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# Expansion around the Mean Field in Quantum Magnetic Systems

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We introduce a new definition of ordered phase in a magnetic system based on properties of the local spin state probability. A statistical functional associated to this quantity depends both on amplitude and direction of the local magnetization. We show that it is possible to introduce an expansion at fixed magnetization amplitude in the inverse of lattice coordination number if the direction is selected by an extremum condition. In the limit of infinite coordination number we recover the mean field results. First order corrections are derived for the Ising model in the presence of a transverse field and for the XY model. Our results concerning critical temperature and order parameter compare favorably with other approaches.

**KEY WORDS:** Phase transitions; spin systems; magnetic systems.

## 1. INTRODUCTION

In this work we discuss a new method to obtain an expansion around the mean field in terms of the inverse coordination number $z$ in the ordered phase of a quantum magnetic system. This expansion is obtained both within a new characterization of the symmetry broken phase.

A systematic series expansion for quantum spin systems as been already developed in the early sixties.[1] In this work an high density expansion, related to $1/z$ is derived close to the critical point. The leading term gives the molecular field approximation and the next to the leading terms correction to the mean field. In the ordered phase they derive a low temperature expansion which is compared with the Dyson's spin wave theory.[2] However in the ordered phase a meaningful expansion in $1/z$

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implies a resummation in the expansion in the power of $\beta = 1/k_B T$ (where $k_B$ is the Boltzman constant).[3,4] This resummation fails in the case of quantum system as discussed precisely in ref. 4.

Our approach, based on the methods first introduced by G. Jona Lasinio[5,6] partially overcomes this difficulty.

For quantum systems defined on a lattice[7,8] the ordered phase is usually defined in terms of the generating functional

$$\Gamma(\{\lambda_i\}) = -\frac{1}{\beta} \ln Tr \left\{ e^{-\beta H} T \exp \left[ \int_0^\beta \sum_i \lambda_i(\tau)\, O_i(\tau)\, d\tau \right] \right\} \tag{1}$$

where $O_i$ is the local symmetry breaking operator associated to the magnetization ($m_i = \langle O_i \rangle$), $\lambda_i$ are the local source fields[2] and $T$ stands for the usual time ordered product in the imaginary time.[9] In the usual approach the standard thermodynamic functional is recovered in the limit of static source fields ($\lambda_i(\tau) \to \lambda_i$). In this limit, the generating functional becomes the free energy in the presence of a symmetry breaking Hamiltonian.

$$\lim_{\lambda_i(\tau) \to \lambda_i} \Gamma(\{\lambda_i\}) = -\frac{1}{\beta} \ln Tr \left\{ \exp \left[ -\beta \left( H - \sum_i \lambda_i O_i \right) \right] \right\} \tag{2}$$

As an alternative approach we discuss the limit of impulsive fields ($\lambda_i(\tau) \to \beta \lambda_i \delta(0^+)$). In this limit the generating functional becomes

$$\lim_{\lambda_i(\tau) \to \beta \lambda_i \delta(0^+)} \Gamma(\{\lambda_i\}) = -\frac{1}{\beta} \ln Tr \left\{ e^{-\beta H} \exp \left[ \beta \sum_i \lambda_i O_i \right] \right\} \tag{3}$$

and can be interpreted as the statistical generating functional of the local operator $O_i$. The possible ambiguities, due to the high power of the Dirac delta function, in the expansion of the time ordered product, are overcome if the step function verifies the identity $\theta(0) = 1/2$.[10]

The two approaches are obviously equivalent in the classical case where the local symmetry breaking operators commutes with the system Hamiltonian.

In both approaches just described the free energy is recovered in the limit of vanishing source fields. For a quantum magnetic spin system we find convenient to relate $O_i$ to the local spin density matrix operator

$$\begin{aligned} O_i &= (2\rho_i - 1) \\ O_i &= \sigma_i \cdot n_i \end{aligned} \tag{4}$$

[2] In the present work when a local quantity appear between {} it means that the whole ensemble of these local quantity should be considered.

The statistical average of $\rho_i$ is the Local Spin State Probability (LSSP) which is of direct interest in quantum information theory.[11,12] Recently[13] we have shown how the behavior of the LSSP changes in the presence of an ordered phase. Here we show how to characterize the ordered phase in terms of the LSSP properties.

