

Ordered Phase in the Fermionized Heisenberg Antiferromagnet

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Abstract

Thermal properties of the ordered phase of the spin 1/2 isotropic Heisenberg Antiferromagnet on a d-dimensional hypercubical lattice are studied within the fermionic representation when the constraint of single occupancy condition is taken into account by the method suggested by Popov and Fedotov. Using saddle point approximation in path integral approach we discuss not only the leading order but also the fluctuations around the saddle point at one-loop level. The influence of taking into account the single occupancy condition is discussed at all steps.

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1 Introduction

The two-dimensional spin-1/2 Heisenberg antiferromagnet (HAFM) on the square lattice has been extensively studied during the last few years. The motivation for this study stems from the discovery of high T_c superconductivity in the ceramic compounds, where the competition between superconductivity and antiferromagnetic order has been observed experimentally [1].

Contrary to early suggestions there is nowadays strong evidence that the ground state of the fully isotropic quantum spin -1/2 HAFM on a two dimensional regular lattice is the Néel state (the classical ground state (the Néel state) is not disordered by quantum fluctuations.).

This evidence is mainly based on numerical work [2]. Recently it has gained an additional support by results obtained analytically with the help of various techniques e.g. large spin expansion,

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field theory of the quantum nonlinear σ -model [3], effective Hamiltonian approach [4], a modified mean field approach (saddle point approximation) based on bosonic [5] or fermionic representations [6] of spin operators.

The main problem in the technique based on these representations is to take into account the so-called single occupancy condition.

The aim of this work is to study the thermal properties of the ordered (magnetic) phase of the spin 1/2 isotropic HAFM on a d -dimensional hypercubical lattice ¹ with periodic boundary conditions within the fermionic representation when the constraint of single occupancy condition is taken into account by the method suggested by Popov and Fedotov [7]. We use saddle point approximation and discuss not only the leading order but also the fluctuations around the saddle point at the one-loop approximation level. We show that at zero temperatures one-loop corrections to the saddle point in our path integral description is equivalent to next-to-leading order in the linear spin wave theory. At all steps we discuss the influence of taking into account the single occupancy condition comparing the results of our calculations with those when this condition is disregarded. In particular we show that at finite temperatures taking into account the single occupancy condition considerably reduces the specific heat.

For $T \neq 0$ the two-dimensional spin system has no long range order (the Néel state is destroyed by thermal fluctuations)[8] and its state has to be treated as a paramagnetic one with strong antiferromagnetic correlations at finite distances. So our finite temperature results are relevant for the case when $d \geq 3$ and $T < T_N$, where T_N is the Néel temperature.

In Sec.2 we briefly review the fermionization procedure of spin operators by the method of Popov and Fedotov.

In Sec.3 we discuss the mean field result (the leading order of the saddle point approximation).

In Sec.4 we obtain the one-loop corrections (Gaussian fluctuations) to free energy and show that one can get the spin wave spectrum at zero temperature. We also find the specific heat and discuss the influence of the single occupancy condition on its temperature dependence.

The last section is devoted to brief comments on our results.

2 Fermionization by Popov and Fedotov's method and bosonic path integrals for the partition function.

The Hamiltonian of the isotropic HAFM reads

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

the sum runs over ordered nearest neighbor sites of the d -dimensional finite regular lattice with M sites. For spin variables \mathbf{S}_i we assume periodic boundary conditions, $J > 0$.

Many authors have proposed to use different representations of spin operators by Bose or Fermi operators. However, the fact that the dimensionality of the space in which these operators act is always greater than the dimensionality of the space of spin operators leads to the problem of the elimination of the superfluous states. Usually it is done by putting some constraints on the states.

¹For simplicity we consider a simple hypercubical lattice though our approach may be also used for a non-bipartite lattice

In the present paper we choose fermionic representation of spin operators

$$\hat{\mathbf{S}}_i = \frac{1}{2} \hat{c}_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i\beta}, \quad \alpha, \beta = 1(\uparrow), 2(\downarrow), \quad (2)$$

the summation with respect to repeated Greek indices is assumed, $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices, and if we use this representation in the spin Hamiltonian \hat{H}_S we shall get the fermionic Hamiltonian:

$$\hat{H}_F = \frac{J}{4} \sum_{\langle i,j \rangle} (\hat{c}_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i\beta}) (\hat{c}_{j\gamma}^\dagger \boldsymbol{\sigma}_{\gamma\delta} \hat{c}_{j\delta}) \quad (3)$$

$\hat{c}_{i\alpha}$ and $\hat{c}_{i\alpha}^\dagger$ are fermionic annihilation and creation operators (at site i with spin projection α to the z axis), which obey canonical anticommutation relation

$$\{\hat{c}_{i\alpha}, \hat{c}_{j\beta}^\dagger\} = \delta_{i,j} \delta_{\alpha\beta}.$$

Popov and Fedotov [7] proved that the partition function of the model (1)

$$Z = \text{Tr}_S(e^{-\beta \hat{H}_S}) \quad (4a)$$

can also be written as

$$Z = i^M \text{Tr}_F(e^{-\beta \hat{H}_F - i \frac{\pi}{2} \hat{N}}). \quad (4b)$$

In these formulas $\text{Tr}_S(\text{Tr}_F)$ is a trace in space where spin (fermionic) operators act, $\hat{N} = \sum_{i=1}^M \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} = \sum_{i=1}^M \hat{n}_i$ is the number operator.

