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ANTIFERROMAGNETIC HEISENBERG SPIN $\frac{1}{2}$ MODEL ON A TRIANGULAR LATTICE IN A MAGNETIC FIELD

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Abstract. *The functional approach of Popov Fedotov is applied to a quantum antiferromagnetic Heisenberg spin -$\frac{1}{2}$ model in the presence of an in plane magnetic field. We calculate the ground state energy, sublattice and uniform magnetization. We find that the quantum fluctuation is enhanced as the magnetic field increases at the intermediate field strength.*

I. INTRODUCTION

The spin $S = \frac{1}{2}$ antiferromagnetic Heisenberg model on a triangular lattice has attracted particular interest because its small spin, low dimensionality and geometrical frustration can anhance quantum fluctuations and lead to a rich phase diagram [1]. An interesting field of study is that of the behavior of frustrated quantum magnetic systems in the presence of external magnetic field [2, 4]. This topic has become more important by the experimental discovery of exotic properties for the approximately isotropic material Cs_2CuBr_4 and the anisotropic Cs_2CuCl_4 [3, 4]. Obviously, the behavior of quantum magnets in aspect in their potential technological application. From a theoretical viewpoint, competition between magnetic field geometrical frustration and small spin provides a difficult challenge to the physicicts. Several methods such as analytical studies using spin wave theory [5-7] and numerical studies using exact diagonalization [8, 9], coupled cluster method [10, 11], density matrix renormalization group [12] and variation approaches [13] have been used. However, a clear understanding of the model has not been achieved. For an analytical approachs to the spin model, the non- canonical commutation relations of spin operators pose a severe difficulty because the standerd many-body method based on the Wicks theorem. In order to circumvent this difficulty one represents the operators in terms of canonical operator of either bosonic or fermionic character. However, this mapping extends the Hiltbert space into unphysical sectors, which have to be removed by imposing a constraint the method proposed by Popov-Fedotov enables one to enforce the constraint exactly within an analytical calculation by introducing an imaginary chemical potential [14]. Motivated by the above mentioned experimental and theoretical works, in this report we focus on the spin $\frac{1}{2}$ antiferromagnetic Heisenberg model on a triangular lattice in the presence of in plane external magnetic field by Popov-Fedotov functional intergral approach.

II. THE MODEL AND FORMALISM

The antiferromagnetic Heisenberg model on a triangular lattice in the presence paper is described by the Hamiltonian:

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j - \sum_i \vec{B}\vec{S}_i \tag{1}$$

where $\vec{S}_i$ is a spin located at site i and the summation $\langle ij \rangle$extends over all nearest neighbor pairs. The magnetice field is applied along the z axis i.e $\vec{B} = (0, 0, B)$.

We know that the classical ground states of the system at zero external field ($B = 0$) takes a well known planar structure with nearest neighbouring spins aligning at angles of to each others. We choose the z-x plane of a fixed global coordinate system to decribe the magnetic order. Supposing that in the classical ground states a spin at site i is directed along some unit vector, we choose this classical spin orientation as local z direction which may very from site to site.

Then the relation between the spin $\vec{S}_i$ in the local coordinate system and the spin $\vec{S}_i$ in the global coordinate system is given by:

$$\begin{array}{l} S_i^{'x} = S_i^x \cos\theta_i + S_i^z \sin\theta_i \\ S_i^{'y} = S_i^y \\ S_i^{'z} = S_i^x \sin\theta_i + S_i^z \cos\theta_i \end{array} \tag{2}$$

where θ_i is the angle between the local z and the global z axis. In the zero field case, the classical ground state consists of three sublattice A, B, C with an angle of 120^o between the sublattice spin, i.e we have $\theta_A = 0; \theta_B = {}^{2\pi}/_3$ and $\theta_C = {}^{4\pi}/_3$. As the magnetic field is applied along the global z- axis, the spins on sublattices B and C are expected to rotate toward the z- axis by the same angle and the angle is determined variationnally and is given by:

$$\begin{array}{l} \cos\theta = \frac{B-3J}{6J}, B \leq B_c = 9J \\ \cos\theta = 1, B \geq B_c \end{array} \tag{3}$$

The classical ground state energy is found to be:

$$E_{cl} = -\frac{B^2 N}{18J} - \frac{3}{2} JNS^2; B \leq B_c \tag{4}$$

Respectively the classical uniform magnetization is given by:

$$M_z = \frac{B}{9J} N \tag{5}$$

Now we rewrite the Hamiltonian (1) in the new spin coordinate (2) as:

$$H = -\frac{1}{2} \sum_{\langle ij, \alpha\beta \rangle} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta - B \sum_i (S_i^z \cos\theta_i - S_i^x \sin\theta_i) \tag{6}$$

