

Magnetic properties of antiferromagnetic quantum Heisenberg spin systems with a strict single particle site occupation

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Abstract. We work out the magnetization and susceptibility of Heisenberg- and XXZ-model antiferromagnet spin-1/2 systems in D dimensions under a rigorous constraint of single particle site occupancy. Quantum and thermal fluctuations are taken into account up to the first order in a loop expansion beyond the Néel state mean field solution. We discuss the results, their validity in the vicinity of the critical point and compare them with the results obtained by means of a spin wave approach.

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1 Introduction

Recent work on quantum spin systems discuss the possible existence of spin liquid states and in two-dimensional space dimensions the competition or phase transition between spin liquid states and an antiferromagnetic Néel state which is naturally expected to describe Heisenberg type systems [1–4]. It is also known that undoped superconducting systems show an antiferromagnetic phase [5].

In the following we focus our attention on a Néel phase description of quantum spin systems described by Heisenberg models. More precisely we present below a detailed study of the magnetization and the parallel magnetic susceptibility of Heisenberg antiferromagnetic spin-1/2 systems on D -dimensional lattices at finite temperature. The aim of the work is the study of the physical pertinence of the Néel state ansatz as a mean-field approximation in the temperature interval $0 < T < T_c$ where T_c is the critical temperature. In order to get a precise answer to this point we work out the quantum fluctuation contributions beyond the mean-field approximation under the constraint of *strict* single site occupancy [6–8,15] which allows to avoid a Lagrange multiplier approximation [10]. The results are also extended to anisotropic XXZ systems and compared to those obtained in the framework of the spin wave approach.

The paper is organized as follows. In Section 2 we present the derivation of the partition function under the single particle site occupation constraint. The mean-field and first order loop expansion term contributions are derived in Section 3. In Section 4 we determine the magne-

tization and the magnetic susceptibility, and discuss the results obtained at the different levels of approximation. Comments are presented and conclusions are drawn in Section 5. Details of calculations are presented in the appendix, Section 6.

2 Fermionization of the Heisenberg model and the partition function

The Heisenberg antiferromagnet Hamiltonian (HAFM) in the presence of a local magnetic field \vec{B}_i reads

$$H = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_i \vec{B}_i \cdot \vec{S}_i \quad (1)$$

where $J_{ij} < 0$ and the sums in the first term run over nearest-neighbour sites $\langle i,j \rangle$ on a D -dimensional hypercubic lattice.

The $S = 1/2$ spin vector operators are expressed in terms of fermionic creation and annihilation operators $\{f_{i\lambda}, f_{i\alpha}^\dagger\}$

$$\vec{S}_i = f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\lambda} f_{i\lambda} \quad (2)$$

where the $\vec{\sigma}_{\alpha\lambda}$ vector components are Pauli matrices.

The transformation is rigorous if $\sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1$. The Fock space constructed with the fermionic operators f, f^\dagger is not in bijective correspondence with the Hilbert space of the spin states. Indeed, in Fock space and for spin-1/2 particles, the occupation of each site i can be characterized by the states $|n_{i,\uparrow}, n_{i,\downarrow}\rangle$ with $n_{i,\alpha} \in \{0, 1\}$, that is states

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$|0, 0\rangle$, $|1, 0\rangle$, $|0, 1\rangle$ and $|1, 1\rangle$. But in the case of single occupancy the states $|0, 0\rangle$ and $|1, 1\rangle$ which are excluded as *unphysical* in the present case have to be eliminated. This is done by means of a projection procedure proposed by Popov and Fedotov [6] and generalized to $SU(N)$ symmetry in reference [8].

Introducing the projection operator $\tilde{P} = e^{i\frac{\pi}{2}\tilde{N}}$ where $\tilde{N} = \sum_{i,\sigma} f_{i\sigma}^\dagger f_{i\sigma}$ is the number operator the partition function \mathcal{Z} reads

$$\mathcal{Z} = \text{Tr} \left[e^{-\beta H} \tilde{P} \right]$$

where β is the inverse temperature. On each site i the contributions of states $|0, 0\rangle$ and $|1, 1\rangle$ to \mathcal{Z} eliminate each other. Indeed

$$\begin{aligned} & \langle 0, 0 | e^{-\beta H} \cdot e^{i\frac{\pi}{2} * 0} | 0, 0 \rangle_i + \langle 1, 1 | e^{-\beta H} \cdot e^{i\frac{\pi}{2} * 2} | 1, 1 \rangle_i \\ & + \langle 1, 0 | e^{-\beta H} \cdot e^{i\frac{\pi}{2}} | 1, 0 \rangle_i + \langle 0, 1 | e^{-\beta H} \cdot e^{i\frac{\pi}{2}} | 0, 1 \rangle_i \\ & = i(\langle 1, 0 | e^{-\beta H} | 1, 0 \rangle_i + \langle 1, 0 | e^{-\beta H} | 1, 0 \rangle_i). \end{aligned}$$

Hence the partition function

$$\mathcal{Z} = \frac{1}{i} \cdot \text{Tr} \left[e^{-\beta(H - \mu \tilde{N})} \right] \quad (3)$$

with the imaginary ‘‘chemical potential’’ $\mu = i\frac{\pi}{2\beta}$ describes a system with strictly one particle per lattice site, in contrast with the usual method which introduces an average projection by means of a real Lagrange multiplier [9, 10].