Let us briefly repeat their arguments. It is sufficient to consider only one site (we omit the site index). For spin $\frac{1}{2}$, spin operators $\hat{S}^a (a = x, y, z)$ act in two dimensional space. But the space where fermionic operators act is four dimensional; we have states

$$|0, 0\rangle, \quad \hat{c}_\uparrow^\dagger |0, 0\rangle = |\uparrow, 0\rangle, \quad \hat{c}_\downarrow^\dagger |0, 0\rangle = |0, \downarrow\rangle, \quad \hat{c}_\uparrow^\dagger \hat{c}_\downarrow^\dagger |0, 0\rangle = |\uparrow, \downarrow\rangle.$$

States $|\uparrow, 0\rangle, |0, \downarrow\rangle$ can be identified with eigenstates of \hat{S}^z operator with spin up and spin down, we call them *physical* and denote $|phys\rangle$. Then states $|0, 0\rangle$ and $|\uparrow, \downarrow\rangle$ are superfluous or *unphysical* and their contribution should be excluded.

The physical states span a two-dimensional physical subspace, characterized by the single occupancy condition

$$\hat{n} |phys\rangle = |phys\rangle.$$

The direct product of the physical subspaces of all the sites form the sectors in which the Hamiltonians \hat{H}_S and \hat{H}_F coincide.

In order to prove the basic formula Eq.(4b) we write

$$\hat{H}_F = \hat{H}_{F_i} + \hat{H}'_{F_i}, \quad \hat{N} = \hat{n}_i + \hat{N}'_i,$$

where $\hat{H}_{F_i}(\hat{n}_i)$ is that part of the $\hat{H}_F(\hat{N})$ which contains the fermionic operators of the i -th site and $\hat{H}'_{F_i}(\hat{N}'_i)$ is the remaining part. For the Hamiltonian of HAFM we have

$$\hat{H}_{F_i} |unphys\rangle_i = 0.$$

Therefore, the trace in Eq.(4b) taken over unphysical states of the i -th site vanishes

$$\text{Tr}_{i \text{ unphys}} \{ e^{-\beta \hat{H}_F - i \frac{\pi}{2} \hat{N}} \} = e^{-\beta \hat{H}'_F - i \frac{\pi}{2} \hat{N}'_i} \text{Tr}_{i \text{ unphys}} \{ (-i)^{\hat{n}_i} \} = 0,$$

since $\text{Tr}_{i \text{ unphys}} \{ (-i)^{\hat{n}_i} \} = (-i)^0 + (-i)^2 = 0$.

As a result, in the calculation of the trace all the unphysical states are eliminated, while on the physical states $\hat{H}_F = \hat{H}_S$ and $\hat{N}|phys\rangle = M|phys\rangle$. Therefore

$$\text{Tr}_F (e^{-\beta \hat{H}_F - i \frac{\pi}{2} \hat{N}}) = (-i)^M \text{Tr}_{phys} (e^{-\beta \hat{H}_F}) = \frac{1}{i^M} \text{Tr}_S (e^{-\beta \hat{H}_S})$$

which proves Eq.(4b).

The evaluation of fermionic trace Tr_F requires only the standard technique because this trace is unrestricted. It can be represented as a path integral in terms of Grassmann fields η and $\bar{\eta}$ [11]

$$Z = i^M \int \mathcal{D}\mu_\eta \exp \left\{ - \int_0^\beta d\tau \left[\sum_{i,\alpha} \bar{\eta}_{i\alpha}(\tau) \left(\partial_\tau + i \frac{\pi}{2\beta} \right) \eta_{i\alpha}(\tau) + \mathcal{H}_F(\bar{\eta}, \eta; \tau) \right] \right\}, \quad (5)$$

where

$$\begin{aligned} \mathcal{H}_F(\bar{\eta}, \eta; \tau) &= \frac{J}{4} \sum_{\langle i,j \rangle} (\bar{\eta}_{i\alpha}(\tau) \boldsymbol{\sigma}_{\alpha\beta} \eta_{i\beta}(\tau)) (\bar{\eta}_{j\gamma}(\tau) \boldsymbol{\sigma}_{\gamma\delta} \eta_{j\delta}(\tau)) \\ &= J \sum_{\langle i,j \rangle} \mathbf{S}_i(\tau) \cdot \mathbf{S}_j(\tau) \end{aligned} \quad (6)$$

and

$$\mathbf{S}_i(\tau) \equiv \frac{1}{2} \bar{\eta}_{i\alpha}(\tau) \boldsymbol{\sigma}_{\alpha\beta} \eta_{i\beta}(\tau), \quad (7)$$

$$\mathcal{D}\mu_\eta = \prod_{0 \leq \tau \leq \beta} \prod_{i,\alpha} d\bar{\eta}_{i\alpha}(\tau) d\eta_{i\alpha}(\tau).$$

Now let us do the Fourier transformation

$$\mathbf{S}_i(\tau) = \frac{1}{\beta} \sum_{\mathbf{q} \in BZ} \sum_m \mathbf{S}(\mathbf{q}, \Omega_m) e^{-i\Omega_m \tau} e^{i\mathbf{q} \cdot \mathbf{r}_i}, \quad (8)$$

where \mathbf{q} is the wave vector in reciprocal space (we can restrict it to the first Brillouin zone (BZ)), $\Omega_m = \frac{2\pi m}{\beta}$ is a Matsubara frequency for Bose field.

