\frac{1}{2}$ operators as bilinear combination of auxiliary Fermi operators as follows:

$$S_i^\alpha = \frac{1}{2} \sum_{\sigma,\sigma'} a_{i\sigma}^\dagger \sigma_{\sigma\sigma'}^\alpha a_{i\sigma'} \quad (5)$$

$\sigma \equiv (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices, and $\sigma, \sigma' = \uparrow, \downarrow$ is the spin index. Hereafter we let $\hbar = 1$. The Pauli principle allows the number of auxiliary fermion at each site i to be 0, 1, 2 so the Fock state of the auxiliary fermion $a_{i\sigma}$ is spanned by four states: two physical states: $|\uparrow\rangle = a_{i\uparrow}^\dagger |0\rangle$; $|\downarrow\rangle = a_{i\downarrow}^\dagger |0\rangle$ and two unphysical states: $|0\rangle$; $|2\rangle = a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger |0\rangle$ where $|0\rangle$ is the vacuum $a_{i\sigma} |0\rangle = 0$. The unphysical states have to be eliminated with the aid of the constraint:

$$\hat{N}_i = \sum_{\sigma} a_{i\sigma}^\dagger a_{i\sigma} = 1 \quad (6)$$

The constraint (6) has to be enforced on each site independently and is done by introducing the projection operator $\hat{P} = \frac{1}{i^N} e^{i\frac{\pi}{2}\hat{N}}$, where $\hat{N} = \sum_{i,\sigma} a_{i\sigma}^\dagger a_{i\sigma}$ to the partition function:

$$Z = Tr \left[e^{-\beta\hat{H}} \hat{P} \right] \quad (7)$$

H is the Hamiltonian (3), written in terms of the fermions operators (5). The contributions of the unphysical states to the partition function automatically cancel out one with other because the trace over the unphysical states of each site vanishes:

$$Tr_{unphys} \left[e^{-\beta(\hat{H} - \frac{i\pi}{2\beta}\hat{N})} \right] = (-i)^0 + (-i)^2 = 0 \quad (8)$$

Therefore, the partition function describing the Hamilton (1) with strictly one spin per lattice site reads:

$$Z = \frac{1}{i^N} Tr \left[e^{-\beta(\hat{H} - \mu\hat{N})} \right] \quad (9)$$

where N denotes the number of sites. The constraint (6) is enforced by means of the purely imaginary Lagrange multipliers $\mu = \frac{i\pi}{2\beta}$ playing the role of imaginary chemical potentials of fermions. As a result, the fermionic Matsubara frequencies are modified as follows:

$$\tilde{\omega}_F = \omega_F - \frac{\pi}{2\beta} = \frac{2\pi}{\beta} \left(n + \frac{1}{4} \right) \quad (10)$$

III. MEAN FIELD APPROXIMATION

In order to get rid off the 4-fermion terms in the partition function (9) we perform a Hubbard-Stratonovich transformation and introduce of the Bose auxiliary fields φ_i :

$$e^{\frac{1}{2} \int_0^\beta d\tau \sum_{ij\alpha\beta} J_{ij}^{\alpha\beta} S_i^\alpha(\tau) S_j^\beta(\tau)} = \frac{1}{Z_0} \int [\mathcal{D}\varphi] e^{-\int_0^\beta d\tau \left\{ \frac{1}{2} \sum_{ij\alpha\beta} (J^{-1})_{ij}^{\alpha\beta} \varphi_i^\alpha(\tau) \varphi_j^\beta(\tau) + 2 \sum_{i\alpha} S_i^\alpha \varphi_i^\alpha \right\}} \quad (11)$$

where:

$$Z_0 = \int_{\varphi(\beta)=\varphi(0)} [\mathcal{D}\varphi] e^{-\int_0^\beta d\tau S_0[\varphi(\tau)]} \quad (12)$$

and:

$$S_0[\varphi] = \frac{1}{2} \sum_{ij\alpha\beta} (J^{-1})_{ij}^{\alpha\beta} \varphi_i^\alpha \varphi_j^\beta \quad (13)$$

