Fermionized Heisenberg model on a non-Bravais lattice with exact local constraint: Application to a honeycomb lattice

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Fermionized Heisenberg model on a non-Bravais lattice with exact local constraint: Application to a honeycomb lattice

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Abstract. We study magnetic order of the Heisenberg model on a non-Bravais lattice based on the Popov-Fedotov trick for exactly treating the local constraint on on-site spin number. The spin operators are represented by auxiliary fermions and an imaginary chemical potential is introduced. The following steps are sketched: i) Parameterizing classical ground state by a magnetic ordering vector and angles between the spins within a unit cell. ii) Going to a local coordinate system. ii) Using functional integral representation with Hubbard-Stratonovich for partition function and calculating determinants of block matrices by Silvester-Powel method. For illustration we obtain some explicit expressions for ferromagnetic Heisenberg model on a honeycomb lattice and compare them with the slave boson results.

1. Introduction

The principle difficulty in the treatment of spin systems is due to the fact that spin operators are neither Fermi nor Bose ones [1]. To overcome this problem, various representations of spin operators such as Fermi, Bose...have been introduced [1]. However the representations of spin as a combination of auxiliary Fermi or Bose operators induces the unphysical states which should be excluded from the consideration by imposing some local constraint condition on each spin lattice point. In practice for simplicity one usually replaces the local constraint requirement by a so-called global one, that treats the constraint condition only in average over all spin sites leading to uncontrollable approximations for quantum spin systems [1]. In 1988 Popov-Fedotov proposed [2] a new method of expressing spin-1/2 (spin-1) lattice systems in term of two (three) component fermions with imaginary chemical potential. Latter, the Popov-Fedotov technique was generalized for arbitrary spin [3, 4]. Recently, Popov-Fedotov concept has successfully been developed in combination with bold diagrammatic Monte Carlo simulation to address frustrated quantum spin systems [5]. A more general fermionization technique has been proposed for strongly correlated systems [6, 7]. The previous applications

of the Popov-Fedotov approach have been done to some particular spin-1/2 systems on Bravais lattice structure such as three dimensional ferromagnet [8], antiferromagnetic Heisenberg model on cubic and square lattice [9, 10] and on triangular lattice [11]. The goal of this paper is to apply the Popov-Fedotov trick to the Heisenberg model a non-Bravais lattice, in particular on a honeycomb one. It is motivated by the fact that many novel honeycomb lattice magnetic materials are obtained with poorly understood properties [12]. On the other hand due to the possibility of emerging Dirac magnon and electronic insulators, the physics of magnons in non-Bravais lattice becomes a subject of active research [13, 14]. The outline of this work is following: in the next section we sketch a general formalism. The third section is devoted to an application to a honeycomb lattice. The discussions are presented in section IV. The extended version of this paper will be published elsewhere.

2. The formalism

We consider a Heisenberg model on a non-Bravais lattice. The Hamiltonian reads

$$H = \sum_{ij} J_{ij} \vec{S}_i \vec{S}_j , \tag{1}$$

where $\vec{S}_i$ is the spin vector operator.

In order to study the fluctuations around the classical state it is convenient to characterize the classical ground state by some set of parameters. In a general non-Bravais lattice with planar spin configuration we may assign each classical *i*-spin in a unit cell to an ordering vector $\vec{Q}$ and and the angle ϕ_i between i-spin and some fixed direction.

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

with $\vec{u}$ and $\vec{v}$ being two orthogonal unit vectors.

Inserting (2) into Hamiltonian (1) we obtain the classical energy in terms of the ordering vector $\vec{Q}$ and the angle ϕ_i:

$$E_{cl} = \frac{1}{2} S^2 \sum_{ij} J_{ij} \cos\left(\vec{Q}\left(\vec{r}_i - \vec{r}_j\right) + \left(\phi_i - \phi_j\right)\right). \tag{3}$$