Here primes are dropped. The couppling constants are given by:

$$\left\{\begin{array}{l} J_{ij}^{yy} = -J \\ J_{ij}^{xx} = J_{ij}^{zz} = -J\cos(\theta_i - \theta_j) \\ J_{ij}^{xz} = -J_{ij}^{zx} = J\sin(\theta_i - \theta_j) \\ J_{ij}^{xy} = J_{ij}^{yx} = J_{ij}^{yz} = J_{ij}^{zy} = 0 \end{array}\right. \tag{7}$$

Following Popov-Fedotov [14], we represent the spin operators in terms of auxiliary fermions:

$$S_i^{\mu} = \frac{1}{2}\sum_{\sigma,\sigma'} a_{i\alpha}^{+}(\sigma^{\mu})_{\alpha\beta} a_{i\beta} \tag{8}$$

where σ^{μ} $(\mu = x, y, z)$ - are Pauli matrices, and $\alpha =\uparrow, \downarrow$ is the spin index. The representation on (6) fullfills the comminication relations for the spin operators. However the Fock space of the auxiliary fermions is spanned by the physical states $|\uparrow\rangle_i = a_{i\uparrow}^{+}|0\rangle\,; |\downarrow\rangle_i = a_{i\downarrow}^{+}|0\rangle$ and the unphysical states $|0\rangle\,; |2\rangle_i = a_{i\uparrow}^{+}a_{i\downarrow}^{+}|0\rangle$ with $|0\rangle$ being the vacuum. The fermionic operators $a_{i\alpha}^{+}, a_{i\alpha}$ must satisfly the local constraint $\sum\limits_{\alpha} a_{i\alpha}^{+}a_{i\alpha} = 1$ in order to exclude the unphysical states. Note that the constraint has to be enforced on each site i independently. This prohibit an infinite order resummation of the perturbation series in J. The problem can be evaded within a mean field like treatment of the constraint, where the local constraint is replace by the thermal average:

$$\sum_{\alpha}\left\langle a_{i\alpha}^{+}a_{i\alpha}\right\rangle = 1 \tag{9}$$

The quation (7) is introduced into the Hamiltonian (1) through a chemical potential μ, which is equal to zero due to the particle hole symmetry of (1). In the Popov-Fedotov scheme an imaginary valued chemmical potential $\mu = i\frac{\pi}{2}T$ is introduced. One starts from a grant canomical ensemble:

$$\tilde{H} = H - \mu\sum_{i} a_{i\alpha}^{+}a_{i\alpha} \tag{10}$$

The contribution from the unphysical states $|0\rangle$ and $|2\rangle$ to the partition function Z is proportional to:

$$\sum_{n_i=0,2} e^{i\frac{\pi}{2}n_i} = 0 \tag{11}$$

so the unphysical contributions from all sites cancel and only the physical states survive in Z. We apply the standard integrant formulation for the Hamiltonian (8) of the spin system in the Neel state in a similar way to [15-19]. To second order (one loop contribution) in the fluctuations $\delta\vec{\varphi}$ of $\vec{\varphi}_i(\tau) = \vec{\varphi}_{io}(0) + \delta\vec{\varphi}_i(\tau)$ the effective action reads:

$$S_{eff}\left[\vec{\varphi}\right] = S + \frac{\delta S_{eff}}{\delta\varphi_i^{\alpha}}\delta\varphi_i^{\alpha} + \frac{1}{2}\frac{\delta^2 S^2{}_{eff}}{\delta\varphi_i^{\alpha}\delta\varphi_i^{\beta}}\delta\varphi_i^{\alpha}\delta\varphi_i^{\beta}\beta \tag{12}$$

where $\vec{\varphi}_i$ are the Hubbard-Stratonovich auxiliary fields. The mean field action reads:

$$S_{mf} = \frac{\beta}{2} \sum_{ij,\alpha\beta} \left(J^{-1}\right)_{ij}^{\alpha\beta} \left[\left(\varphi_{io}^{\alpha} - B_i^{\alpha}\right)\left(\varphi_{jo}^{\beta} - B_j^{\beta}\right)\right] - \sum_i \ln 2 \cosh \frac{\beta}{2}\varphi_{io} \tag{13}$$

where:

$$\vec{B}_i = B\left(-\sin\theta_i, 0, \cos\theta_i\right) \tag{14}$$

The local Hubbard-Stratonovich auxiliary fields $\vec{\varphi}_i$ can be related to the local magnetizations $\vec{m}_i$ as follows:

$$\overrightarrow{m}_i = \frac{1}{2}\frac{\tanh\frac{\beta\varphi_{io}}{2}}{\varphi_{io}}.\overline{\Phi}_{io}\frac{\partial\tilde{B}_i}{\partial B_i^{\alpha}} \tag{15}$$