In the equation (11) and (13) $(J^{-1})_{ij}^{\alpha\beta}$ denotes the inverse of the coupling matrix $J_{ij}^{\alpha\beta}$. Starting from (9), this leads to:

$$Z = \frac{1}{Z_0} \frac{1}{i^N} \int [\mathcal{D}\varphi] [\mathcal{D}\eta] e^{-\int_0^\beta S[\varphi(\tau), \eta(\tau)] d\tau} \quad (14)$$

where

$$S[\varphi(\tau), \eta(\tau)] = S_0[\varphi] + S_1[\varphi, \eta] \quad (15)$$

$$S_1[\varphi, \eta] = \sum \eta_{i\sigma}^*(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) \eta_{i\sigma}(\tau) + \frac{1}{2} \sum_{i\alpha\sigma\sigma'} \eta_{i\sigma}^*(\tau) \sigma_{\sigma\sigma'}^\alpha \eta_{i\sigma'}(\tau) \varphi_i^\alpha \quad (16)$$

and $\eta_{i\sigma}^*$, $\eta_{i\sigma}$ stand for the Grassmann variables. After integration over the bilinear Grassmann variables the partition function (14) becomes:

$$Z = \frac{1}{i^N} \frac{1}{Z_0} \int_{\varphi(\beta)=\varphi(0)} [\mathcal{D}\varphi] e^{-S_{eff}[\varphi]} \quad (17)$$

where the effective action $S_{eff}[\varphi]$ is given by

$$S_{eff}[\varphi] = \int_0^\beta S_0[\varphi] d\tau - \ln \det \beta \hat{K} \quad (18)$$

The matrix \hat{K} reads:

$$\hat{K}_i(\omega_{n_1} - \omega_{n_2}) = \begin{pmatrix} i\omega_{n_1} \delta_{n_1, n_2} + \frac{1}{2}\varphi_i^z(\omega_{n_1} - \omega_{n_2}) & \frac{1}{2}\varphi_i^x(\omega_{n_1} - \omega_{n_2}) - i\varphi_i^y(\omega_{n_1} - \omega_{n_2}) \\ \frac{1}{2}\varphi_i^x(\omega_{n_1} - \omega_{n_2}) + i\varphi_i^y(\omega_{n_1} - \omega_{n_2}) & i\omega_{n_2} \delta_{n_1, n_2} - \frac{1}{2}\varphi_i^z(\omega_{n_1} - \omega_{n_2}) \end{pmatrix} \quad (19)$$

$\omega_{n_1}, \omega_{n_2}$ refer to modified fermionic Matsubara frequencies defined in (10). \widehat{K}_i can be written in the form:

$$\widehat{K}_i = \widehat{K}_{io} + \widehat{M}_i \quad (20)$$

where

$$\widehat{K}_{io}(\omega_1, \omega_2) = \begin{pmatrix} i\omega_{n_1} + \frac{1}{2}\varphi_{io}^z & \frac{1}{2}\varphi_{io}^- \\ \frac{1}{2}\varphi_{io}^+ & i\omega_{n_2} - \frac{1}{2}\varphi_{io}^z \end{pmatrix} \delta_{n_1, n_2} \quad (21)$$

$$\widehat{M}_i = \frac{1}{2} \begin{pmatrix} \delta\varphi_i^z(\omega_{n_1} - \omega_{n_2})\delta\varphi_i^-(\omega_{n_1} - \omega_{n_2}) \\ \delta\varphi_i^+(\omega_{n_1} - \omega_{n_2}) - \delta\varphi_i^z(\omega_{n_1} - \omega_{n_2}) \end{pmatrix} \quad (22)$$

with

$$\delta\varphi_i(\omega_{n_1} - \omega_{n_2}) = \varphi_i(\omega_{n_1} - \omega_{n_2}) - \varphi_i(0) \quad (23)$$

and

$$\delta\varphi_i^\pm(\omega) = \delta\varphi_i^x(\omega) \pm i\delta\varphi_i^y(\omega) \quad (24)$$

Then the second term in the effective action (18) can be developed into a series:

$$\ln \det \beta \widehat{K}_i = Tr \ln \widehat{K}_{io} + Tr \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \left(\widehat{K}_{io}^{-1} \widehat{M}_i \right)^n \quad (25)$$