The magnetic ordering vector $\vec{Q}$ and the angle ϕ_i can be derived by minimizing the classical energy E_{cl} with respect to $\vec{Q}$ and ϕ_i. Depending on exchange interaction J_{ij} and on lattice structure there may exist different sets of parameters $\{\vec{Q}, \phi_i\}$ corresponding to different ordered phases. Following Miyake [16] we transform the spin components from the laboratory reference frame $\left\{S_i^x, S_i^y, S_i^z\right\}$ to the local reference frame $\left\{S_i^{x'}, S_i^{y'}, S_i^{z'}\right\}$ with the spin quantization on each site being along its classical direction:

$$\begin{cases} S_i^z = S_i^{z'} \cos\theta_i - S_i^{x'} \sin\theta_i , \\ S_i^x = S_i^{z'} \sin\theta_i - S_i^{x'} \cos\theta_i , \\ S_i^y = S_i^{y'} . \end{cases} \tag{4}$$

The transformation (4) simplified auxiliary particle formalisms so that one needs introduce only one type of auxiliary bosons or fermions for each spin in the unit cell for all possible ordered phases such as Neel, spiral, canted state...
Substituting (4) in (1), one obtains the following Hamiltonian:

$$H = -\frac{1}{2}\sum_{\substack{i,j \\ \alpha,\beta=x,y,z}} J_{\mathrm{ij}}^{\alpha\beta} S_i^{\alpha} S_j^{\beta}, \tag{5}$$

where

$$\begin{cases} J_{\mathrm{ij}}^{xx} = J_{\mathrm{ij}}^{zz} = X_{\mathrm{ij}} = -J_{ij}\cos\left(\Delta_{ij}\right), \\ J_{\mathrm{ij}}^{yy} = Y_{\mathrm{ij}} = -J_{\mathrm{ij}}, \\ J_{\mathrm{ij}}^{zx} = -J_{\mathrm{ij}}^{zx} = W_{\mathrm{ij}} = J_{\mathrm{ij}}\sin\left(\Delta_{ij}\right), \\ J_{\mathrm{ij}}^{xy} = J_{\mathrm{ij}}^{yx} = J_{\mathrm{ij}}^{yz} = J_{\mathrm{ij}}^{zy} = 0. \end{cases} \tag{6}$$

with

$$\Delta_{ij} = \vec{Q}\left(\vec{r}_j - \vec{r}_i\right) + \left(\phi_j - \phi_i\right). \tag{7}$$

Then following Popov-Fedotov [2] we write the spin operators in term of auxiliary Fermi operators operators $a_{i\sigma}^{+}$, $a_{i\sigma}$

$$S_i^{\alpha} = \frac{1}{2}\sum a_{i\sigma}^{+}\sigma_{\sigma\sigma'}^{\alpha} a_{i\sigma'}, \tag{8}$$

where $\sigma = \left(\sigma^x, \sigma^y, \sigma^z\right)$ are the Pauli matrices, and σ, $\sigma' = \uparrow$, $\downarrow$ is the spin index. Because the Fock state of the fermion $a_{i\sigma}$ is spanned by four states: two unphysical states: $|0\rangle$; $|2\rangle = a_{i\uparrow}^{+} a_{i\downarrow}^{+}|0\rangle$ and two physical one: $|\uparrow\rangle = a_{i\uparrow}^{+}|0\rangle$; $|\downarrow\rangle = a_{i\downarrow}^{+}|0\rangle$ where $|0\rangle$ is the vacuum state, the unphysical states have to be excluded by the constraint:

$$\hat{N}_i = \sum_{\sigma} a_{i\sigma}^{+} a_{i\sigma} = 1. \tag{9}$$

The constraint (9) has to be enforced for each site i and can be done by introducing the projection operator $\hat{\mathrm{P}} = \frac{1}{i^N} e^{i\frac{\pi}{2}\hat{N}}$ to the partition function:

$$\mathrm{Z} = \mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{\mathrm{H}}}\hat{\mathrm{P}}\right], \tag{10}$$

where $\hat{N} = \sum_i \hat{N}_i$ and H is the Hamiltonian in the fermion representation (8) [2].

As a result, the fermionic Matsubara frequences are modified:

$$\tilde{\omega}_F = \frac{2\pi}{\beta}\left(n + \frac{1}{4}\right). \tag{11}$$

The further calculations have been carried out closely following Ref. [11].