3 Mean field and one-loop approximations

Following the usual procedure we transform the Heisenberg Hamiltonian into a bilinear fermionic expression using a Hubbard-Stratonovich decoupling. Starting from (3) this leads to

$$\begin{aligned} \mathcal{Z} &= \frac{1}{\mathcal{Z}_0} \int \prod_i \mathcal{D}\vec{\varphi}_i \int_{\xi_{i\sigma}(\beta) = i\xi_{i\sigma}(0)} \\ &\times \mathcal{D}(\xi_{i\sigma}^*, \xi_{i\sigma}) e^{-\int_0^\beta d\tau \left[\sum_{i,\sigma} \xi_{i\sigma}^* \frac{\partial}{\partial \tau} \xi_{i\sigma} + S_0[\varphi(\tau)] + \sum_i \vec{\varphi}_i \cdot \vec{S}_i(\tau) \right]} \end{aligned} \quad (4)$$

where τ is an imaginary time and

$$\begin{aligned} \mathcal{Z}_0 &= \int \prod_i \mathcal{D}\vec{\varphi}_i e^{-\int_0^\beta d\tau S_0[\vec{\varphi}(\tau)]} \\ S_0[\vec{\varphi}(\tau)] &= \frac{1}{2} \sum_{i,j} J_{ij}^{-1} (\vec{\varphi}_i(\tau) - \vec{B}_i) \cdot (\vec{\varphi}_j(\tau) - \vec{B}_j) \end{aligned}$$

where $\vec{\varphi}$ stands for the Hubbard-Stratonovich decoupling fields and ξ for the *Grassmann* variables.

After integration over the bilinear fermionic $\{\xi_{i\sigma}\}$ terms which appear in the action \mathcal{Z} takes the form

$$\mathcal{Z} = \frac{1}{\mathcal{Z}_0} \int \mathcal{D}\vec{\varphi} e^{-S_{eff}[\vec{\varphi}]}$$

where

$$\begin{aligned} S_{eff}[\vec{\varphi}] &= \int_0^\beta d\tau S_0[\vec{\varphi}(\tau)] \\ &- \sum_i \ln 2\text{ch} \frac{\beta}{2} \|\vec{\varphi}_i(\omega = 0)\| + \text{Tr} \left\{ \sum_{n=1}^{\infty} \frac{1}{n} (G_0 M_1)^n \right\} \end{aligned} \quad (5)$$

and $(\vec{\varphi}_i(\omega) = 0)$ is the Fourier transform of $\vec{\varphi}_i(\tau)$. The propagator G_0 and M_1 are defined in matrix form in appendix A.1.

In a loop expansion beyond the mean-field approximation $\vec{\varphi}$ the effective action given by (5) is expanded in a Taylor series

$$\begin{aligned} S_{eff}[\vec{\varphi}] &= \\ & S_{eff} \Big|_{[\vec{\varphi}]} + \frac{\partial S_{eff}}{\partial \vec{\varphi}} \Big|_{[\vec{\varphi}]} \delta\vec{\varphi} + \frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \vec{\varphi}^2} \Big|_{[\vec{\varphi}]} \delta\vec{\varphi}^2 + \mathcal{O}(\delta\vec{\varphi}^3) \end{aligned}$$

to second order (one-loop contribution) in the fluctuations $\delta\vec{\varphi}^2$ of $\vec{\varphi} = \vec{\varphi} + \delta\vec{\varphi}$. Since the mean field $\vec{\varphi}$ is chosen in such a way that $\frac{\partial S_{eff}}{\partial \vec{\varphi}} \Big|_{[\vec{\varphi}]} \delta\vec{\varphi} = 0$ one gets the set of coupled self-consistent equations

$$\sum_j J_{ij}^{-1} [\vec{\varphi}_j - \vec{B}_j] = \frac{1}{2} \frac{\vec{\varphi}_i}{\varphi_i} \text{th} \left[\frac{\beta \varphi_i}{2} \right]$$

which fixes the fields $\vec{\varphi}$.

In the following we consider a Néel mean-field order $\vec{\varphi}_i(\tau) = (-1)^{\vec{\pi} \cdot \vec{r}_i} \varphi^z \vec{e}_z = \varphi_i^z \vec{e}_z$ where $\vec{\pi}$ is the Brillouin spin sublattice vector. The magnetic field applied to the system is also chosen to be aligned along the direction \vec{e}_z . The partition function can be decomposed into a product of three terms

$$\mathcal{Z} = \mathcal{Z}_{MF} \cdot \mathcal{Z}_{zz} \cdot \mathcal{Z}_{+-}$$

where \mathcal{Z}_{MF} , \mathcal{Z}_{zz} and \mathcal{Z}_{+-} are given by

$$\begin{aligned} \mathcal{Z}_{MF} &= e^{-S_{eff} \Big|_{[\vec{\varphi}]}} \\ \mathcal{Z}_{zz} &= \frac{1}{\mathcal{Z}_0^{zz}} \int \mathcal{D}\varphi^z e^{-\frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \varphi^{z2}} \Big|_{[\vec{\varphi}]} \delta\varphi^{z2}} \\ \mathcal{Z}_{+-} &= \frac{1}{\mathcal{Z}_0^{+-}} \int \mathcal{D}(\varphi^+, \varphi^-) e^{-\frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \varphi^+ \partial \varphi^-} \Big|_{[\vec{\varphi}]} \delta\varphi^+ \cdot \delta\varphi^-} \end{aligned}$$

with

$$\begin{aligned} S_{eff} \Big|_{[\vec{\varphi}]} &= \\ & \frac{\beta}{2} \sum_{i,j} J_{ij}^{-1} [(\vec{\varphi}_i^z - B_i^z) \cdot (\vec{\varphi}_j^z - B_j^z)] - \sum_i \ln 2\text{ch} \frac{\beta}{2} \|\vec{\varphi}_i^z\| \end{aligned}$$