We remark that, the choice of $\sigma_i \cdot n_i$ as the symmetry breaking operator naturally introduces a direction in the two dimensional local Hilbert space which characterize the spin state ($\Gamma(\{\lambda_i\}) \to \Gamma(\{\lambda_i\}, \{n_i\})$). This direction will be fixed by a minimum condition on the free energy. The presence of a direction naturally leads to define a magnetization vector, whose amplitude is the magnetization.

This new approach can be extended to the study of ordered phases of other quantum systems defined on a lattice, like the Hubbard and Holstein models, in the strong coupling limit. In these models the role of the local spin is played by the doubly degenerate ground state of the local Hamiltonian which corresponds to a particular choice of the chemical potential.

In our approach the expansion is obtained by considering, first, a Legendre transform which introduces a new functional which depends of magnetization instead on the source field.

$$\Omega(\{m_i\}, \{n_i\}) = \Gamma(\{\lambda_i\}, \{n_i\}) - \sum_i \lambda_i m_i \tag{5}$$

The Legendre transform establishes an inversion relation between the source field and the magnetization.

$$\lambda_i(\{m_i\}, \{n_i\}) = -\frac{1}{\beta}\frac{\partial \Omega}{\partial m_i} \tag{6}$$

Taking into account the relation between source field and magnetization, which is fixed in the free spin limit ($H = 0$), for $S = 1/2$ we obtain the self consistent solution for the magnetization

$$m_i = \tanh(\beta\lambda_i(m)) \tag{7}$$

A systematic expansion of $\Omega$, and then of $\lambda_i(m)$ can be achieved splitting the system Hamiltonian in a mean field contribution and a fluctuations operator. The zero-th order term of this expansion recovers the mean field solution. This method is fully explained in Section 2.

Our results are compared with the traditional approach in the XY and quantum Ising models. In the first case (Section 3) we compare the result for the critical temperature obtained in the first order of $1/z$ expansion with the one obtained at the same level from an R.P.A. calculation. In the second case (section 4) we compare with results obtained in the work of Stratt[14] which is based on an improvement of classical mean field theory proposed by Kirkwood.[15, 16] These results are, actually, easily derived within the previously quoted "traditional" approach by means of an expansion around the mean field. The only difference is that the symmetry breaking terms lies along the $z$ axis (while the external field lies on the $x$ axis) and the relation between $\lambda_z$ and $m_z$ are fixed at zero spin interaction. The comparison is always in favour of our approach especially close to the critical temperature. The improvement is shown to be related to the presence of two variational parameters.

## 2. THE DEFINITION OF THE ORDERED PHASE

In this paper we consider a spin system described by the following Hamiltonian

$$H = -\tfrac{1}{2} \sum_{ij,\alpha} J_{ij}^{\alpha} \sigma_i^{\alpha} \sigma_j^{\alpha} - \sum_{i,\alpha} h_i^{\alpha} \sigma_i^{\alpha} \tag{8}$$

Here for a given site $i$, $j$ runs on the $z$ next neighbours sites, the interaction strength $J_{ij}^{\alpha}$ is assumed to scale with $1/z$ and the index $\alpha$ is associated to the three spin components. With a suitable choice of $J_{ij}^{\alpha}$ we may recover respectively the Ising, the XY and the Heisenberg model are recovered.

To study systems described by the Hamiltonian of Eq. (8), we start from the definition of a generating functional of Eq. (1) where we choose to work with the more general operator that can be used to violate the Hamiltonian's symmetry $(O_i = \sigma_i \cdot n_i)$, where $\{n_i^{\alpha}\} = (\sin\theta_i \cos\varphi_i, \sin\theta_i \sin\varphi_i, \cos\theta_i)$ and the component of the $\sigma$ vector are the Pauli operators. In the traditional approach the limit of a static source field is considered and a thermodynamic functional is obtained.

$$F(\{\lambda_i\}, \{n_i\}) = \frac{1}{\beta} \ln Tr \left\{ \exp\left[ -\beta \left( H - \sum_i \lambda_i \sigma_i \cdot n_i \right) \right] \right\} \tag{9}$$

Instead, our alternative definition takes into account the limit of an impulsive source field and leads to the generating functional

$$\Gamma(\{\lambda_i\}, \{n_i\}) = \frac{1}{\beta} \ln Tr \left\{ e^{-\beta H} \exp\left[ \beta \sum_i \lambda_i (\sigma_i \cdot n_i) \right] \right\} \tag{10}$$