From (17) and (24), at the one loop approximation one obtains the effective action as follows:

$$\begin{aligned} S_{eff} &= \frac{\beta}{2} \sum_{\Omega_n} \bar{\Phi}_o \hat{A}_{ij}(\Omega_n) \Phi_o - Tr \ln K_o \\ &+ \frac{\beta}{2} \sum_{ij, \Omega_n} \left\{ \bar{\Phi}_{io} \hat{C}_{ij}(\Omega_n) \delta\Phi_j(\Omega_n) + \delta\bar{\Phi}_i(-\Omega_n) \hat{C}_{ij}(\Omega_n) \Phi_{jo} \right\} \end{aligned} \quad (26)$$

where

$$\hat{A}_{ij}(\Omega_n) = \delta_{\Omega_n, 0} (\hat{J}^{-1})_{ij} \quad (27)$$

$$\hat{C}_{ij}(\Omega_n) = \delta_{\Omega_n, 0} (\hat{J}^{-1})_{ij} + \frac{2}{\beta} \hat{K}_{i1} \delta_{ij} \delta_{\Omega_n, 0} \quad (28)$$

$$\hat{D}_{ij}(\Omega_n) = \delta_{\Omega_n, 0} (\hat{J}^{-1})_{ij} + \frac{1}{\beta} \hat{K}_{i2} \delta_{ij} \delta_{\Omega_n, 0} \quad (29)$$

The matrix \widehat{K}_{i1} is given by:

$$\widehat{K}_{i1} = -\frac{1}{4} \frac{\beta}{|\varphi_{io}|} \tanh \frac{\beta|\varphi_{io}|}{2} \hat{I} \quad (30)$$

while the matrix \widehat{K}_{i2} has the following components:

$$K_{i2}^{--} = \frac{1}{16} (\varphi_{io}^+)^2 Q_{i\Omega} \quad (31)$$

$$K_{i2}^{++} = \frac{1}{16} (\varphi_{io}^-)^2 Q_{i\Omega} \quad (32)$$

$$K_{i2}^{zz} = \frac{1}{8} \left[\left((\varphi_{io}^z)^2 - (\varphi_{io}^+) (\varphi_{io}^-) \right) Q_{i\Omega} - 4P_{i\Omega} \right] \quad (33)$$

$$K_{i2}^{-+} = -\frac{1}{16} \left[(\varphi_{io}^z)^2 (\varphi_{io}^z + 2i\Omega) Q_{i\Omega} + P_{i\Omega} \right] \quad (34)$$

$$K_{i2}^{+-} = -\frac{1}{16} \left[(\varphi_{io}^z)^2 (\varphi_{io}^z - 2i\Omega) Q_{i\Omega} + P_{i\Omega} \right] \quad (35)$$

$$K_{i2}^{z+} = \frac{1}{8} \sum_{i,\Omega} [\varphi_{io}^- (\varphi_{io}^z + i\Omega)] Q_{i\Omega} \quad (36)$$

$$K_{i2}^{+z} = \frac{1}{8} \sum_{i,\Omega} [\varphi_{io}^- (\varphi_{io}^z - i\Omega)] Q_{i\Omega} \quad (37)$$

$$K_{i2}^{z-} = \frac{1}{8} \sum_{i,\Omega} [\varphi_{io}^+ (\varphi_{io}^z - i\Omega)] Q_{i\Omega} \quad (38)$$

$$K_{i2}^{-z} = \frac{1}{8} \sum_{i,\Omega} [\varphi_{io}^+ (\varphi_{io}^z + i\Omega)] Q_{i\Omega} \quad (39)$$

We use the following notations in the above expressions:

$$Q_{i,\Omega \neq 0} = \frac{2\beta}{|\varphi_{io}| (\varphi_{io}^2 + \Omega^2)} \tanh \frac{\beta |\varphi_{io}|}{2} \quad (40)$$

$$Q_{i,\Omega=0} = \frac{2\beta}{|\varphi_{io}|^3} \tanh \frac{\beta |\varphi_{io}|}{2} - \frac{\beta^3}{\varphi_{io}^2} \frac{1}{\cosh^2 \frac{\beta \varphi_{io}}{2}} \quad (41)$$

$$P_{i,\Omega \neq 0} = \frac{\varphi_{io}^2}{4} Q_{i,\Omega \neq 0} \quad (42)$$

$$P_{i,\Omega=0} = -\frac{\varphi_{io}^2}{4} Q_{i,\Omega=0} + \frac{\beta}{|\varphi_{io}|} \tanh \frac{\beta |\varphi_{io}|}{2} \quad (43)$$