$$\frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \varphi^z \partial \varphi^z} \Big|_{[\bar{\varphi}]} \delta \varphi^{z^2} = \sum_{\omega} \sum_{i,j} \frac{\beta}{2} \left[J_{ij}^{-1} - \left(\frac{\beta}{4} \text{th} \left(\frac{\beta}{2} \bar{\varphi}_i^z \right) \right) \delta_{ij} \delta(\omega=0) \right] \delta \varphi_i^z(-\omega) \delta \varphi_j^z(\omega)$$

$$\begin{aligned} \frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \varphi^+ \partial \varphi^-} \Big|_{[\bar{\varphi}]} \delta \varphi^+ \delta \varphi^- = \\ \sum_{\omega} \sum_{i,j} \frac{\beta}{2} \left[\frac{1}{2} J_{ij}^{-1} - \left(\frac{1}{2} \frac{\text{th} \left(\frac{\beta}{2} \bar{\varphi}_i^z \right)}{\bar{\varphi}_i^z - i\omega} \right) \delta_{ij} \right] \delta \varphi_i^+(-\omega) \delta \varphi_j^-(\omega) \\ + \sum_{\omega} \sum_{i,j} \frac{\beta}{2} \left[\frac{1}{2} J_{ij}^{-1} \right] \delta \varphi_i^+(\omega) \delta \varphi_j^-(\omega) \quad (6) \end{aligned}$$

\mathcal{Z}_{MF} is the mean field contribution, \mathcal{Z}_{zz} and \mathcal{Z}_{+-} are the one-loop contributions respectively for the longitudinal part $\delta \varphi^z$ and the transverse parts of $\bar{\varphi}$, $\delta \varphi^{+-}$, which take account of the fluctuations around the mean-field value $\bar{\varphi}^z$.

The contributions \mathcal{Z}_{zz} and \mathcal{Z}_{+-} are quadratic in the field variables $\delta \varphi^z, \delta \varphi^{+-}$ and can be worked out in the presence of a staggered magnetic field B_i^z . Studies involving a uniform magnetic field acting on antiferromagnet quantum spin systems can also be found in reference [8].

4 Magnetization and susceptibility of d-dimensional systems

4.1 Magnetization

The fields $\{\bar{\varphi}_i\}$ can be related to the magnetizations $\{\bar{m}_i\}$ as shown in Appendix A.2 and the free energy can be expressed in terms of this order parameter, see Appendix A.3. The magnetization m on site i is the sum of a mean field contribution $\bar{m} = -\frac{1}{\beta} \frac{\partial \ln \mathcal{Z}_{MF}}{\partial B^z}$, a transverse contribution $\delta m_{+-} = -\frac{1}{\beta} \frac{\partial \ln \mathcal{Z}_{+-}}{\partial B^z}$ and a longitudinal contribution $\delta m_{zz} = -\frac{1}{\beta} \frac{\partial \ln \mathcal{Z}_{zz}}{\partial B^z}$. For a small magnetic field \bar{B} a linear approximation leads to $m = \bar{m} + \delta m_{zz} + \delta m_{+-}$ where

$$\begin{aligned} \bar{m} &= \frac{1}{2} \text{th} \frac{\beta}{2} D|J| \bar{m} \\ \delta m_{zz} &= -\frac{1}{N_p \beta} \sum_{\vec{k} \in SBZ} \frac{8\bar{m} \Delta \tilde{m}_0 (1 - 4\bar{m}^2) \left(\frac{\beta D|J| \gamma_{\vec{k}}}{2} \right)^2}{\left[1 - \left(\frac{\beta D|J| \gamma_{\vec{k}}}{2} \right)^2 (1 - 4\bar{m}^2)^2 \right]} \\ \delta m_{+-} &= \frac{(1 + 2D|J| \Delta \tilde{m}_0)}{4\bar{m}} - \frac{1}{N_p} \\ &\quad \times \sum_{\vec{k} \in SBZ} \frac{(1 + 2D|J| \Delta \tilde{m}_0 (1 - \gamma_{\vec{k}}^2))}{\sqrt{1 - \gamma_{\vec{k}}^2}} \\ &\quad \times \frac{1}{\left[\text{th} \left(\beta D|J| \bar{m} \sqrt{1 - \gamma_{\vec{k}}^2} \right) \right]} \end{aligned}$$

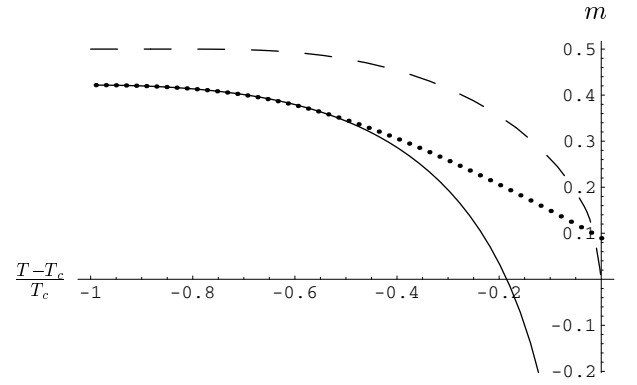


Fig. 1. Magnetization in a 3D Heisenberg antiferromagnet cubic lattice. Dashed line: Mean field magnetization, Dotted line: Spin wave magnetization, Full line: One-loop corrected magnetization.

N_p is the number of spin-1/2 sites, $\Delta \tilde{m}_0 = \frac{\beta}{4} \frac{(1 - 4\bar{m}^2)}{1 - \frac{\beta}{2} D|J| (1 - 4\bar{m}^2)}$ and $\gamma_{\vec{k}} = \frac{1}{D} \sum_{\vec{\eta} \in n.n.} \cos(\vec{k} \cdot \vec{\eta})$, see Appendix A.3 for details of the derivation.