Summation over ordered nearest neighbors can be written as

$$\sum_{\langle i,j \rangle} = \frac{1}{2} \sum_{i,\boldsymbol{\delta}} , \quad (9)$$

since j is a nearest neighbor of i : $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}$, and $\boldsymbol{\delta}$ represents the displacement of $z = 2d$ nearest neighbors of each site. Then

$$\int_0^\beta d\tau \mathcal{H}_F(\bar{\eta}, \eta; \tau) = \frac{JMd}{\beta} \sum_{\mathbf{q} \in BZ} \sum_m \gamma_{\mathbf{q}} \mathbf{S}(\mathbf{q}, \Omega_m) \mathbf{S}(-\mathbf{q}, -\Omega_m), \quad (10)$$

where the so-called structure function $\gamma_{\mathbf{q}} = \frac{1}{z} \sum_{\delta} e^{i\mathbf{q}\delta} = \gamma_{-\mathbf{q}} = \frac{1}{d}(\cos q_1 + \cos q_2 + \dots + \cos q_d)$. From Eq.(8) it follows that

$$\mathbf{S}(-\mathbf{q}, -\Omega_m) = \mathbf{S}^*(\mathbf{q}, \Omega_m) \quad (11)$$

and if we write

$$\mathbf{S}(\mathbf{q}, \Omega_m) = \text{Re}\mathbf{S}(\mathbf{q}, \Omega_m) + i\text{Im}\mathbf{S}(\mathbf{q}, \Omega_m) \quad (12)$$

then

$$\int_0^\beta d\tau \mathcal{H}_F(\bar{\eta}, \eta; \tau) = \frac{dJM}{\beta} \sum_{\mathbf{q} \in BZ} \sum_m \gamma_{\mathbf{q}} [(\text{Re}\mathbf{S}(\mathbf{q}, \Omega_m))^2 + (\text{Im}\mathbf{S}(\mathbf{q}, \Omega_m))^2]. \quad (13)$$

The standard way to decouple four fermion terms is to use Hubbard-Stratonovich representations and introduce some auxiliary Bose fields. The decoupling scheme is not unique and the particular choice of the Bose fields depends which mean field solutions (ordered or disordered for our model) we are going to discuss. Of course, before one starts to use some approximation (usually saddle point approximation) all representations are equivalent and if we are able to calculate the path integrals exactly we shall get the same result.

In the present paper we are considering the ordered phase (the disordered phase which is the most relevant for $d \leq 2$ will be discussed elsewhere [9]) and the Hubbard-Stratonovich decoupling can be done with the help of an auxiliary vector field $\mathcal{M}(\mathbf{q}, \Omega_m)$ which plays the role of the staggered magnetization

$$e^{-\int_0^\beta d\tau \mathcal{H}_F(\bar{\eta}, \eta; \tau)} = \int \mathcal{D}\mu_{\mathcal{M}} \exp \left\{ \sum_{\mathbf{q}, m} \left[-|\mathcal{M}(\mathbf{q}, \Omega_m)|^2 + \sqrt{-\frac{dJM}{\beta}} \gamma_{\mathbf{q}} [\mathcal{M}^*(\mathbf{q}, \Omega_m) \mathbf{S}(\mathbf{q}, \Omega_m) + \mathbf{S}^*(\mathbf{q}, \Omega_m) \mathcal{M}(\mathbf{q}, \Omega_m)] \right] \right\}, \quad (14)$$

and the path integration measure

$$\mathcal{D}\mu_{\mathcal{M}} = \prod_m \prod_{\mathbf{q} \in BZ} \prod_{a=x,y,z} \frac{d\text{Re}\mathcal{M}^a(\mathbf{q}, \Omega_m) d\text{Im}\mathcal{M}^a(\mathbf{q}, \Omega_m)}{\pi}. \quad (15)$$

For Fermi fields Fourier transformations are

$$\eta_{i\alpha}(\tau) = \sum_n \eta_{i\alpha}(\nu_n) e^{-i\nu_n \tau}, \quad (16a)$$

$$\bar{\eta}_{i\alpha}(\tau) = \sum_n \bar{\eta}_{i\alpha}(\nu_n) e^{i\nu_n \tau}, \quad (16b)$$

where $\nu_n = \frac{2\pi(n+1)}{\beta}$ is a Matsubara frequency for Fermi fields. Then

$$\mathbf{S}(\mathbf{q}, \Omega_m) = \frac{\beta}{2M} \sum_{i, n', n} \bar{\eta}_{i\alpha}(\nu_{n'}) \sigma_{\alpha\beta} \eta_{i\beta}(\nu_n) e^{-i\mathbf{q}\mathbf{r}_i} \delta_{\Omega_m, \nu_{n'} - \nu_n}. \quad (17)$$

and for the partition function we get

$$Z = i^M \int \mathcal{D}\mu_\eta \mathcal{D}\mu_{\mathcal{M}} \exp \left\{ - \sum_{\mathbf{q}, m} |\mathcal{M}(\mathbf{q}, \Omega_m)|^2 + \sum_{i,j} \sum_{n', n} \bar{\eta}_{i\alpha}(\nu_{n'}) \mathcal{K}_{n', n; i, j}^{\alpha\beta}(\mathcal{M}) \eta_{j\alpha}(\nu_n) \right\}, \quad (18)$$