We also introduce the three component spinors:

$$\left\{ \begin{array}{l} \Phi_{io} = \begin{pmatrix} \varphi_{io}^+ \\ \varphi_{io}^- \\ \varphi_{io}^z \end{pmatrix}; \quad \bar{\Phi}_{io} = (\varphi_{io}^+, \varphi_{io}^-, \varphi_{io}^z) \\ \delta\Phi_i = \begin{pmatrix} \delta\varphi_i^+ \\ \delta\varphi_i^- \\ \delta\varphi_i^z \end{pmatrix}; \quad \delta\bar{\Phi}_i = (\delta\varphi_i^+, \delta\varphi_i^-, \delta\varphi_i^z) \end{array} \right. \quad (44)$$

The mean field equation for the auxiliary field φ_{io} can be derived by minimizing the effective action in the application of the least action principle:

$$\frac{\delta S_{eff}}{\delta \Phi_k(\Omega)} \Big|_{\delta\Phi_i = \delta\bar{\Phi}_i = 0 \forall i} = \frac{\delta S_{eff}}{\delta \bar{\Phi}_k(-\Omega)} \Big|_{\delta\Phi_i = \delta\bar{\Phi}_i = 0 \forall i} = 0 \quad (45)$$

From (28) and (44) one obtains:

$$\sum_j (\hat{J}^{-1})_{ij} \Phi_{jo} = \frac{\Phi_{io}}{2|\varphi_{io}|} \tanh \frac{\beta |\varphi_{io}|}{2} \quad (46)$$

In order to relate the auxiliary field φ_i to the local magnetization \mathbf{m}_i , we add the source term $\sum_i \lambda_i^\alpha S_i^\alpha(\tau)$ to the Hamiltonian (1). The sublattice magnetization is given by following:

$$\mathbf{m}_i^\alpha = \langle \mathbf{S}_i^\alpha \rangle = -\frac{1}{\beta} \frac{\partial \ln Z(\lambda)}{\partial \lambda_i^\alpha} \Big|_{\lambda_k=0 \forall k} \quad (47)$$

which leads to the relation:

$$\langle \varphi_k^\nu \rangle = \sum_{i,\alpha} (J)_{ki}^{\nu\alpha} \mathbf{m}_i^\alpha \quad (48)$$

Because we are working in the local coordinates with $\mathbf{e}_{i\alpha}$ pointing along the sublattice classical magnetization in the mean-field approximation $\mathbf{m}_{i\alpha} = m_{i\alpha} \mathbf{e}_z$ and $\varphi_{i\alpha} = \varphi_{i\alpha} \mathbf{e}_z$. Combining (45) and (47) the mean-field equation of the magnetization $m_{i\alpha}$ is given by

$$m_{i\alpha} = \frac{1}{2} \tanh \frac{\beta \sum_{ij} (\hat{J})_{ij}^{zz} m_{j\alpha}}{2} \quad (49)$$

In the absence of the external magnetic field all the sublattices are equivalent so $m_{A\alpha} = m_{B\alpha} = m_\alpha$ for the hypercubic lattice and $m_{A\alpha} = m_{B\alpha} = m_{C\alpha} = m_\alpha$ for the triangular lattice. Inserting $(J)_{ij}^{zz} = \alpha J$, from (48) one gets:

$$m_\alpha = \frac{1}{2} \tanh \frac{3J\beta m_\alpha}{2} \quad (50)$$

with z being the coordination number of the lattice. ($z = 2D$ for the D -dimensional hypercubic lattice and $z = 6$ for the triangular lattice). For average projection, with $\mu = 0$, we find on a similar procedure:

$$m_\alpha = \frac{1}{2} \tanh \frac{z\alpha J\beta m_\alpha}{4} \quad (51)$$

Putting $\alpha = 1$ and $z = 2D$ for the D -dimensional hypercubic lattice we recover the results obtained by the other authors [8, 9, 10, 24] while for $\alpha = 1/2$ and $z = 6$ we obtain the results for the triangular lattice. From (49) the phase transition temperature T_C reads:

$$k_B T_C = \frac{z\alpha J}{4} \quad (52)$$

which is twice larger than the Néel temperature obtained in the case of average projection. The temperature dependence of the sublattice magnetization have been calculated by solving the equations (49) and (50). The results are shown in Fig.1. One can see that the exact constraint treatment changes sizably the finite temperature results. This is due to thermal fermion number fluctuations into unphysical states, which are reduced in exact projection.