At low temperature ($T \rightarrow 0$) the magnetization goes over to the corresponding spin-wave expression [7, 11–13], which reads

$$\begin{aligned} m &= 1 - \frac{1}{N_p} \sum_{\vec{k} \in SBZ} \frac{1}{\text{th} \left(\frac{\beta D|J|}{2} \sqrt{1 - \gamma_{\vec{k}}^2} \right)} \cdot \frac{1}{\sqrt{1 - \gamma_{\vec{k}}^2}} \\ &= \bar{m} + \delta m \end{aligned}$$

where $\bar{m} = 1/2$ is the mean-field contribution and δm is generated by thermal and quantum fluctuations.

Figure 1 shows the magnetization m in the mean-field, the one-loop and the spin wave approach for temperatures $T \leq T_c$ where $T_c = D|J|/2$ corresponds to the critical point. One observes a sizable contribution of the quantum and thermal fluctuations generated by the loop contribution over the whole range of temperatures as well as an excellent and expected agreement between the quantum corrected and the spin wave result at very low temperatures.

The magnetization shows a singularity in the neighbourhood of the critical point. This behaviour can be read from the analytical expressions of δm_{+-} and δm_{zz} and is generated by the $|\vec{k}| = 0$ mode which leads to $\gamma_{\vec{k}} = 1$ and by cancellation of \bar{m} . The Néel state mean-field approximation is a realistic description at very low T . With increasing temperature this is no longer the case. The chosen ansatz breaks a symmetry whose effect is amplified as the temperature increases and leads to the well-known divergence disease observed close to T_c . Hence if higher order contributions in the loop expansion cannot cure the singularity the Néel state antiferromagnetic ansatz does not describe the physical symmetries of the system at the mean-field level at temperatures in the neighbourhood of the critical point. Consequently it is not a pertinent mean-field approximation for the description of the system.

The discrepancy can be quantified by means of the quantity $\frac{|\Delta m|}{\bar{m}}$ where $\Delta m = m - \bar{m} = \delta m_{zz} + \delta m_{+-}$.

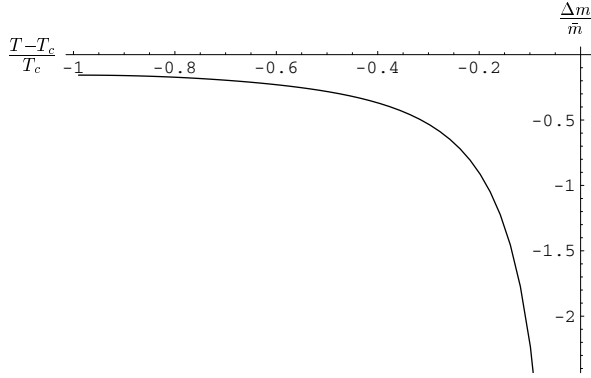


Fig. 2. Ginzburg criterion $\frac{\Delta m}{\bar{m}}$ for the 3D Heisenberg model.

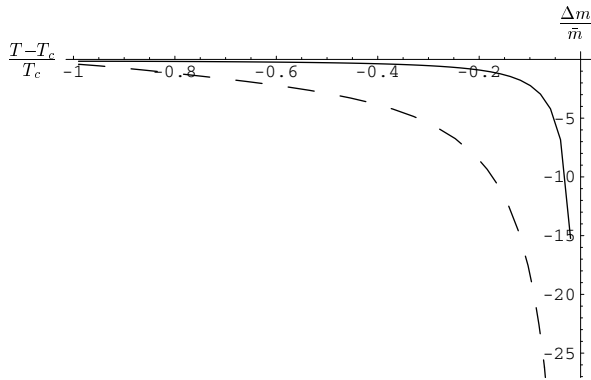


Fig. 3. Comparison of the Ginzburg criterion for 2D (dashed line) and 3D (full line) Heisenberg model.

Figure 2 shows the result. The relation $\frac{|\Delta m|}{\bar{m}} < 1$ (Ginzburg criterion) fixes a limit temperature $T_{\text{lim}}^{\bar{m}}$ above which the quantum and thermal fluctuations generate larger contributions than the mean-field. For 3D systems this leads to $T_{\text{lim}} \simeq 0.8T_c$, for 2D systems the criterion is never satisfied except maybe for very low temperature, see Figure 2.

The pathology is the stronger the smaller the space dimensionality. It is also easy to see on the expression of the magnetization that, as expected, the contributions of the quantum fluctuations decrease with increasing D . As can be seen in the Figure 3, the saddle point breaks down earlier in two than in three dimensions.

In fact, the Heisenberg model spin wave spectrum shows a Goldstone mode as a consequence of the symmetry breaking by the Néel state. When $|\vec{k}|$ goes to zero

$$\omega_{\vec{k}} = ZDS\sqrt{1 - \gamma_{\vec{k}}^2}$$

$$\lim_{\vec{k} \rightarrow \vec{0}} \omega_{\vec{k}} \sim |\vec{k}|.$$

The zero mode destroys the long range order in 1D and 2D as expected from the Mermin-Wagner theorem [14].