The first momentum of $\Gamma$ is related to the density matrix

$$\langle \rho_i \rangle = \frac{1}{2} + \frac{1}{2} \frac{\partial \Gamma}{\partial \lambda_i} \bigg|_{\lambda = 0} \tag{11}$$

whose physical interpretation is the probability of having a spin in the $i$th site in a given state $|S_i\rangle = \cos(\theta_i/2)\,|\uparrow\rangle_i + e^{i\varphi_i}\sin(\theta_i/2)\,|\downarrow\rangle_i$ when the system is at thermal equilibrium:

$$\langle\rho_i\rangle = \frac{Tr(e^{-\beta H}\,|S_i\rangle\langle S_i|)}{Tr(e^{-\beta H})} \tag{12}$$

It is important to note that the trace is over a complete set of whole system while the projection operator is associated to the spin state of a fixed site $i$.

The functional $\Gamma$ is clearly related to the free energy of the system in the limit of vanishing source field. From (10) we define the magnetization in the presence of a source field

$$m_i = \frac{\partial\Gamma}{\partial\lambda_i} \tag{13}$$

By means of a Legendre Transform we define a new functional $\Omega(m) = \Gamma(\lambda) - \sum_i \lambda_i m_i$ whose independent variables are the magnetization amplitude $m_i$ and direction $n_i$

$$\Omega(\{m_i\},\{n_i\}) = \frac{1}{\beta}\ln Tr\left\{e^{-\beta H}\exp\left[\beta\sum_i \lambda_i(\sigma_i\cdot n_i - m_i)\right]\right\} \tag{14}$$

The source field $\lambda_i$ as a function of $m_i$ and $n_i$ is given by

$$\lambda_i = -\frac{\partial\Omega}{\partial m_i} \tag{15}$$

It is convenient to invert the relation between $\lambda_i$ and the independent variable $m_i$ in the limit of free spins, i.e., when both the interaction between spin on different sites of the lattice and the external field vanish ($H = 0$). Defining, for any operator $O$ the expectation value at zero Hamiltonian $\langle O\rangle_0$ as

$$\langle O\rangle_0 = \frac{Tr[e^{\beta\sum_i \lambda_i(0)\,\sigma_i\cdot n_i}O]}{Tr[e^{\beta\sum_i \lambda_i(0)\,\sigma_i\cdot n_i}]} \tag{16}$$

we obtain for $m_i = \langle\sigma_i\cdot n_i\rangle_0$

$$m_i = \tanh(\beta\lambda_i(0)) \tag{17}$$

The thermodynamic value of the magnetization $m_i$ is obtained in the limit of vanishing source fields $\lambda_i$ and thus, taking into account (15), by the extremum condition $\frac{\partial\Omega}{\partial m_i} = 0$.

Our procedure can be summarized as follows. We first consider $1/z$ expansion for $\Omega$

$$\Omega = \sum_k \frac{1}{z^k} \Omega^{(k)} \tag{18}$$

From Eq. (15) a corresponding expansion can be obtained for the source fields $\lambda_i^{(k)} = -\partial\Omega^{(k)}/\partial m_i$. This condition gives an explicit equation for $\lambda_i^{(k)}$ if the knowledge of $\Omega^{(k)}$ implies only the knowledge of $\lambda_i^{(s)}$ with $s < k$ for $k > 0$. Hence, we need an ansatz for $\lambda_i^{(0)}$ and for the magnetization direction which will be verified self consistently. This ansatz is suggested by the well known mean field approximation.

First of all it is convenient to split the Hamiltonian of the system in three different contributions. These contributions are represented by a mean field contribution ($H_{mf}$), a constant ($H_0$) and a bilinear non local operator ($H_f$) which is related to the fluctuations around the mean field.

$$\begin{aligned}
H &= H_{mf} + H_f + H_0 \\
H_{mf} &= -\sum_{ij,\alpha} J_{ij}^{\alpha} m_j^{\alpha} (\sigma_i^{\alpha} - m_i^{\alpha}) - \sum_{i,\alpha} \mu_i^{\alpha} (\sigma_i^{\alpha} - m_i^{\alpha}) \\
H_f &= -\tfrac{1}{2} \sum_{ij,\alpha} J_{ij}^{\alpha} (\sigma_i^{\alpha} - m_i^{\alpha})(\sigma_j^{\alpha} - m_j^{\alpha}) \\
H_0 &= -\tfrac{1}{2} \sum_{ij,\alpha} J_{ij}^{\alpha} m_i^{\alpha} m_j^{\alpha} - \sum_{i,\alpha} \mu_i^{\alpha} m_i^{\alpha}
\end{aligned} \tag{19}$$