where

$$\mathcal{K}_{n', n; i, j}^{\alpha\beta}(\mathcal{M}) = \left[\delta^{\alpha\beta} \left(-i\nu_n \beta + i\frac{\pi}{2} \right) \delta_{n'n} + \sum_{\mathbf{q}} \sqrt{-\frac{dJ\beta}{M}} \gamma_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}_i} \mathcal{M}(\mathbf{q}, \nu_{n'} - \nu_n) \sigma_{\alpha\beta} \right] \delta_{ij}, \quad (19)$$

and the measure for the path integration with respect to Grassmann variables now reads

$$\mathcal{D}\mu_\eta = \prod_{i, n, \alpha} d\bar{\eta}_{i\alpha}(\nu_n) d\eta_{i\alpha}(\nu_n). \quad (20)$$

Integrating with respect to them we obtain

$$Z = i^M \int \mathcal{D}\mu_{\mathcal{M}} e^{-S_{eff}[\mathcal{M}]} = e^{-\beta F}, \quad (21)$$

where

$$S_{eff}[\mathcal{M}] = \sum_{\mathbf{q}, m} |\mathcal{M}(\mathbf{q}, \Omega_m)|^2 - \text{Tr} \ln \mathcal{K}(\mathcal{M}) \quad (22)$$

and F is a free energy.

3 The leading order of the saddle point approximation

In order to deal with the AFM solution we shall choose a frequency independent solution along the z-axis ($\boldsymbol{\pi} = \underbrace{(\pi, \pi, \dots, \pi)}_d$)

$$\mathcal{M}(\mathbf{q}, \Omega_m) = \hat{z} \sqrt{dM\beta J} m \delta_{\mathbf{q}, \boldsymbol{\pi}}. \quad (23)$$

The real parameter m is a staggered magnetization. Then

$$(\mathcal{K}^{MF}(\mathcal{M}))_{n', n; i, j}^{\alpha\beta} = \left[\delta^{\alpha\beta} \left(-i\nu_n \beta + i\frac{\pi}{2} \right) + (-1)^i dJ\beta m \sigma_{\alpha\beta}^z \right] \delta_{n'n} \delta_{ij}, \quad (24)$$

and $(-1)^i = (-1)^{(\mathbf{r}_i)_1 + \dots + (\mathbf{r}_i)_d}$. So the free energy in the mean field leading order takes a form

$$F^{MF}(m) = dJMm^2 - \frac{1}{\beta} \sum_m \ln [1 + e^{\beta E_m}] - \frac{M}{\beta} \ln i, \quad (25)$$

where $\{E_m\}$ is the spectrum of the mean field Hamiltonian

$$\hat{H}^{MF} = \sum_{j, \alpha} \left(\omega_{j, \alpha} \hat{c}_{j\alpha}^\dagger \hat{c}_{j\alpha} + i\frac{\pi}{2\beta} \hat{c}_{j\alpha}^\dagger \hat{c}_{j\alpha} \right), \quad (26)$$

$$\begin{aligned}\omega_{j1} &= (-1)^j dJ\mathcal{m}, \\ \omega_{j2} &= -(-1)^j dJ\mathcal{m}.\end{aligned}$$

The summation with respect to eigenvalues can be done easily with the result

$$\sum_m \ln [1 + e^{\beta E_m}] = M \ln \left(\frac{2}{i} \cosh (d\beta J\mathcal{m}) \right). \quad (27)$$

So for the free energy in the leading order we get

$$F^{MF}(\mathcal{m}) = dJM\mathcal{m}^2 - \frac{M}{\beta} \ln (\cosh (d\beta J\mathcal{m})) - \frac{M}{\beta} \ln 2 \quad (28)$$

Minimization of $F^{MF}(\mathcal{m})$ yields the mean field staggered magnetization equation

$$\mathcal{m} = \frac{1}{2} \tanh (d\beta J\mathcal{m}). \quad (29)$$

Exactly the same result for magnetization one obtains in the mean field approach to the $S = 1/2$ Heisenberg model with the Hamiltonian Eq.(1) working in terms of spin variables.

If the single occupancy condition is disregarded instead of Eqs.(28) and Eqs.(29) we get

$$F_0^{MF}(\mathcal{m}_0) = dJM\mathcal{m}_0^2 - \frac{2M}{\beta} \ln \left(\cosh \left(\frac{d}{2}\beta J\mathcal{m}_0 \right) \right) - \frac{2M}{\beta} \ln 2 \quad (30)$$

and

$$\mathcal{m}_0 = \frac{1}{2} \tanh \left(\frac{d}{2}\beta J\mathcal{m}_0 \right). \quad (31)$$