In the case of the XXZ-model the Hamiltonian of the system can be written

$$H^{XXZ} = -\frac{J}{2} \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + (1 + \delta) S_i^z S_j^z)$$

where δ governs the anisotropy. In this case the excitation spectrum shows a finite $|\vec{k}| = 0$ energy $\omega_{\vec{k}}$

$$\omega_{\vec{k}} = ZDS\sqrt{1 - \left(\frac{J}{J + \Delta}\gamma_{\vec{k}}\right)^2}$$

$$\lim_{\vec{k} \rightarrow \vec{0}} \omega_{\vec{k}} \sim \sqrt{1 - \left(\frac{1}{1 + \delta}\right)^2 \left(1 - \frac{\vec{k}^2}{2D}\right)}.$$

In Appendix A.4 we develop explicitly the expressions of the free energy, magnetization and susceptibility. By examination the expressions show that the zero momentum mode is no longer responsible for a breakdown of the saddle point procedure near $T_c^{XXZ} = \frac{D|J + \Delta|}{2}$. However the magnetization of the XXZ-model remains infinite near T_c^{XXZ} . This is due to the common disease shared with the Heisenberg model that the mean field magnetization appearing in the denominator of δm_{+-} goes to zero near the critical temperature. One concludes that the mean-field Néel state solution makes only sense at low temperatures, that is for $T \lesssim T_{\text{lim}}$, whatever the degree of symmetry breaking induced by the mean-field ansatz.

4.2 Susceptibility

We consider the parallel susceptibility χ_{\parallel} which characterizes a magnetic system on which a magnetic field is applied in the Oz direction. The expression of χ_{\parallel} decomposes again into three contributions

$$\chi_{\parallel} = -\frac{1}{N_p} \frac{\partial^2 \mathcal{F}}{\partial B^2} \Big|_{B=0} = \chi_{MF} + \chi_{zz} + \chi_{+-}$$

with

$$\chi_{\parallel MF} = \Delta m_{\chi_0} = \frac{\frac{\beta}{4}(1 - 4\bar{m}^2)}{1 + \frac{\beta}{2}D|J|(1 - 4\bar{m}^2)}$$

$$\chi_{\parallel zz} = -\frac{1}{N_p\beta} \sum_{\vec{k} \in SBZ} \frac{8 \left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2 \Delta m_{\chi_0}^2 (1 + 4\bar{m}^2)}{\left[1 - \left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2 (1 - 4\bar{m}^2)^2\right]}$$

$$\chi_{\parallel +-} = \frac{1}{N_p} \sum_{\vec{k} \in SBZ} \left\{ -\frac{1}{2} \frac{\beta(1 - 2D|J|\Delta m_{\chi_0})^2}{\text{sh}^2(\beta D|J|\bar{m})} \right.$$

$$+ \frac{1}{\text{sh}^2(\beta D|J|\bar{m}\sqrt{1 - \gamma_{\vec{k}}^2})} \left[\frac{\beta}{2}(1 - 2D|J|\Delta m_{\chi_0})^2 \right.$$

$$\left. \left. - \beta(D|J|\Delta m_{\chi_0}\gamma_{\vec{k}})^2 \frac{\text{sh } 2\beta D|J|\bar{m}\sqrt{1 - \gamma_{\vec{k}}^2}}{\beta D|J|\bar{m}\sqrt{1 - \gamma_{\vec{k}}^2}} \right] \right\}.$$

The behaviour of χ_{\parallel} is shown in Figure 4 in which we compare the mean-field, spin wave and the one-loop corrected contributions for a system on a 3D cubic lattice.

$$G_0 = \begin{bmatrix} -\frac{1}{\det G_p} [ip\delta_{p,q} - \frac{1}{2}\varphi_i^z(p-q=0)\delta_{p,q}] & \frac{1}{\det G_p} \frac{1}{2}\varphi_i^-(p-q=0)\delta_{p,q} \\ \frac{1}{\det G_p} \frac{1}{2}\varphi_i^+(p-q=0)\delta_{p,q} & -\frac{1}{\det G_p} [ip\delta_{p,q} + \frac{1}{2}\varphi_i^z(p-q=0)\delta_{p,q}] \end{bmatrix}$$

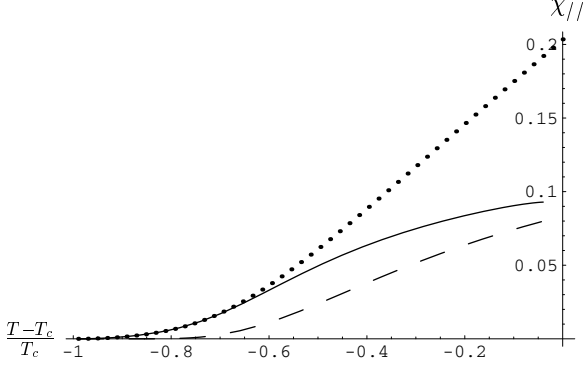


Fig. 4. Parallel magnetic susceptibility at 3D for Heisenberg model. Dotted line: Spin wave susceptibility. Dashed line: mean field susceptibility $\chi_{\parallel MF}$. Full line: total susceptibility ($\chi_{\parallel MF} + \delta\chi_{\parallel}$).

One observes again a good agreement between the quantum corrected and the spin wave expressions at low temperatures. For higher temperatures the curves depart as expected. The mean-field contribution remains in qualitative agreement with the total contribution.

5 Conclusion

In the present work we aimed to work out the expression of physical observables (magnetization and susceptibility) starting from a specific mean field ansatz and including contribution up to first order in a loop expansion in order to investigate the effect of fluctuation corrections to mean field effects at Gaussian approximation. The mean field is chosen as a Néel state which is an a priori reasonable choice for spin systems described in terms of unfrustrated bipartite Heisenberg model. The results are compared to those obtained in the framework of spin wave theory.

The number of particles per site is fixed by means of a rigorous constraint implemented in the partition function. It has been shown elsewhere [7, 15] that this fact introduces a large shift of the critical temperature compared to the case where the constraint is generated through an ordinary Lagrange multiplier term.

At low temperature the magnetization and the magnetic susceptibility are close to the spin wave value as expected, also in agreement with former work [7]. Quantum corrections are sizable at low temperatures. With increasing temperature increasing thermal fluctuations add up to the quantum fluctuations.