$$\Phi_{io} = -\tilde{B}_i + \sum_k \hat{J}_{ki}\left(\frac{\partial\bar{B}}{\partial B_i^{\alpha}}\right) m_i^{\alpha} \tag{16}$$

here we use the following notations:

$$\Phi_{io} = \begin{pmatrix} \varphi_{io}^x + i\varphi_{io}^y \\ \varphi_{io}^x - i\varphi_{io}^y \\ \varphi_{io}^z \end{pmatrix}$$

$$\tilde{B}_i = \begin{pmatrix} B_i^x + iB_i^y \\ B_i^x - iB_i^y \\ B_i^z \end{pmatrix} \tag{17}$$

$$\bar{\Phi}_{io} = \left(\Phi_{io}\right)^T$$
$$\tilde{B}_i = \left(\tilde{B}_i\right)^T$$

The quantum fluctuation contribution is given by third term of eq (10) and can be derived in the analogous way as in [23,24] and the detail calculations are not given explicitly here. The quantum fluctuation contribution to the ground state energy is given by:

$$E_{fl} = \left(-\frac{1}{2} + \frac{1}{3N}\sum_{\substack{\vec{k}\in BZ \\ \alpha=1,2,3}} \omega_{\alpha}(\vec{k})\right) 3NJS; B \leq B_C \tag{18}$$

where $\omega_{\alpha}(\vec{k})$ are the three modes of the spin wave excitations, which are eigenvalues of a 3x3 matrix. In the small B with the $\sqrt{3}\times\sqrt{3}$ spin structure we can obtain the analytical result. The sublattice magnetization is defined as the average spin component within the same sublattice along its quantization axis:

$$\left\langle S_Q^{z'}\right\rangle = \frac{3}{N}\sum_{i\in Q}\left\langle S_i^{z'}\right\rangle = \frac{1}{2} - \langle\Delta S_Q\rangle, (Q = A, B, C sublattice) \tag{19}$$

and:

$$\langle \Delta S_A \rangle = -\frac{1}{2} + \frac{1}{24} \sum_{\vec{k},\alpha} \frac{2-\gamma(k)}{\omega_\alpha(k)} \tag{20}$$

where $\gamma(k)$ is the structure factor,

$$\gamma(k) = \frac{1}{6} \sum_{\vec{\delta}} e^{i\vec{k}\vec{\delta}}$$

with $\vec{\delta}$ are nearest neigbor vectors.

$\langle \Delta S_B \rangle = \langle \Delta S_C \rangle$ are given in the somehow similar form.

The uniform magnetization is along the external field orientation and can be written as:

$$\langle S^z \rangle = \frac{1}{3N} \sum_i \langle S_i^z \rangle = \frac{B}{9J} - \frac{1}{3} \langle \Delta S_A \rangle - \frac{2}{3} \langle \Delta S_B \rangle \cos\theta \tag{21}$$

III. DISCUSSIONS AND CONCLUSIONS

We have to evalute the Eq. (18) numerically to discuss the quantum corrections to the ground state energy. It is clear from (4) that the classical ground state energy decreases monotonically as the external magnetic field B increases. The numerical result of Eq. (18) show that the quantum correction to the energy is very small. At $T = 0$ as the magnetic fields B increases, the quantum fluctuation energy increases, for example, at $B = 0$: $\frac{E_{fl}}{3NJ} = -0.055$ and at $B = 4J$: $\frac{E_{fl}}{3NJ} = -0.041$.

As regard to the quantum correction at $T = 0$ to the sublattice magnetization from Eqs. (15-17); (20) we get that the sublattice magnetization $\langle \Delta S_Q \rangle$ decreases, with increasing the external magnetic field B and decreases more rapidly than $\Delta S_B, \Delta S_C$, for example, at $B = 0$: $\Delta S_A = \Delta S_B = \Delta S_C = 0.27$ and at $B = 4J$:[$\Delta S_A = 0.076; \Delta S_B = \Delta S_C = 0.175$).

The numerical result from Eqs. (15-17) and (21) for the uniform magnetization including the leading order quantum fluctuation show almost linearly increasing of the uniform magnetization with the magnetic fields. At $B = 0$: $\langle S^z \rangle = 0$ and at $B = 4J$: $\langle S^z \rangle = 0.170$.

The above result at $T = 0$ are in agreement with the previous spin wave theory of Gan et al [22]. The numerical calculation for $T \neq 0K$ is on the progress and will be published elsewhere. On expected significant difference between the Popov-Fedotov formalism with an exact local constraint and other approaches with a relaxed constraint [23].

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