We sketch here the main procedure.

First we represent the partition function (10) in a fuctional integral form, where the fermions operators are replaced by Grassmann variables. Then we eliminate the 4-fermion terms in the partition function by a Hubbard-Stratonovich transformation, introducing the Bose auxiliary field $\vec{\varphi}_i$ which plays the role of the magnetization. Then we perform integration over the Grassmann variable to get:

$$Z = \left(\frac{1}{i^N}\right)\frac{1}{Z_0}\int D\left[\vec{\varphi}_i\right] e^{-S_{eff}[\vec{\varphi}_i]}, \tag{12}$$

where the effective action $S_{eff}\left[\vec{\varphi}\right]$ reads:

$$S_{eff}\left[\vec{\varphi}\right] = S_o\left[\vec{\varphi}\right] - \ln\det\beta\hat{K}. \tag{13}$$

Here we use the following notations:

$$Z_0 = \int\limits_{\varphi(\beta)=\varphi(o)} D\left[\varphi\right] e^{-\int_0^\beta d\tau\, S_o[\varphi]}, \tag{14}$$

with:

$$S_o\left[\varphi\right] = \frac{1}{2}\sum_{\substack{ij\\ \alpha\beta}}\left(J^{-1}\right)_{ij}^{\alpha\beta}\varphi_i^\alpha\varphi_j^\beta. \tag{15}$$

$\left(J^{-1}\right)_{ij}^{\alpha\beta}$ is the inverse of the interaction matrix $J_{ij}^{\alpha\beta}$.

$$\hat{K} \equiv \hat{K}_i\left(\omega_1,\omega_2\right) = \left(-i\omega_1 - \frac{i\pi}{2\beta}\right)\delta_{\omega_1,\omega_2}\hat{I} + \frac{1}{2}\vec{\sigma}\ \vec{\varphi}_i\left(\omega_1-\omega_2\right). \tag{16}$$

The form (13) of the effective action $S_{eff}\left[\varphi\right]$ allows us to apply a perturbation technique, decomposing the matrix $\hat{K}$ into nonperturbation and perturbation parts:

$$\hat{K} = \hat{K}_o + \hat{M}. \tag{17}$$

The explicit forms of $\hat{K}_o$ and $\hat{M}$ depend on the way of decomposing the auxiliary field $\vec{\varphi}_i$. One can set:

$$\vec{\varphi}_i\left(\Omega\right) = \vec{\varphi}_{io}\left(\Omega=0\right) + \delta\vec{\varphi}_i\left(\Omega\right), \tag{18}$$

where $\vec{\varphi}_{io}\left(\Omega=0\right)$ is the mean field part and $\delta\vec{\varphi}_i\left(\Omega\right)$ is the fluctuation part of the auxiliary field. The mean field $\vec{\varphi}_{io}\left(\Omega\right)$ is defined by minimizing the effective action (13):

$$\left.\frac{\delta S_{eff}\left[\varphi\right]}{\delta\varphi_i^\alpha}\right|_{\delta\varphi_i^\alpha=0} = 0. \tag{19}$$

The chosen value φ_{io} is related to the classical ground state magnetization per site m_{io}^{α} as follows:

$$\varphi_{io}^{\alpha} = -\sum_{j\beta} m_{jo}^{\beta} J_{j\alpha}^{\beta\alpha}. \tag{20}$$

In the local reference frame only the z-components of $\vec{m}_{io}$ and $\vec{\varphi}_{io}$ are non-zero, $m_{io}^{\alpha} = m_{oo}\delta_{\alpha,z}; \varphi_{io}^{\alpha} = \varphi_{oo}\delta_{\alpha,z}$.