4 One-loop corrections

Now we write

$$\mathcal{M}(\mathbf{q}, \Omega_m) = \hat{z} \sqrt{dM\beta J\mathcal{m}} \delta_{\mathbf{q}, \boldsymbol{\pi}} + \delta \mathcal{M}(\mathbf{q}, \Omega_m), \quad (32)$$

where $\delta \mathcal{M}(\mathbf{q}, \Omega_m)$ are fluctuations of the magnetization around the mean-field value (the leading order) \mathcal{m} satisfying Eq.(29). Then

$$\mathcal{K}_{n',n;i,j}^{\alpha\beta}(\delta \mathcal{M}) = \left[\delta^{\alpha\beta} \left(-i\nu_n \beta + i\frac{\pi}{2} \right) + (-1)^j dJ\beta \mathcal{m} \sigma_{\alpha\beta}^z \right] \delta_{n'n} \delta_{ij} + \delta \mathcal{N}_{ij}^{\alpha\beta}(\nu_{n'} - \nu_n), \quad (33)$$

where

$$\delta \mathcal{N}_{ij}^{\alpha\beta}(\nu_{n'} - \nu_n) \equiv \sum_{\mathbf{q} \in BZ} \sqrt{-\frac{dJ\beta}{M}} \gamma_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}_i} \delta \mathcal{M}(\mathbf{q}, \nu_{n'} - \nu_n) \sigma_{\alpha\beta} \delta_{ij}. \quad (34)$$

The partition function

$$Z = e^{-\beta F^{MF}} \int \mathcal{D}\mu_{\mathcal{M}} e^{-S_{eff}^{(2)}[\delta\mathcal{M}]}, \quad (35)$$

where

$$S_{eff}^{(2)}[\delta\mathcal{M}] = \sum_m \sum_{\mathbf{q} \in BZ} |\delta\mathcal{M}(\mathbf{q}, \Omega_m)|^2 - \text{Tr} \ln \mathcal{K}(\delta\mathcal{M}), \quad (36)$$

$$\mathcal{D}\mu_{\mathcal{M}} \equiv \prod_m \prod_{\mathbf{q} \in BZ} \frac{d\text{Re}\delta\mathcal{M}(\mathbf{q}, \Omega_m) d\text{Im}\delta\mathcal{M}(\mathbf{q}, \Omega_m)}{\pi}. \quad (37)$$

The superscript (2) means that only the terms of the second order with respect to $\delta\mathcal{M}$ are kept. Thus we take into account only so-called Gaussian fluctuations.

Let us define a matrix G such that its matrix elements has a form

$$G_{n'n; i, j}^{\alpha\beta} = \left[-i\nu_n\beta + i\frac{\pi}{2} - (-1)^\alpha(-1)^j dJ\beta\mathcal{m} \right]^{-1} \delta_{ij} \delta_{\alpha\beta} \delta_{n'n}. \quad (38)$$

This matrix is the one particle propagator evaluated at the saddle point. Then Eq.(33) written in the matrix form (with respect to spin index α and lattice site index i) takes a form

$$\mathcal{K}_{n'n} = G_{n'n}^{-1} - \delta\mathcal{N}(\nu_{n'} - \nu_n) \quad (39)$$

and

$$\begin{aligned} \text{Tr} \ln \mathcal{K}(\delta\mathcal{M}) &= \text{Tr} \ln G^{-1} + \text{Tr} \ln(1 - G\delta\mathcal{N}) \\ &= \text{Tr} \ln G^{-1} - \text{Tr}[G\delta\mathcal{N}] - \frac{1}{2}\text{Tr}[G\delta\mathcal{N}G\delta\mathcal{N}] - \dots \end{aligned}$$

The term which describes the Gaussian fluctuations in more explicit form reads

$$\text{Tr}[G\delta\mathcal{N}G\delta\mathcal{N}] = \sum_{n, m} \text{Sp}[(\overline{\mathcal{M}} - i\tilde{\nu}_n\beta)^{-1} \delta\mathcal{N}(\Omega_m) (\overline{\mathcal{M}} - i\tilde{\nu}_n\beta + i\Omega_m\beta)^{-1} \delta\mathcal{N}(-\Omega_m)], \quad (40)$$

where $\overline{\mathcal{M}}$ is a matrix in the space of i and α indices with the matrix element

$$\overline{\mathcal{M}}_{ij}^{\alpha\beta} = -(-1)^\alpha(-1)^j dJ\beta\mathcal{m} \delta_{ij} \delta_{\alpha\beta}, \quad (41)$$

and Sp is a trace in this space (its element we denote as $|i\alpha\rangle$),

$$\tilde{\nu}_n \equiv \nu_n + \frac{\pi}{2\beta}.$$

So in the one-loop approximation we have for $S_{eff}^{(2)}[\delta\mathcal{M}]$

$$S_{eff}^{(2)} = \sum_{m, \mathbf{q} \in BZ} |\delta\mathcal{M}(\mathbf{q}, \Omega_m)|^2 + \tilde{S}_{eff}^{(2)}[\delta\mathcal{M}] \quad (42)$$

and

$$\tilde{S}_{eff}^{(2)}[\delta\mathcal{M}] = \frac{1}{2} \sum_{i, \alpha, \beta, m} T_{\alpha\beta}(i, m) \langle i\alpha | \delta\mathcal{N}(\Omega_m) | i\beta \rangle \langle i\beta | \delta\mathcal{N}(-\Omega_m) | i\alpha \rangle, \quad (43)$$

where

$$\begin{aligned}
T_{\alpha\beta}(i, m) &\equiv \sum_n \langle i\alpha | (\overline{m} - i\tilde{\nu}_n\beta)^{-1} | i\alpha \rangle \langle i\beta | (\overline{m} - i\tilde{\nu}_n\beta + i\Omega_m\beta)^{-1} | i\beta \rangle \\
&= \sum_n \frac{1}{i\tilde{\nu}_n\beta + (-1)^\alpha (-1)^i dJ\beta m} \frac{1}{i\tilde{\nu}_n\beta - i\Omega_m\beta + (-1)^\beta (-1)^i dJ\beta m}. \quad (44)
\end{aligned}$$