IV. FLUCTUATION CORRECTIONS

In the local coordinates in the mean-field approximation we have $\varphi_{i\alpha}^\pm = 0$ and $\varphi_{i\alpha}^z = \varphi_\alpha$ for every site i , therefore the matrix \hat{K}_{i2} (30)-(38) has only two nonzero components:

$$K_{i2}^{+-} = (K_{i2}^{-+})^* = -\frac{\beta}{4} \frac{1}{(\varphi_{i\alpha} + i\Omega)} \tanh \frac{\beta\varphi_\alpha}{2} \quad (53)$$

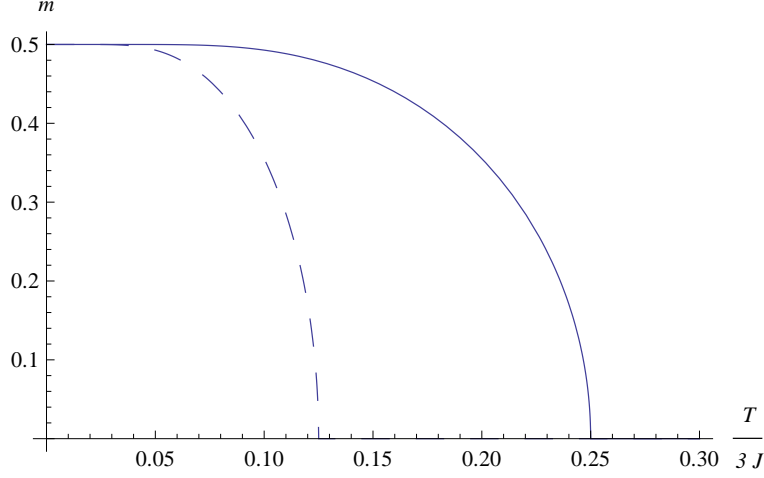


Fig. 1. Temperature dependence of magnetization. Full line: exact projection. Dotted line: average projection.

After the Fourier transform the last term of the effective action (25) reads:

$$S_{eff}^{(2)} = \frac{\beta}{2} \sum_{\mathbf{p}, \Omega} \delta\bar{\Phi}(-\mathbf{p}, -\Omega) \hat{D}(\mathbf{p}, \Omega) \delta\Phi(\mathbf{p}, \Omega) \quad (54)$$

where the kernel $\hat{D}(\mathbf{p}, \Omega)$ is given by:

$$\hat{D}(\mathbf{p}, \Omega) = \hat{J}^{-1}(\mathbf{p}) + \frac{1}{\beta} \hat{K}_2(\Omega) \quad (55)$$

Here we have:

$$\hat{K}_2(\Omega) = \begin{pmatrix} 0 & K_2^{+-}(\Omega) & 0 \\ K_2^{-+}(\Omega) & 0 & 0 \\ 0 & 0 & K_2^{zz} \end{pmatrix} \quad (56)$$

with:

$$K_2^{+-}(\Omega) = K_2^{-+}(\Omega) = -\frac{m_o}{2(\alpha z J m_o + i\Omega)} \quad (57)$$

$$K_2^{zz} = -\frac{\beta}{4} (1 - 4m_o^2) \quad (58)$$

From (4) the inverse of the coupling matrix $\hat{J}^{-1}(\mathbf{p})$ in the momentum representation is defined as follows:

$$(J^{-1}(\mathbf{p}))^{++} = (J^{-1}(\mathbf{p}))^{--} = \frac{\alpha\gamma^2(\mathbf{p}) + B(\mathbf{p})}{C(\mathbf{p})} \quad (59)$$

$$(J^{-1}(\mathbf{p}))^{+-} = (J^{-1}(\mathbf{p}))^{-+} = \frac{\alpha\gamma^2(\mathbf{p}) - B(\mathbf{p})}{C(\mathbf{p})} \quad (60)$$

$$(J^{-1}(\mathbf{p}))^{+z} = (J^{-1}(\mathbf{p}))^{-z} = -(J^{-1}(\mathbf{p}))^{z+} = -(J^{-1}(\mathbf{p}))^{z-} = \frac{2\sqrt{1 - \alpha^2 f(\mathbf{p})} \gamma(\mathbf{p})}{C(\mathbf{p})} \quad (61)$$

$$(J^{-1}(\mathbf{p}))^{zz} = \frac{4\alpha\gamma(\mathbf{p})}{C(\mathbf{p})} \quad (62)$$