At higher temperature the fluctuation contribution of quantum and thermal nature grow to a singularity in the neighbourhood of the critical temperature. The assumption that the Néel mean-field contributes for a major part to the magnetization and the susceptibility is no longer valid. Approaching T_c the mean field contribution to the

magnetization goes to zero and strong diverging fluctuations are generated at the one-loop order. This behaviour is common to the Heisenberg and XXZ magnetization. In addition the Néel order breaks $SU(2)$ symmetry of the Heisenberg Hamiltonian inducing low momentum fluctuations near T_c which is not the case in the XXZ-model.

The influence of fluctuations decreases with the dimension D of the system due to the expected fact that the mean-field contribution increases relatively to the loop contribution.

In dimension $D = 2$ the magnetization verifies the Mermin and Wagner theorem [14] for $T \neq 0$, the fluctuations are larger than the mean field contribution for any temperature. In a more realistic description another mean-field ansatz may be necessary in order to describe the correct physics. Indeed, in the neighbourhood of $T = 0$ Ghaemi and Senthil [3] have shown that a second order phase transition from a Néel mean field to an ASL (algebraic spin liquid) may be at work depending on the strength of interaction parameter which enter the Hamiltonian of the system. This confirms that another mean field solution like ASL may be a better starting point as a Néel state.

The authors would like to thank Drs. D. Cabra and T. Vekua for instructive discussions.

Appendix

A.1 Matrices G_0 and M_1

After integration over the fermionic degrees of freedom in equation (4) the partition function takes the form

$$\begin{aligned} \mathcal{Z} &= \frac{1}{Z_0} \int \mathcal{D}\varphi e^{-\{\int_0^\beta d\tau S_0[\varphi(\tau)] - \ln \det[\beta M]\}} \\ &= \frac{1}{Z_0} \int \mathcal{D}\varphi e^{-S_{eff}[\varphi]} \end{aligned}$$

where

$$M_{i,(p,q)} = \begin{bmatrix} ip\delta_{p,q} + \frac{1}{2}\varphi_i^z(p-q) & \frac{1}{2}\varphi_i^-(p-q) \\ \frac{1}{2}\varphi_i^+(p-q) & ip\delta_{p,q} - \frac{1}{2}\varphi_i^z(p-q) \end{bmatrix}$$

p and q refer to modified fermionic Matsubara frequencies, $p = \omega_f - \mu = \frac{2\pi}{\beta}(n + 1/4)$ and n is an integer, see [6]. M can be put in the form

$$M = -G_0^{-1}(1 - G_0 M_1)$$

where

see equation above

$$M_1 = \begin{bmatrix} \frac{1}{2}\delta\varphi_i^z(p-q) & \frac{1}{2}\delta\varphi_i^-(p-q) \\ \frac{1}{2}\delta\varphi_i^+(p-q) & -\frac{1}{2}\delta\varphi_i^z(p-q) \end{bmatrix}$$

with $\delta\vec{\varphi}_i(p-q) = \vec{\varphi}_i(p-q) - \vec{\varphi}_i(p-q=0)\delta_{p,q}$. The second term in the expression of M corresponds to the quantum contributions. The expression $\ln \det(\beta M)$ can be developed into a series

$$\begin{aligned} \ln \det(\beta M) &= \ln \det \beta [-G_0^{-1}(1 - G_0 M_1)] \\ &= \ln \det(-\beta G_0^{-1}) + \text{Tr} \ln(1 - G_0 M_1) \\ &= \ln \det(-\beta G_0^{-1}) - \text{Tr} \left\{ \sum_{n=1}^{\infty} \frac{1}{n} (G_0 M_1)^n \right\}. \end{aligned}$$

The first term $\ln \det(-\beta G_0^{-1})$ leads to the expression $\sum_i \ln 2 \text{ch} \frac{\beta}{2} \|\vec{\varphi}_i(\omega=0)\|$. The first term in the sum gives the contributions at the one-loop level.

A.2 Relation between the Hubbard-Stratonovich mean fields $\vec{\varphi}_i$ and the mean-field magnetizations \vec{m}_i

Using $\vec{m}_i = -\frac{\partial \mathcal{F}_{MF}}{\partial B_i^z}$ one gets

$$\begin{aligned} \vec{\varphi}_j^z &= \frac{2}{\beta} \text{th}^{-1} 2\vec{m}_i \\ \vec{\varphi}_j^z - B_j &= \sum_i J_{i,j} \vec{m}_i \\ \frac{2}{\beta} \text{th}^{-1} 2\vec{m}_i &= B_i + \sum_j J_{i,j} \vec{m}_j. \end{aligned}$$

Starting from the Néel state $\vec{m}_i = (-1)^i \vec{m} + (-1)^i \Delta \vec{m}(B)$. For a weak magnetic field the second term can be linearized $\Delta \vec{m}(B) = \Delta \vec{m}_0 B$. The coupling strength matrix acting between nearest neighbour sites is taken as $J_{ij} = J \sum_{\vec{\eta} \in n.n.} \delta(\vec{r}_i - \vec{r}_j \pm \vec{\eta})$ with $J < 0$. Then

$$\begin{aligned} \vec{m}_i &= (-1)^i \vec{m} + (-1)^i \Delta \vec{m}(B) \\ &= \frac{1}{2} \text{th} \frac{\beta}{2} [(-1)^i B + Z |J| (-1)^i \\ &\quad (\vec{m} + \Delta \vec{m}(B))] \\ (-1)^i (\vec{m} + \Delta \vec{m}(B)) &= \frac{1}{2} \text{th} \frac{\beta}{2} (-1)^i \\ &\quad [B + 2.D.|J|. (\vec{m} + \Delta \vec{m}(B))]. \end{aligned}$$