Then (19) and (20) lead to the following mean-field equation for the magnetization:

$$m_{io} = \frac{1}{2}\tanh\frac{\beta}{2}\sum_{j} J_{ij}^{zz} m_{jo}. \tag{21}$$

The mean-field free energy reads:

$$F_{MF} = \frac{1}{2}\sum_{ij} J_{ij}^{zz} m_{io} m_{jo} + \ln 2\cosh\left(\frac{1}{2}\beta\varphi_{io}\right). \tag{22}$$

We can obtain the partition function at the one-loop approximation by integrating over the fluctuation field $\delta\vec{\varphi}_i(\Omega)$:

$$Z_{fl} = \left[\det \hat{D}_{ij}(\Omega)\right]^{1/2}; \hat{D}_{ij}(\Omega) = \hat{I} + \hat{J}_{ij}\hat{K}_{ij}(\Omega). \tag{23}$$

In order to separate the transverse and longitudinal fluctuations we will work in $(+, -, z)$ basics instead of the Descartes basics (x, y, z). The elements of the interaction matrix $\hat{J}_{ij}$ in $(+, -, z)$ basics are given in terms of (X_{ij}, Y_{ij}, W_{ij}) defined in (6) as follows:

$$\begin{cases} J_{ij}^{++} = J_{ij}^{--} = X_{ij} - Y_{ij}, \\ J_{ij}^{+-} = J_{ij}^{-+} = X_{ij} + Y_{ij}, \\ J_{ij}^{zz} = X_{ij}, \\ J_{ij}^{+z} = J_{ij}^{-z} = -J_{ij}^{z+} = -J_{ij}^{z-} = -W_{ij}. \end{cases} \tag{24}$$

The non-zero components of the matrix $\hat{K}_{ij}(\Omega)$ are given by:

$$\begin{cases} K_{ij}^{+-}(\Omega) = \left(K_{ij}^{-+}\right)^{*} = \dfrac{\beta}{2}\dfrac{m_{io}}{\varphi_{io} + i\Omega}\delta_{ij}, \\ K_{ij}^{zz}(\Omega) = -\dfrac{1}{4}\left(1 - 4m_{io}^{2}\right)\delta_{ij}\delta_{\Omega,o}. \end{cases} \tag{25}$$

From (23) one can get the fluctuation contribution to the free energy:

$$F_{fl} = \frac{1}{2\beta}\ln\det\hat{D}_{ij}(\Omega). \tag{26}$$

It is convenient to perform the Fourier transformation over $\hat{D}_{ij}$ and then to calculate $\det \hat{D}(\vec{p})$ instead of calculating $\det \hat{D}_{ij}$. In the case of a Bravais lattice all sites are equivalent so $\hat{D}(\vec{p})$ is a 3 x 3 matrix. Therefore it is straightforward to calculate $\ln \det \hat{D}(\vec{p})$ and obtain explicit analytical expressions for the fluctuation contributions to the free energy [11]. A non-Bravais lattice is quite different. If there are *n* spin in an unit cell then the matrix $\hat{D}(\vec{p})$ is 3*n* x3*n* block matrix. Following Silvester [17] and Powell [18] one can reduce the determinant of a matrix with N^2 blocks to the product of the determinants of N distinct combinations of single block. For example [17]:

$$\det\begin{pmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{pmatrix} = \det\left(\hat{A}\hat{D} - \hat{B}\hat{D}^{-1}\hat{C}\hat{D}\right). \tag{27}$$

In the following, the formula (27) will be used for the case of the Heisenberg model in a honeycomb lattice.

3. Application to ferromagnetic honeycomb lattice

We consider the ferromagnetic Heisenberg model defined by the Hamiltonian:

$$H = J\sum_{ij} \vec{S}_i \vec{S}_j. \tag{28}$$

Here, $\langle ij \rangle$ are paid of nearest neighbors with ferromagnetic coupling constant $J < 0$ on the honeycomb lattice (Fig. 1)

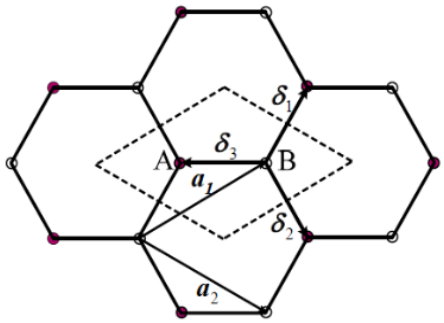

Fig.1 The honeycomb lattice is defined by the basic vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and two sublattices *A* and *B*.