In equation (58)-(61) we use the following notations:

$$\gamma(\mathbf{p}) = \frac{2}{z} \sum_{\boldsymbol{\delta}} \cos \boldsymbol{\delta} \mathbf{p} \quad (63)$$

where $\boldsymbol{\delta}$ is the nearest neighbor vectors $\boldsymbol{\delta} = (1, 0, 0, \dots); (0, 0, \dots, 1)$ for the hypercubic and: $\boldsymbol{\delta}_1 = (1, 0); \boldsymbol{\delta}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$ and $\boldsymbol{\delta}_3 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$ for the triangular lattice.

$$f(\mathbf{p}) = \frac{2i}{z} \sum_{\boldsymbol{\delta}} \sin(\mathbf{p}\boldsymbol{\delta}) \quad (64)$$

$$B(\mathbf{p}) = \alpha^2 \gamma^2(\mathbf{p}) + (1 - \alpha^2) f^2(\mathbf{p}) \quad (65)$$

$$C(\mathbf{p}) = 4zJ\gamma(\mathbf{p})B(\mathbf{p}) \quad (66)$$

Substituting (53) into (25) and integrating over the fluctuation field $\delta\Phi(\Omega_n)$ we obtain the free energy in the one-loop approximation:

$$\begin{aligned} F &= \frac{Nz\alpha Jm_o^2}{2} - \frac{N}{\beta} \ln \left(2 \cosh \frac{z\alpha Jm_o\beta}{2} \right) \\ &+ \frac{1}{4\beta} \sum_{\mathbf{p}} \ln \left[1 - \frac{(z\alpha)^2}{16} J^2 \beta^2 (1 - 4m_o^2)^2 \gamma^2(\mathbf{p}) \right] \\ &+ \frac{1}{\beta} \sum_{\mathbf{p}} \ln \frac{\sinh \frac{\beta\varepsilon(\mathbf{p})}{2}}{\sinh \frac{z\alpha Jm_o}{2}} \end{aligned} \quad (67)$$

where the magnon energy is given by:

$$\begin{cases} \varepsilon(\mathbf{p}) &= z\alpha Jm_o\omega(\mathbf{p}) \\ \omega(\mathbf{p}) &= \left[1 + \frac{1-\alpha}{\alpha} \gamma(\mathbf{p}) - \frac{1}{\alpha} \gamma^2(\mathbf{p}) \right]^{1/2} \end{cases} \quad (68)$$

For $z = 2D$ and $\alpha = 1$, from (66) and (67) we get the well known results for the D -dimensional hypercubic lattice [8]. For $z = 6$ and $\alpha = 1/2$, equation (67) gives the magnon dispersion for *TLMFM* [19]. In the limit $T \rightarrow 0K$, from (66) one gets the ground state energy per bond for *TLMFM*:

$$\varepsilon_o = -\frac{3}{8} + \frac{1}{4} \frac{1}{N} \sum_{\mathbf{p}} \omega(\mathbf{p}) \quad (69)$$

The numerical evaluation of equation (68) gives $\varepsilon_o = -0,1818$; which is in agreement with the results obtained by other methods [19-23]. Adding the sources term $\sum_i \boldsymbol{\lambda}_i \mathbf{S}_i$ to the Hamiltonian (1) in a similar way in the preceding section we obtain for the sublattice magnetization in one-loop approximation as follows:

$$m = \left(m_o + \frac{1}{4m_o} \right) + \frac{z\alpha J\Delta m}{4m_o} - \frac{1}{4N} \sum_{\mathbf{p}} \frac{1}{\tanh \frac{\beta\varepsilon(\mathbf{p})}{2}} \left(\frac{2}{\omega(\mathbf{p})} + \frac{\gamma(\mathbf{p})}{\omega(\mathbf{p})} + \frac{z\alpha J\Delta m}{2} \right) \quad (70)$$

where:

$$\Delta m = \frac{2\beta(1 - 4m_o^2)}{4 - \beta z \alpha J(1 - 4m_o^2)} \quad (71)$$

Putting $z = 4$ and $\alpha = 1$, from (69) and (70) we get the results in Ref.[9] for the square lattice. For the triangular lattice $z = 6$ and $\alpha = 1/2$ taking the limit of zero temperature $\Delta m = 0$; $m_o = \frac{1}{2}$, we have:

$$m = 1 - \frac{1}{4N} \sum_p \left(\frac{2}{\omega(p)} + \frac{\gamma(p)}{\omega(p)} \right) \quad (72)$$

which is exactly the magnetization obtained in linear spin wave approximation [19]. On the contrary, at finite temperatures exact treatment of the constraint changes the results considerably.