The summation with respect to Matsubara frequencies can be easily done with the following result

$$\begin{aligned}
\Phi(A, B; \Omega_m) &\equiv \sum_n \frac{1}{i\tilde{\nu}_n\beta - A} \frac{1}{i\tilde{\nu}_n\beta - B - i\Omega_m\beta} \\
&= \frac{1}{i\Omega_m\beta - A + B} \frac{\sinh[\frac{1}{2}(A - B)]}{i \sinh[\frac{1}{2}(A + B)] + \cosh[\frac{1}{2}(A - B)]},
\end{aligned}$$

if $A \neq B$, and

$$\Phi(A, A; \Omega_m) = -\delta_{m0} \frac{1 - i \sinh A}{2 \cosh^2 A}. \quad (45)$$

We need to know only the expression for the special choice: $B = -A$. In this case

$$\Phi(A, -A; \Omega_m) = -\frac{2A \tanh A}{(\Omega_m\beta)^2 + 4A^2} - \frac{i\Omega_m\beta \tanh A}{(\Omega_m\beta)^2 + 4A^2}. \quad (46)$$

So we get ($A \equiv dJ\beta m$)

$$T_{11}(j, m) = -\delta_{m0} \frac{1 - i(-1)^j \sinh A}{2 \cosh^2 A} \equiv -\delta_{m0} [\kappa - i(-1)^j \rho], \quad (47a)$$

$$T_{22}(j, m) = -\delta_{m0} [\kappa + i(-1)^j \rho], \quad (47b)$$

$$T_{12}(j, m) = -\frac{2A \tanh A}{(\Omega_m\beta)^2 + 4A^2} - \frac{i(-1)^j \Omega_m\beta \tanh A}{(\Omega_m\beta)^2 + 4A^2} \equiv \xi(m) + i(-1)^j \zeta(m) \quad (48a)$$

and

$$T_{21}(j, m) = \xi(m) - i(-1)^j \zeta(m). \quad (48b)$$

Taking into account the Eq.(29) for the mean field magnetization we get

$$\kappa = \frac{1}{2}(1 - 4m^2).$$

If the single occupancy condition is neglected we get instead ($A_0 \equiv dJ\beta m_0$)

$$\kappa_0 = \frac{1}{4 \cosh^2 \frac{A_0}{2}} = \frac{1}{4}(1 - 4m_0^2)$$

and

$$\xi_0(m) = -\frac{2A_0 \tanh \frac{A_0}{2}}{(\Omega_m \beta)^2 + 4A_0^2}, \quad \zeta_0(m) = -\frac{\Omega_m \beta \tanh \frac{A_0}{2}}{(\Omega_m \beta)^2 + 4A_0^2}.$$

From Eqs.(29) and (31) it follows that $\xi(m)|_{A=A_0} = \xi_0(m)$ and $\zeta(m)|_{A=A_0} = \zeta_0(m)$. From Eq.(34) we have

$$\langle i1 | \delta \mathcal{N}(\Omega_m) | i1 \rangle = \sum_{\mathbf{q} \in BZ} \sqrt{-\frac{dJ\beta}{M}} \gamma_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}_i} \delta \mathcal{M}^z(\mathbf{q}, \Omega_m), \quad (49a)$$

$$\langle i2 | \delta \mathcal{N}(\Omega_m) | i2 \rangle = - \sum_{\mathbf{q} \in BZ} \sqrt{-\frac{dJ\beta}{M}} \gamma_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}_i} \delta \mathcal{M}^z(\mathbf{q}, \Omega_m), \quad (49b)$$

$$\langle i1 | \delta \mathcal{N}(\Omega_m) | i2 \rangle = \sum_{\mathbf{q} \in BZ} \sqrt{-\frac{dJ\beta}{M}} \gamma_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}_i} [\delta \mathcal{M}^x(\mathbf{q}, \Omega_m) - i\delta \mathcal{M}^y(\mathbf{q}, \Omega_m)], \quad (50a)$$

$$\langle i2 | \delta \mathcal{N}(\Omega_m) | i1 \rangle = \sum_{\mathbf{q} \in BZ} \sqrt{-\frac{dJ\beta}{M}} \gamma_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}_i} [\delta \mathcal{M}^x(\mathbf{q}, \Omega_m) + i\delta \mathcal{M}^y(\mathbf{q}, \Omega_m)], \quad (50b)$$

and $\tilde{S}_{eff}^{(2)}$ defined in Eq.(43) can be rewritten as

$$\tilde{S}_{eff}^{(2)} = \tilde{S}_L^{(2)} + \tilde{S}_T^{(2)},$$

where the longitudinal part

$$\tilde{S}_L^{(2)} = \frac{1}{2} \sum_{i,m} \{ T_{11}(m) \langle i1 | \delta \mathcal{N}(\Omega_m) | i1 \rangle \langle i1 | \delta \mathcal{N}(-\Omega_m) | i1 \rangle + T_{22}(m) \langle i2 | \delta \mathcal{N}(\Omega_m) | i2 \rangle \langle i2 | \delta \mathcal{N}(-\Omega_m) | i2 \rangle \}$$

and the transverse part

$$\tilde{S}_T^{(2)} = \frac{1}{2} \sum_{i,m} \{ T_{12}(m) \langle i1 | \delta \mathcal{N}(\Omega_m) | i2 \rangle \langle i2 | \delta \mathcal{N}(-\Omega_m) | i1 \rangle + T_{21}(m) \langle i2 | \delta \mathcal{N}(\Omega_m) | i1 \rangle \langle i1 | \delta \mathcal{N}(-\Omega_m) | i2 \rangle \}.$$