We find convenient to express $H_{mf}$ in terms of the modulus $v_i$ and the direction $n'_i$ of a self consistent field whose components are $v_i^{\alpha} = \sum_j J_{ij}^{\alpha} m_j^{\alpha} + \mu_i^{\alpha}$

$$H_{mf} = -\sum_i v_i (\sigma \cdot n'_i) + \sum_i v_i m_i (n_i \cdot n'_i) \tag{20}$$

Next step is to split the statistical weight into two factors by means of a time ordered product. So $\Omega$ becomes

$$\begin{aligned}
\Omega &= \ln Tr[e^{\beta \sum_i \lambda_i (\sigma_i \cdot n_i - m_i)} e^{-\beta H_{mf}} \Lambda] - \beta H_0 \\
\Lambda &= T \exp\left[ -\int_0^{\beta} d\tau \, H_f(\tau) \right]
\end{aligned} \tag{21}$$

where $H_f(\tau)$ evolves in the quasi time $\tau$ as

$$\begin{aligned}
H_f(\tau) &= U(-\tau) \, H_f U(\tau) \\
U(\tau) &= \exp\left( \tau \sum_i v_i (\sigma \cdot n'_i) \right)
\end{aligned} \tag{22}$$

As far as the first step of the iteration process is concerned, $\Omega^{(0)}$ should depend only on $\lambda_i(0)$. This condition is satisfied if $\lambda_i^{(0)} - \lambda_i(0) = -\nu_i$ and $n_i = n_i'$. Within this ansatz the statistical weight appearing in Eq. (21) reduces to that of the $H = 0$ limit and consequently all the contributions arising from the expansion of the time ordered product of zero order in $1/z$, vanish. In fact, these terms are characterized by the presence of, at least, two independent sites but the average of a fluctuation operator on each of these sites with the $H = 0$ statistical weight vanishes because of (17). Therefore $\Omega^{(0)}$ becomes

$$\Omega^{(0)} = -\frac{1}{\beta}\sum_i \left[\frac{1+m_i}{2}\ln\left(\frac{1+m_i}{2}\right) + \frac{1-m_i}{2}\ln\left(\frac{1-m_i}{2}\right)\right] - H_0 \tag{23}$$

Moreover it must be observed that this ansatz at equilibrium implies $\lambda_i(0) = \nu_i$ and then from (17)

$$m_i^{(0)} = \tanh(\beta \nu_i) \tag{24}$$

From the condition $n_i = n_i'$ we obtain a magnetization direction selection $n_i = n_i^{(0)}$ associated to the zero order approximation. The self consistency of the ansatz is obtained verifying that the extremum conditions $\partial\Omega^{(0)}/\partial m = \partial\Omega^{(0)}/\partial\theta = \partial\Omega^{(0)}/\partial\varphi = 0$ are satisfied at equilibrium.

Next step is the calculation of $\Omega^{(1)}$ once $\lambda_i^{(0)}$ is known. It is important to note that possible corrections arising from the expansion of the statistical weight of (21) cancel if we restrict the magnetization direction space in a small region around $n_i^{(0)}$ and $m_i^{(0)}$ of order $1/z$. For this reason the first correction to the mean field calculation of $\Omega$ is.

$$\Omega^{(1)} = \frac{1}{\beta}\Lambda^{(1)} \tag{25}$$

where $\Lambda^{(1)}$ takes into account all contributions of order $1/z$ deriving from the time ordered product. In the simple case of a hypercubic lattice we have

$$\Lambda^{(1)} = \int_0^\beta \int_0^\tau \langle H_f(\tau)\, H_f(\tau')\rangle_0 \, d\tau\, d\tau' \tag{26}$$

It is important to note that our expansion method even if limited in the neighbourhood of the mean field magnetization direction implies a finite term of $1/z$ contribution. This is a remarkable improvement with respect to a straightforward extension of the method of ref. 3 which gives according to refs. 4 and 17 an infinite number of $1/z$ contributions when applied to quantum magnetic system.