By means of a Taylor expansion around $B = 0$:

$$\begin{aligned} (-1)^i (\vec{m} + \Delta \vec{m}(B)) &= \frac{1}{2} \text{th} \frac{\beta}{2} (-1)^i . 2.D|J| \vec{m} \\ &+ \frac{1}{2} . \frac{\beta}{2} (-1)^i [1 + 2.D|J| \Delta \vec{m}_0] \\ &\times \left[1 - \text{th}^2 \frac{\beta}{2} (-1)^i 2D|J| \vec{m} \right] . B \\ &+ \mathcal{O}(B^2). \end{aligned}$$

By identification one gets $\Delta \vec{m}_0 = \frac{\beta}{4} [1 + 2.D|J| \Delta \vec{m}_0] [1 - 4\vec{m}^2]$ and finally

$$\begin{aligned} \vec{m} &= \frac{1}{2} \text{th} \frac{\beta}{2} D|J| \vec{m} \\ \Delta \vec{m}(B) &= \Delta \vec{m}_0 . B \\ \Delta \vec{m}_0 &= \frac{\frac{\beta}{4} (1 - 4\vec{m}^2)}{1 - \frac{\beta}{2} D|J| (1 - 4\vec{m}^2)} \end{aligned}$$

where D is the lattice dimension.

A.3 The free energy and the terms $\delta\varphi^z$ and $\delta\varphi^{+-}$ in equation (6)

Substituting $\vec{m}_i = (-1)^i (\vec{m} + \Delta \vec{m}(B))$ in $\frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \varphi^{z2}} \Big|_{[\vec{\varphi}]}$ $\delta\varphi^{z2}$ and $\frac{1}{2} \frac{\partial^2 S_{eff}}{\partial \varphi^+ \partial \varphi^-} \Big|_{[\vec{\varphi}]}$ $\delta\varphi^+ \delta\varphi^-$ of equation 6 leads to

$$\begin{aligned} (1) &= \left(\frac{\beta}{4} \text{th}' \left(\frac{\beta}{2} \vec{\varphi}_\alpha^z \right) \right) \\ &= \frac{\beta}{4} (1 - 4(\vec{m} + \Delta \vec{m}(B))^2) \\ (2) &= \left(\frac{1}{2} \frac{\text{th} \left(\frac{\beta}{2} \vec{\varphi}_\alpha^z \right)}{\vec{\varphi}_\alpha^z - i\omega} \right) \\ &= [2a]_\omega + (-1)^\alpha [2b]_\omega \\ [2a]_\omega &= \frac{(\vec{m} + \Delta \vec{m}(B)) . (B + 2D|J|(\vec{m} + \Delta \vec{m}(B)))}{[(B + 2D|J|(\vec{m} + \Delta \vec{m}(B)))^2 + \omega^2]} \\ [2b]_\omega &= \frac{i\omega(\vec{m} + \Delta \vec{m}(B))}{[(B + 2D|J|(\vec{m} + \Delta \vec{m}(B)))^2 + \omega^2]}. \end{aligned}$$

Integrating out the fluctuations $\vec{\delta\varphi}$ away from the mean field $\vec{\varphi}^z$ leads to

$$\begin{aligned} \vec{m} &= \frac{1}{2} \text{th} \frac{\beta}{2} D|J| \vec{m} \\ \Delta \vec{m}(B) &= \Delta \vec{m}_0 . B \\ \Delta \vec{m}_0 &= \frac{\frac{\beta}{4} (1 - 4.\vec{m}^2)}{1 - \frac{\beta}{2} D|J| (1 - 4.\vec{m}^2)} \\ \mathcal{F}_{MF} &= N_p D|J| (\vec{m} + \Delta \vec{m}(B))^2 \\ &\quad - \frac{N_p}{\beta} \ln \text{ch} \left(\frac{\beta}{2} [B + 2D|J|(\vec{m} + \Delta \vec{m}(B))] \right) \\ \delta \mathcal{F}_{zz} &= \frac{1}{2\beta} \sum_{\vec{k} \in SBZ} \ln \left[1 - \left(\frac{\beta D|J| \gamma_{\vec{k}}}{2} \right)^2 \right. \\ &\quad \left. \times [1 - 4(\vec{m} + \Delta \vec{m}(B))^2]^2 \right] \end{aligned}$$

$\delta\mathcal{F}_{+-} =$

$$\frac{2}{\beta} \sum_{\vec{k} \in SBZ} \ln \left(\frac{\text{Sinh}\left(\frac{\beta}{2} ([B + 2D|J|(\bar{m} + \Delta\tilde{m}(B))])^2\right)}{\text{Sinh}\left(\frac{\beta}{2} [B + 2D|J|(\bar{m} + \Delta\tilde{m}(B))]\right)} - \frac{[2D|J|\gamma_{\vec{k}}(\bar{m} + \Delta\tilde{m}(B))]^2)^{1/2}}{\text{Sinh}\left(\frac{\beta}{2} [B + 2D|J|(\bar{m} + \Delta\tilde{m}(B))]\right)} \right).$$

A.4 The XXZ-model

The XXZ Hamiltonian

$$H^{XXZ} = -\frac{J}{2} \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + (1 + \delta) S_i^z S_j^z)$$

leads to a critical temperature

$$T_c^{XXZ} = \frac{D|J + \Delta|}{2}$$

$$\Delta = J\delta$$

and a mean magnetization

$$\bar{m} = \frac{1}{2} \text{th} \frac{\beta}{2} D|J + \Delta| \bar{m}$$

$$\Delta\tilde{m}(B) = \Delta\tilde{m}_0 \cdot B = B \cdot \frac{\frac{\beta}{4} (1 - 4\bar{m}^2)}{1 - \frac{\beta}{2} D|J + \Delta| (1 - 4\bar{m}^2)}.$$