V. CONCLUSIONS

In the present work we have studied the Néel state of the spin $\frac{1}{2}$ isotropic Heisenberg antiferromagnetic model on hypercubic and triangular lattices using Popov-Fedotov approach in one-loop approximation. Working in local coordinates we considered both lattices in an unified procedure. For the hypercubic lattice we recover the results of the other authors. Some results for the triangular lattice have been derived by us before, but in more complicated way [25]. We employed an auxiliary fermion representation for spin $\frac{1}{2}$ operators. The exact projection into the physical states is performed by introducing an imaginary chemical potential as proposed by Popov and Fedotov. We obtained the explicit expressions for the free energy and the sublattice magnetization taking into account the fluctuations. The results show that exact projection gives a significant effect at finite temperatures. However, in the limit of low temperature the difference of the results for the cases when the constraint is treated exactly and when it is done in thermal average is negligibly small. This is due to the suppression of the fermion number fluctuations into the unphysical states, as discussed in Ref.[24].

ACKNOWLEDGMENT

This work is supported in part by NAFOSTED.

REFERENCES

- [1] A. Auerbach, *Interacting electrons and quantum magnetism*, Springer Verlag, (1994).
- [2] A. A. Abrikosov, *Physics* **2** (1965) 5
- [3] D. P. Arovas and A. Auerbach, *Phys. Rev.* **B38** (1988) 316.
- [4] V. N. Popov and S. A. Fedotov, *Sov. Phys., JETP* **67** (1988) 535.
- [5] O. Veits *et al.*, *J. France* **4** (1994) 493 .
- [6] M. N. Kicelev, *Int. J. Mod. Phys.* **B20** (2006) 381.
- [7] S. Tejima and A. Oguchi, *J. Phys. Soc. Jpn.* **64** (1995) 4923.
- [8] S. Azakov *et al.*, *Int. J. Mod. Phys.* **B14** (2000) 13.
- [9] R. Dillenschneider and J. Richert, *Eur. Phys. J.* **B49** (2006) 187.
- [10] R. Dillenschneider and J. Richert, *Phys. Rev.* **B73** (2006) 2440 .
- [11] J. Stein and R. Oppermann, *Phys. Rev.* **B46** (1992) 8409.
- [12] M. N. Kicelev, H. Feldmann and R. Oppermann, *Phys. Rev.* **B65** (2002) 184410.

- [13] R. Oppermann and A. Muller-Groeling, *Phys. Lett.* **A168** (1992) 75.
- [14] M. N. Kicelev, K. Kikoin and L. W. Molenkamp, *Phys.Rev.* **B68** (2002) 184410.
- [15] N. A. Forture *et al.*, *Phys. Rev. Lett.* **102** (2009) 257201.
- [16] R. Coldea *et al.*, *Phys. Rev. Lett.* **86** (2001) 1335.
- [17] Y. Shimizu *et al.*, *Phys. Rev. Lett.* **91** (2003) 107001 .
- [18] Y. Shirata, H. Tanaka, A. Matsuo and K. Kindo, arXiv: cond-matt. 1110. 3889.
- [19] Th. Jolicoeur and J. C. le Guillou, *Phys. Rev.* **B40** (1989) 2727.
- [20] J. Alicea, A. V. Chubukov and O. A. Starykh, *Phys. Rev. Lett.* **102** (2009) 137201.
- [21] L. Wang and S. G. Chung, arXiv: cond-matt. 1110. 0377
- [22] D. J. J. Farnell *et al.*, *J. Phys: Condens. Matter.* **21** (2009) 406002.
- [23] T. Sakai and H. Nakano, *Phys. Rev.* **B83** (2011) 100405 (R).
- [24] J. Brinckmann and P. Wolfle, arXiv: cond-mat. 0803. 3312.
- [25] T. V. Quang, P. T. T. Nga and N. T. Thang, *Comm. Phys.* **19** (2009) 71

Received 31 December 2011.