In terms of the two quasi-time spin correlations functions

$$C_i^{\alpha,\alpha'}(\tau-\tau') = \langle(\sigma_i^\alpha(\tau)-m_i^\alpha)(\sigma_i^\alpha(\tau')-m_i^\alpha)\rangle_0$$

$$\Lambda^{(1)} = \frac{1}{2}\sum_{ij\alpha\alpha'} J_{ij}^\alpha J_{ij}^{\alpha'} \int_0^\beta \int_0^\tau C_i^{\alpha\alpha'}(\tau-\tau')\, C_j^{\alpha\alpha'}(\tau-\tau')\, d\tau\, d\tau' \tag{27}$$

It is worth to note that the correlation functions must be defined out of equilibrium and than with a statistical weight which does not commute with the evolution operator. This is an important difference with the standard Green functions methods.

In the Ising model, where the symmetry breaking operator commutes with the Hamiltonian, correlations functions do not depend on the imaginary time and we simply recover the second term of high temperature expansion at fixed order parameter of ref. 3.

We shall limit ourselves, for sake of simplicity, to the case in which the symmetry breaking direction is associated to a single angular variable $\theta$. Those $n_i = n_i^{(0)}$ implies $\theta_i = \theta_{i,0}$. Corrections to the mean field imply the solution of the variational problem in $m$ and $\theta$ which takes into account Eq. (27). This problem can be solved by an iterative procedure based on an expansion of the extremum condition with respect to the angular variable in the neighbourhood of $\theta_i = \theta_{i,0}$ and the correction to the angular variable $\theta$ is given by the solution of the following equation

$$\left.\frac{\partial^2 H_0}{\partial\theta^2}\right|_{\theta=\theta_0} \Delta\theta = \left.\frac{\partial\Omega^{(1)}}{\partial\theta}\right|_{\theta=\theta_0} \tag{28}$$

where $\Delta\theta$ is the correction to $\theta_{i,0}$. The zero-th order term is missing in (28) because $\theta_i = \theta_{i,0}$ is a solution of the stationary condition for $H_0$. Finally the self consistent equation for the magnetization is given as

$$m_i = \tanh\left(\beta v|_{\theta=\theta_0} + \beta \left.\frac{\partial v}{\partial\theta_i}\right|_{\theta=\theta_0} \Delta\theta + \left.\frac{\partial\Lambda^{(1)}}{\partial m_i}\right|_{\theta=\theta_0}\right) \tag{29}$$

This iterative approach can be generalized to any arbitrary order in power of $1/z$.

A similar procedure can be developed for the traditional definition of the thermodynamic functional of Eq. (9). The only difference arise when the expansion with respect to fluctuation Hamiltonian is introduced. In this case, the evolution in the imaginary time of Eq. (22) is related to $\lambda_i(0)$ instead of $\beta v_i$. In the limit of infinite coordination number this is irrelevant but when corrections beyond the mean field are taken into account the inverse susceptibility $\partial\lambda_i(0)/\partial m_i = 1/(1-m^2)$ appears in the extremum condition. As a consequence the expansion is not well behaved for $0 \leqslant m \leqslant 1$. However, it is worth to note that $m = 1$ is of the physical interest only in low temperature limit where both these approaches diverge.

As we shall see in the quantum Ising model, in the traditional approach is also possible to work with a fixed direction $n_i$. This is, actually, the choice made in ref. 14.

We shall compare results of these different approaches in the following sections.

## 3. XY MODEL IN AN HYPERCUBIC LATTICE

The XY model shows the spontaneous breakdown of a continuous symmetry associated to the rotation around the $z$ axis. As a consequence of the Mermin and Wagner theorem[18] this transition is expected, for non vanishing temperature, only for dimensionality $z > 4$ for an hypercubic lattice. Mean field theory and Random Phase Approximation can be found in ref. 19. This model can be also interpreted as a lattice spin gas model at half filling and the analogous of the magnetic order is the presence of a superfluid phase. Moreover the lattice gas model corresponds to the infinite repulsion limit of the boson Hubbard model at half filling.[20] This model is of current interest because of recent experimental realizations with the optical lattices.[21] From this point of view our results give a first correction in $1/z$ to the superfluid density at half filling for infinite on site interaction.[22]