A.4.1 Free energy

$$\mathcal{F}_{MF} = N_p D|J + \Delta| (\bar{m} + \Delta\tilde{m}(B))^2 - \frac{N_p}{\beta} \times \ln \text{ch} \left(\frac{\beta}{2} [B + 2D|J + \Delta|(\bar{m} + \Delta\tilde{m}(B))] \right)$$

$$\delta\mathcal{F}_{zz} = \frac{1}{2\beta} \sum_{\vec{k} \in SBZ} \ln \left[1 - \left(\frac{\beta D|J + \Delta| \gamma_{\vec{k}}}{2} \right)^2 [1 - 4(\bar{m} + \Delta\tilde{m}(B))^2]^2 \right]$$

$\delta\mathcal{F}_{+-} =$

$$\frac{2}{\beta} \sum_{\vec{k} \in SBZ} \ln \left(\frac{\text{Sinh}\left(\frac{\beta}{2} ([B + 2D|J + \Delta|(\bar{m} + \Delta\tilde{m}(B))])^2\right)}{\text{Sinh}\left(\frac{\beta}{2} [B + 2D|J + \Delta|(\bar{m} + \Delta\tilde{m}(B))]\right)} - \frac{[2D|J|\gamma_{\vec{k}}(\bar{m} + \Delta\tilde{m}(B))]^2)^{1/2}}{\text{Sinh}\left(\frac{\beta}{2} [B + 2D|J + \Delta|(\bar{m} + \Delta\tilde{m}(B))]\right)} \right).$$

A.4.2 Magnetization

$$m = \bar{m} + \delta m_{zz} + \delta m_{+-}$$

$$\bar{m} = -\frac{1}{N_p} \left. \frac{\partial \mathcal{F}_{MF}}{\partial B} \right|_{B=0}$$

$$\delta m_{zz} = -\frac{1}{N_p} \left. \frac{\partial \mathcal{F}_{zz}}{\partial B} \right|_{B=0}$$

$$= -\frac{1}{N_p \beta} \sum_{\vec{k} \in SBZ} \frac{8 \cdot \bar{m} \Delta\tilde{m}_0 (1 - 4\bar{m}^2) \left(\frac{\beta D|J + \Delta| \gamma_{\vec{k}}}{2} \right)^2}{\left[1 - \left(\frac{\beta D|J + \Delta| \gamma_{\vec{k}}}{2} \right)^2 (1 - 4\bar{m}^2) \right]}$$

$$\delta m_{+-} = \frac{(1 + 2D|J + \Delta| \Delta\tilde{m}_0)}{4\bar{m}}$$

$$- \frac{1}{N_p} \sum_{\vec{k} \in SBZ} \frac{\left(1 + 2D|J + \Delta| \Delta\tilde{m}_0 (1 - \left(\frac{J}{J + \Delta} \gamma_{\vec{k}} \right)^2) \right)}{\sqrt{1 - \left(\frac{J}{J + \Delta} \gamma_{\vec{k}} \right)^2}}$$

$$\times \frac{1}{\left[\text{th} \left(\beta D|J| \bar{m} \sqrt{1 - \left(\frac{J}{J + \Delta} \gamma_{\vec{k}} \right)^2} \right) \right]}.$$

A.4.3 Susceptibility

$$\chi_{\parallel} = -\frac{1}{N_p} \left. \frac{\partial^2 \mathcal{F}}{\partial B^2} \right|_{B=0} = \chi_{MF} + \chi_{zz} + \chi_{+-}$$

$$\chi_{\parallel MF} = \Delta m_{\chi 0} = \frac{\frac{\beta}{4} (1 - 4\bar{m}^2)}{1 + \frac{\beta}{2} D|J + \Delta| (1 - 4\bar{m}^2)}$$

$$\chi_{\parallel zz} = -\frac{1}{N_p \beta} \sum_{\vec{k} \in SBZ} \frac{8 \left(\frac{\beta D|J + \Delta| \gamma_{\vec{k}}}{2} \right)^2 \Delta m_{\chi 0}^2 (1 + 4\bar{m}^2)}{\left[1 - \left(\frac{\beta D|J + \Delta| \gamma_{\vec{k}}}{2} \right)^2 (1 - 4\bar{m}^2) \right]}$$

$$\chi_{\parallel +-} = \frac{1}{N_p} \sum_{\vec{k} \in SBZ} \left\{ -\frac{1}{2} \frac{\beta (1 - 2D|J + \Delta| \Delta m_{\chi 0})^2}{\text{sh}^2(\beta D|J + \Delta| \bar{m})} + \frac{1}{\text{sh}^2 \left(\beta D|J + \Delta| \bar{m} \sqrt{1 - \left(\frac{J}{J + \Delta} \gamma_{\vec{k}} \right)^2} \right)} \right.$$

$$\times \left[\frac{\beta}{2} (1 - 2D|J + \Delta| \Delta m_{\chi 0})^2 - \beta (D|J| \Delta m_{\chi 0} \gamma_{\vec{k}})^2 \right.$$

$$\left. \times \frac{\text{sh} 2\beta D|J + \Delta| \bar{m} \sqrt{1 - \left(\frac{J}{J + \Delta} \gamma_{\vec{k}} \right)^2}}{\beta D|J + \Delta| \bar{m} \sqrt{1 - \left(\frac{J}{J + \Delta} \gamma_{\vec{k}} \right)^2}} \right]$$

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