The nearest neighbor vectors are given by

$$\vec{\delta}_1 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right);\ \vec{\delta}_2 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right);\ \vec{\delta}_3 = (-1, 0), \tag{29}$$

where the lattice constant is taken to be one.

For finding the classical ground state parameters $\vec{Q}$ and ϕ_i we can set $\phi_A = 0$ and $\phi_B = \phi$. Substituting (29) in to (3) and minimizing the classical energy with respect to the parameter $\vec{Q}$ and ϕ we obtain for the ferromagnetic phase:

$$\vec{Q} = (0,\ 0),\ \phi = 0, \tag{30}$$

with the energy:

$$E_{cl} = \frac{3NJ}{8}, \tag{31}$$

where N is total site number.

The mean – field equation for the magnetization per site reads:

$$m_0 = \frac{1}{2}\mathrm{Tanh}\frac{3|J|m_0}{2}. \tag{32}$$

The mean – field equation for free energy per site is given by:

$$F_{MF} = \frac{3|J|}{2}m_0^2 - \ln 2\cosh\frac{3|J|m_0}{2}. \tag{33}$$

From (32) the Curie temperature is defined by:

$$k_B T_C = \frac{3|J|}{4}, \tag{34}$$

which is twice larger than the Curie temperature derived in the case of replacing the local constraint (9) by the global one as expected [19].

In the nearest neighbor approximation the exchange coupling between the sites of the same sublatice is zero $J_{AA} = J_{BB} = 0$ so $X_{AA} = X_{BB} = 0$.

From (6), (24), (29) and (30) we derive the interaction matrix in Fourier transformation as following:

$$\tilde{J}(\vec{p}) = \begin{pmatrix} 0 & \tilde{J}_{AB}(\vec{p}) \\ \tilde{J}_{BA}(\vec{p}) & 0 \end{pmatrix}, \tag{35}$$

where

$$\tilde{J}_{AB}(\vec{p}) = \left(\tilde{J}_{BA}(\vec{p})\right)^* = \begin{pmatrix} 0 & 2X(\vec{p}) & 0 \\ 2X(\vec{p}) & 0 & 0 \\ 0 & 0 & X(\vec{p}) \end{pmatrix}, \tag{36}$$

and

$$\begin{aligned} X(\vec{p}) &= -3J\gamma(\vec{p}), \\ \gamma(\vec{p}) &= \frac{1}{3}\sum_{\vec{\delta}_i} e^{-i\vec{\delta}_i\vec{p}}. \end{aligned} \tag{37}$$

The Eqs (25) and (35) lead to the following expression for the block matrix $\hat{D}(\vec{p},\Omega)$:

$$\hat{D}(\vec{p},\Omega)=\begin{pmatrix} I & \hat{D}_{AB}(\vec{p},\Omega) \\ \hat{D}_{BA}(\vec{p},\Omega) & I \end{pmatrix}. \tag{38}$$

We use the following notation:

$$\begin{aligned} \hat{D}_{AB}(\vec{p},\Omega)&=\tilde{J}_{AB}(\vec{p}).\hat{K}\ (\Omega), \\ \hat{D}_{BA}(\vec{p},\Omega)&=\tilde{J}_{BA}(\vec{p}).\hat{K}\ (\Omega). \end{aligned} \tag{39}$$

where

$$\hat{K}\ (\Omega)=\begin{pmatrix} 0 & k^{+-}(\Omega) & 0 \\ k^{-+}(\Omega) & 0 & 0 \\ 0 & 0 & k^{zz}(\Omega)\delta_{\Omega,0} \end{pmatrix}, \tag{40}$$

$$\begin{aligned} k^{+-}(\Omega)&=\left(k^{-+}(\Omega)\right)^{*}=\frac{\beta}{2}\frac{m_0}{3|J|m_0+i\Omega}, \\ k^{zz}(\Omega)&=-\frac{1}{4}\left(1-4m_0^2\right). \end{aligned} \tag{41}$$