This model can be obtained from (8) choosing $\mu_i^\alpha = 0\ \forall\alpha$, $J_{ij}^x = J_{ij}^y = J/z$ and $J_{ij}^z = 0$. With the assumption of the invariance of the magnetization under translation ($m_i = m, \forall i$) we obtain for the modulus $v$ and the versor $n'$:

$$\begin{aligned} v &= Jm \\ n'^x &= \cos\varphi \\ n'^y &= \sin\varphi \\ n'^z &= 0 \end{aligned} \tag{30}$$

From (30) we obtain, as expected, that any direction in the XY plane may be chosen as magnetization direction. In the following we choose the $x$ axis as the symmetry breaking direction. Moreover, due to the Eq. (24), the modulus of the magnetization obeys to the usual mean field self consistent equation.

$$m = \tanh(\beta J m) \tag{31}$$

Because of the absence of an external field the magnetization above the critical temperature vanishes while below lies on the symmetry invariance subspace. The zero-th order term of $\Omega$, for site, is obtained by Eq. (23).

$$\Omega^{(0)} = -\frac{1}{\beta}\left[\sum_i \frac{1+m_i}{2}\ln\left(\frac{1+m_i}{2}\right)+\frac{1-m_i}{2}\ln\left(\frac{1-m_i}{2}\right)\right]+\frac{J}{2}m^2 \tag{32}$$

To evaluate the first correction to $\Omega$ we need to evaluate the local correlations functions $C_i^{\alpha,\alpha'}(\tau-\tau')$ for any $\alpha$ and $\alpha'$. Having chosen the $x$-axis as magnetization direction we obtain:

$$\begin{aligned}
&C_i^{x,x}(\tau-\tau') = 1-m^2\\
&C_i^{x,y}(\tau-\tau') = 0\\
&C_i^{y,x}(\tau-\tau') = 0\\
&C_i^{y,y}(\tau-\tau') = \cosh[2\nu(\tau-\tau')]+m\sinh[2\nu(\tau-\tau')]
\end{aligned} \tag{33}$$

Substituting in (27) we obtain for $\Omega^{(1)}$ for single site

$$\Omega^{(1)} = \frac{\beta^2J^2}{4z}\left\{(1-m^2)^2+\frac{1}{2}(1-m^2)+\frac{1}{2\beta J}+\frac{1}{32\beta^2J^2m^2}[(1-m)^2\exp(4\beta Jm)\right.$$
$$\left.+(1+m)^2\exp(-4\beta Jm)-2(1+m^2)]\right\} \tag{34}$$

The first term is equivalent to the Onsager reaction field of the Ising model[3] while the other terms are due to the quantum nature of the systems. From the previous equation, we can also see that, for this model, no correction to the magnetization direction occurs as expected because of the absence of the transverse field.

We can compare this result with the one obtained in the traditional approach based on the thermodynamic functional Eq. (9). Correlation functions can be obtained from (33) substituting $\nu$ with $\lambda(0)$. From these correlation functions, taking into account Eq. (17) it is easy to obtain the first correction, for single site, in $1/z$.

$$F^{(1)} = \frac{\beta^2J^2}{4z}\left\{(1-m^2)^2+\frac{1}{2}(1-m^2)+\frac{m}{2\beta\lambda(0)}\right\} \tag{35}$$

where $\lambda(0)$ can be written as function of $m$ taking into account relation (17).

To compare the results of these two approaches we must, at first, evaluate the value of the magnetization which minimize the two functionals

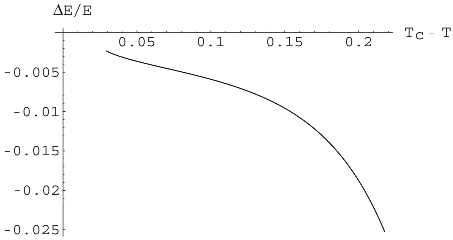


Fig. 1. Comparison between the free energies of our approach and the traditional one for the XY model in a simple cubic lattice (z=6).