So using Eqs.(47) and (49) we obtain

$$\tilde{S}_L^{(2)} = dJ\beta\kappa \sum_{\mathbf{q} \in BZ} \gamma_{\mathbf{q}} |\delta \mathcal{M}^z(\mathbf{q}, 0)|^2 \quad (51)$$

and with the help of Eqs.(48) and (50)

$$\begin{aligned} \tilde{S}_T^{(2)} = & \frac{1}{2} (-dJ\beta) \sum_{m, \mathbf{q} \in BZ} \{ \gamma_{\mathbf{q}} [\delta \mathcal{M}^x((\mathbf{q}, \Omega_m)) - i\delta \mathcal{M}^y((\mathbf{q}, \Omega_m))] [\delta \mathcal{M}^x(-\mathbf{q}, -\Omega_m) + i\delta \mathcal{M}^y(-\mathbf{q}, -\Omega_m)] \xi(m) \\ & + \gamma_{\mathbf{q}} [\delta \mathcal{M}^x((\mathbf{q}, \Omega_m)) + i\delta \mathcal{M}^y((\mathbf{q}, \Omega_m))] [\delta \mathcal{M}^x(-\mathbf{q}, -\Omega_m) - i\delta \mathcal{M}^y(-\mathbf{q}, -\Omega_m)] \xi(m) \\ & - \gamma_{\mathbf{q}} [\delta \mathcal{M}^x((\mathbf{q}, \Omega_m)) - i\delta \mathcal{M}^y((\mathbf{q}, \Omega_m))] [\delta \mathcal{M}^x(-\mathbf{q} - \boldsymbol{\pi}, -\Omega_m) + i\delta \mathcal{M}^y(-\mathbf{q} - \boldsymbol{\pi}, -\Omega_m)] \zeta(m) \\ & - \gamma_{\mathbf{q}} [\delta \mathcal{M}^x((\mathbf{q}, \Omega_m)) + i\delta \mathcal{M}^y((\mathbf{q}, \Omega_m))] [\delta \mathcal{M}^x(-\mathbf{q} - \boldsymbol{\pi}, -\Omega_m) - i\delta \mathcal{M}^y(-\mathbf{q} - \boldsymbol{\pi}, -\Omega_m)] \zeta(m) \} . \end{aligned}$$

So

$$\begin{aligned}
\tilde{S}_{eff}^{(2)} &= dJ\beta\kappa \sum_{\mathbf{q} \in RBZ} |\gamma_{\mathbf{q}}| \{ |\delta\mathcal{M}^z(\mathbf{q}, 0)|^2 - |\delta\mathcal{M}^z(\mathbf{q} + \boldsymbol{\pi}, 0)|^2 \} \\
&+ dJ\beta \sum_m \sum_{\mathbf{q} \in RBZ} |\gamma_{\mathbf{q}}| \left\{ [-|\delta\mathcal{M}^x(\mathbf{q}, \Omega_m)|^2 + |\delta\mathcal{M}^x(\mathbf{q} + \boldsymbol{\pi}, \Omega_m)|^2 \right. \\
&- |\delta\mathcal{M}^y(\mathbf{q}, \Omega_m)|^2 + |\delta\mathcal{M}^y(\mathbf{q} + \boldsymbol{\pi}, \Omega_m)|^2] \xi(m) \\
&+ 2\text{Im} [\delta\mathcal{M}^x(\mathbf{q}, \Omega_m)\delta\mathcal{M}^y(-\mathbf{q} - \boldsymbol{\pi}, -\Omega_m) \\
&- \delta\mathcal{M}^y(\mathbf{q}, \Omega_m)\delta\mathcal{M}^x(-\mathbf{q} - \boldsymbol{\pi}, -\Omega_m)] \zeta(m) \left. \right\} .
\end{aligned} \tag{52}$$

The part of $S_{eff}^{(2)}$ which describes the transverse fluctuations for each \mathbf{q} vector and for each value of m consists of four 2×2 blocks mixing the real and imaginary components of $\delta\mathcal{M}^x$ and $\delta\mathcal{M}^y$ at \mathbf{q} and $\mathbf{q} + \boldsymbol{\pi}$ in pairs. The matrices corresponding to these blocks are given by ($\mathbf{q} \in RBZ$)

$$\begin{pmatrix} 1 - d\beta J |\gamma_{\mathbf{q}}| \xi(m) & \pm d\beta J |\gamma_{\mathbf{q}}| \zeta(m) \\ \pm d\beta J |\gamma_{\mathbf{q}}| \zeta(m) & 1 + d\beta J |\gamma_{\mathbf{q}}| \xi(m) \end{pmatrix} \tag{53}$$

with the eigenvalues

$$\lambda_{\pm}(\mathbf{q}, m) = 1 \pm \frac{2d\mathcal{M}|\gamma_{\mathbf{q}}|}{\sqrt{(\Omega_m J^{-1})^2 + (2d\mathcal{M})^2}} . \tag{54}$$

We see that $\lambda_{-}(\mathbf{q}, m)$ vanishes at $\Omega_m = 0$ when $\mathbf{q} = 0$. The corresponding eigenmodes are the Goldstone modes (spin waves) which appear due to the fact that AFM (ordered) phase is a phase with spontaneously broken symmetry.