Because the diagonal block elements of the matrix $\hat{D}(\vec{p},\Omega)$ (38) is the 3 x 3 unit matrix, from the Eq. (27) and (38) one obtains:

$$\det\hat{D}(\vec{p},\Omega)=\prod_{\vec{p}\in RBZ}A_0(\vec{p})\prod_{\Omega}Q(\vec{p},\Omega), \tag{42}$$

where

$$A_0(\vec{p})=1-9J^2\left|\gamma^2(\vec{p})\right|\left(k^{zz}\right)^2, \tag{43}$$

$$Q(\vec{p},\Omega)=\frac{\left((i\Omega)^2-E_1(\vec{p})\right)\left((i\Omega)^2-E_2(\vec{p})\right)}{\left((i\Omega)^2-(3Jm_0)^2\right)^2}. \tag{44}$$

The magnon energy is given by:

$$E_{1,2}(\vec{p})=3|J|m_0\left(1\pm|\gamma(\vec{p})|\right). \tag{45}$$

The product over the bosonic Matsubara frequencies may be carried out via the Gamma function [20]:

$$\prod_{\Omega}Q(\vec{p},\Omega)=\frac{1}{2}\prod_{\alpha=1,2}\frac{\sinh\left(\frac{\beta}{2}E_\alpha(\vec{p})\right)}{\sinh\left(\frac{3\beta|J|m_0}{2}\right)}. \tag{46}$$

Then the free energy in the one loop approximation reads:

$$F = \frac{3N|J|m_0^2}{2} - \frac{N}{\beta}\ln 2\cosh\frac{3|J|m_0}{2} + \frac{1}{2\beta}\sum_{\substack{\alpha=1,2\\ \vec{p}\in RBZ}} \ln\frac{\sinh\left(\frac{\beta}{2}E_\alpha(\vec{p})\right)}{\sinh\left(\frac{3\beta|J|m_0}{2}\right)} + \frac{1}{2\beta}\sum_{\vec{p}\in RBZ}\ln A_0(\vec{p}). \quad (47)$$

This is the main result of the present paper. Derivation of explicit expressions for the fluctuation contributions to the magnetization, internal energy and specific c_v from the free energy (47) is straightforward.

4. Discussions

The above obtained free energy (47) is different from that derived in the standard spin wave up to $1/S^2$ corrections. However, similar to the Bravais lattice, the results obtained in the previous section by Popov–Fedotov method in the one loop approximation lead in the zero temperature limit exactly to the same one derived in linear wave theory using slave boson representation of spin operator [8-11, 21]. This confirms the fact that at zero temperature the Popov–Fedotov trick does not improve the results of global constraint approximation. At the finite temperature the exact constraint reduces the number of states where an auxiliary fermion may thermally fluctuate into. In result the critical temperature T_C is twice higher than in the global constraint case.

The mean-field magnetization m_0 in the Eq. (47) depends on temperature following (32), while in the other slave particle method m_0 = ½ so the Popov–Fedotov gives a significant effect at finite temperature for all quantities containing m_0. For the honeycomb lattice the interesting properties appear near the Dirac points $\vec{K}_\pm = \left(\frac{2\pi}{3}, \pm\frac{2\pi}{3\sqrt{3}}\right)$. Expanding $\gamma(\vec{p})$ near $\vec{K}_\pm$ we get the linear dispersion of so called Dirac magnon that is similar to the spinless Dirac fermion of Bloch graphene model [13, 14]

$$E_{1,2}(\vec{q}) = \frac{3}{2}|J|m_0\left(\sigma_x q_x - \tau\sigma_y q_y\right). \quad (48)$$

where the $\tau = \pm 1$ correspond to the states near $\vec{K}_\pm$, $\vec{q} = \vec{p} - \vec{K}_\pm$. It is almost the same result of linear spin wave theory applying Holstein-Primakoff transformation of spin operators [13, 14], except the fact that in (48) m_0 depends on temperature via (32) instead of m_0 = ½.

The obtained results on the example of the ferromagnetic Heisenberg model on the honeycomb lattice are encouraging further applications of Popov–Fedotov trick to Heisenberg model on other non Bravais such as Kagome, Chevron-square, Union-Jack, frustrated honeycomb...lattices.

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