and then compare the free energies calculated at the minimum. The results of this comparison are summarized in Fig. 1. We note a slight improvement that is more evident in low temperature. From the knowledge of $\Omega$ it is possible to calculate any physical quantity of the system in both the high and low temperature phases. We begin by considering the critical temperature $T_c$. We expand $\Omega$ in powers of $m$ and determine the critical temperature as the value of $\beta$ at which the $m^2$ coefficient vanishes. From (34) we obtain the following equations

$$\Omega = \Omega_{(0)}(\beta) + \Omega_{(2)}(\beta)\, m^2 + \Omega_{(4)}(\beta)\, m^4 + \cdots \tag{36}$$

where the coefficient are given by

$$\begin{aligned} \Omega_{(0)}(\beta) &= \ln 2 + \frac{\beta^2 J^2}{2z} \\ \Omega_{(2)}(\beta) &= -\frac{1}{2} + \frac{\beta J}{2} - \frac{\beta^2 J^2}{2z} - \frac{\beta^3 J^3}{3z} + \frac{\beta^4 J^4}{6z} \\ \Omega_{(4)}(\beta) &= -\frac{1}{12} + \frac{\beta^2 J^2}{4z} - \frac{4\beta^5 J^5}{15z} + \frac{\beta^6 J^6}{45z} \end{aligned} \tag{37}$$

Hence the critical temperature is given from the solution of

$$1 = \beta_c J - \frac{\beta_c^2 J^2}{z}\left(1 + \frac{2}{3}\beta_c J - \frac{1}{3}\beta_c^2 J^2\right) \tag{38}$$

Neglecting second order contribution in $1/z$ in the solution of (38) we obtain

$$\beta_c J = 1 + \frac{4}{3}\frac{1}{z} \tag{39}$$

Quantum fluctuations introduce two competitive terms that, for high dimensionality, make the XY model critical temperature lower than in the Ising one ($\beta_c J = 1 + 1/z$). The critical temperature can be compared with the one obtained with the approach of the Random Phase Approximation at the same order in $1/z$. For the XY model the random phase approximation[19] gives the following equation for the order parameter

$$\frac{m}{N}\sum_{n} \coth\left[\beta J_0 m \sqrt{1-\frac{J_n}{J_0}}\right] = 1 \tag{40}$$

where $J_n$ is the $n$th eigenvalues of coupling matrix $J_{ij}$ and $J_0$ is the greatest of these eigenvalues. In the random phase approximation we perform an arbitrary resummation with respect to $1/z$. To compare this result for the critical temperature with our approach we must recover the term proportional to the inverse of number of next neighbours. Expanding l.h.s. of (40) to the first non vanishing term we obtain the $1/z$ correction. In the limit of vanishing $m$ we obtain

$$\beta_c J = 1 + \frac{3}{8z} \tag{41}$$

It can be observed that all approximations beyond the mean field approximation reduce the critical temperature. Our approach gives the lowest $T_c$, and hence it is in a better agreement to the to "true critical temperature" obtained from high temperature expansion for different lattices[23] than the others.

Another important thermodynamical quantity is the order parameter near the critical temperature. Neglecting powers greater than $m^4$ in the expansion of $\Omega$ for small $m$ we obtain

$$m = \sqrt{\frac{(\beta - \beta_c)\,\Omega'_{(2)}(\beta_c)}{2\Omega_{(4)}(\beta_c)}} \tag{42}$$

substituting our result we obtain

$$\frac{m}{\sqrt{3J(\beta-\beta_c)}} = 1 - \frac{9}{10z} + 0\left(\frac{1}{z^2}\right) \tag{43}$$

Quantum fluctuations have a significant effect on the slope with respect to the Ising case where the slope is equal to $1 + 1/2z$.

Moreover the expansion in $1/z$ for the free energies of quantum magnetic systems allows to generalize the procedure established in ref. 3 for the evaluation of the critical exponent.

**Table I. Correction to the Critical Index Obtained with the Approach Described Above**

| | $z=6$ | $z=8$ |
|---|---|---|
| $\Delta\gamma/\gamma$ | 0.173 | 0.089 |

The basic point is to rearrange the $1/z$ series expansion in terms of an auxiliary parameter $\mu$ connected with the fluctuation operator $H_f$. Thus from the knowledge of $\Omega$ to a given order in $1/z$ it is possible to obtain an infinite series for $\gamma$ in power of $\mu$. The value of the critical index $\gamma$ is obtained by a truncation of the series at fixed order and an extrapolation to $\mu=1$. Actually the series sums up to 1 for $\mu=1$ except in the square lattice ($z=4$) where the series is divergent. This result can be interpreted as a consequence of absence of an ordered phase for the XY model in two dimension.(18) The knowledge of the first order correction in $1/z$ to the free energy is however consistent only with a truncation to the first order of the expansion in $\mu$. As a consequence the extrapolation to $\mu=1$ gives very unrealistic results, but the relative importance of quantum correctionsis in any case of some interest.