So from Eq.(35) we obtain up to some inessential constant the free energy including one-loop corrections

$$\begin{aligned}
F &= F^{MF} + \frac{2}{\beta} \sum_{\mathbf{q} \in RBZ} \sum_{m>0} \ln(\lambda_{+}(\mathbf{q}, m)\lambda_{-}(\mathbf{q}, m)) + \frac{1}{\beta} \sum'_{\mathbf{q} \in RBZ} \ln(1 - \gamma_{\mathbf{q}}^2) \\
&+ \frac{1}{2\beta} \sum_{\mathbf{q} \in RBZ} \ln(1 - d^2\beta^2 J^2 \kappa^2 \gamma_{\mathbf{q}}^2) ,
\end{aligned} \tag{55}$$

where $\sum'_{\mathbf{q} \in RBZ}$ means that the point $\mathbf{q} = 0$ should be excluded. The summation with respect to Matsubara frequencies can be done with help of the formula

$$\sum_{m>0} \ln \left(1 - \frac{A^2}{(\Omega_m \beta)^2 + B^2} \right) = \ln \left(\frac{B \sinh \frac{\sqrt{B^2 - A^2}}{2}}{\sqrt{B^2 - A^2} \sinh \frac{B}{2}} \right) \tag{56}$$

and we get finally for the free energy

$$F = F^{MF} + \frac{2}{\beta} \sum'_{\mathbf{q} \in RBZ} \ln \left[\frac{\sinh \left(d\mathcal{M}\beta J \sqrt{1 - \gamma_{\mathbf{q}}^2} \right)}{\sinh(d\mathcal{M}\beta J)} \right] + \frac{2}{\beta} \ln \frac{d\mathcal{M}\beta J}{\sinh(d\mathcal{M}\beta J)}$$

$$+\frac{1}{2\beta} \sum_{\mathbf{q} \in RBZ} \ln \left[1 - \frac{d^2}{4} \beta^2 J^2 (1 - 4m^2)^2 \gamma_{\mathbf{q}}^2 \right] . \quad (57)$$

Now taking the limit of zero temperature $\beta \rightarrow \infty$ we get the energy of the ground state per site (there is no contribution to the limiting expression from the last term)

$$\frac{F}{M} \xrightarrow{T \rightarrow 0} \frac{E_0^{(0)}}{M} = -\frac{dJ}{4} + \frac{dJ}{M} \sum_{\mathbf{q} \in RBZ} \left[\sqrt{1 - \gamma_{\mathbf{q}}^2} - 1 \right] , \quad (58)$$

which is exactly the ground state energy per site obtained in linear spin-wave approximation [12] for spin 1/2.

It is easy to check that the same zero temperature result will be obtained when the single occupancy condition is disregarded.

On the contrary, at finite temperatures taking into account the single occupancy condition gives different values of the different thermodynamical quantities, e.g. for the free energy this affects in changing the temperature dependence of the magnetization m and changing the longitudinal part. Figs.1 and 2 show the difference of the results for the cases when single occupancy condition is taken into account (solid line) and when it is disregarded (dashed line). On Fig.1 the temperature dependence of the internal energy and entropy and on Fig.2 of the specific heat are given. From our numerical calculations we found that only in the interval $0 \leq t \leq 0.13$ the difference is negligibly small. In this interval the specific heat goes to zero as $C_v = at^\alpha$ with $\alpha = 3$, as it should [12].

5 Conclusion

We have studied the magnetic (ordered) phase of the isotropic spin 1/2 HAFM defined on the simple d-dimensional hypercubic lattice using fermionized spin operators and saddle point approximation. Single occupancy condition which is needed when spin operators are bosonized or fermionized is taken into account by the method of Popov and Fedotov.

It is shown that inclusion of the one-loop corrections to the leading order of the saddle point approximation leads in the limit of zero temperature exactly to the same expression for the ground state energy which one obtains for the next-to-leading term in the linear spin wave theory, and this result does not depend if the single occupancy condition is disregarded or not.

It is worthwhile to mention that in the mean field theory of the spin 1/2 HAFM where Schwinger bosons are used [5] one obtains the same result of the linear spin wave theory at zero temperature already in the leading order and taking into account the single occupancy condition is crucial in this case.

We demonstrated that in our approach taking into account the single occupancy condition changes finite temperature results considerably.

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Figure captions

Fig.1 Internal energy per site E/M and entropy per site S/M versus dimensionless temperature $t = (\beta J)^{-1}$ for the 3-dimensional cubic lattice. Dashed and solid lines correspond to the cases when single occupancy condition is disregarded and taken into account respectively.

Fig.2 Temperature dependence of the specific heat per site $C_v/(K_B t)$ for the 3-dimensional cubic lattice. Dashed and solid lines correspond to the cases when single occupancy condition is disregarded and taken into account respectively.