## 4. ISING MODEL IN A TRANSVERSE FIELD

Quantum Ising model is defined by the following hamiltonian

$$\begin{aligned} v &= \sqrt{J^2m^2\cos^2\theta + h^2} \\ n'^x &= \frac{h}{v} \\ n'^y &= 0 \\ n'^z &= \frac{Jm\cos\theta}{v} \end{aligned} \tag{44}$$

It is obtained from (8) choosing $J^x_{ij}=J^y_{ij}=0$, $J^z_{ij}=J/z$, and $h^x_i=h$ while $h^z_i=h^y_i=0$.

The model is of direct interest in various fields from quantum computing(24) to spin glass(25, 26) and quantum annealing.(27, 28) As far as critical properties are concerned the work of Suzuki(29) establishes that the statistical mechanics is the same of the classical system in $d+1$ dimension. Although this result is very useful to relate critical properties of a system with and without transverse field, it does not suggest any systematic expansion of thermodynamical quantities. A result which can be interpreted as a first order in $1/z$ expansion for an hypercubic lattice is obtained in ref. 14.

At first we note that, with simple physical considerations, the magnetization must lies in the $xz$ plane and those we shall put $\varphi=0$ in the follows. Then $\Omega^{(0)}$, for each site, turns out to be

$$\Omega^{(0)} = -\left[\left(\frac{1}{2}+m\right)\ln\left(\frac{1}{2}+m\right)+\left(\frac{1}{2}-m\right)\ln\left(\frac{1}{2}-m\right)\right] + \beta\left(\frac{J}{2}m^2\cos^2\theta + hm\sin\theta\right) \tag{45}$$

From the magnetization direction selection $n_i = n'_i$ and taking into account (44) we obtain that two different directions are possible for $\theta$.

$$\sin\theta = \frac{h}{Jm} \qquad \cos\theta = 0 \tag{46}$$

The first case of (46), which implies $h/Jm < 1$, corresponds to the ordered phase while the second to a disordered one. According to (24) m is given by

$$m = \tanh(\beta\sqrt{h^2 + J^2m^2\cos^2\theta}) \tag{47}$$

Substituting the result for $\theta$ obtained from (46) in (47) we obtain

$$\begin{aligned} m &= \tanh(\beta h) \qquad \text{disordered phase} \\ m &= \tanh(\beta Jm) \qquad \text{ordered phase} \end{aligned} \tag{48}$$

It is interesting to note that the amplitude of the magnetization does not depend on the external field in the ordered phase in mean field approximation. As expected, $m$ vanishes in the infinite temperature limit and then the second case of (46) must be taken into account (disordered phase). On the contrary at low temperature $m$ grows and, if $h/J \leqslant 1$, there is a temperature at which the first case of (46) becomes valid (ordered phase). As it can be easily verified from $\Omega$ the critical temperature in the presence of a transverse field is the one at which the magnetization direction aligns with the transverse field, i.e., $h/Jm = 1$ Substituting in (48) we obtain

$$\frac{1}{T_c} = \frac{1}{h}\tanh^{-1}\left(\frac{h}{J}\right) \tag{49}$$

From the condition for an ordered phase $h/J \leqslant 1$ the critical field $h_c$ is $h_c = J$ which corresponds to $T_c = 0$.

To study first order corrections to $\Omega$ we must evaluate the local correlation function $C_i^{z,z}(\tau-\tau')$. A simple calculation gives

$$C_i^{z,z}(\tau-\tau') = \cos^2(\theta) + \sin^2(\theta)[\cosh(2\nu(\tau-\tau')) - m \sinh(2\nu(\tau-\tau'))] \qquad (50)$$

From (50) it is possible to obtain $\Omega^{(1)}$ and then it is possible to obtain corrections to equilibrium magnetization amplitude and direction as shown in Section 2.

For sake of comparison it is worth to summarize main points of ref. 14. This work can be seen as a particular case of the usual approach defined in Eq. (9) in which the direction of the symmetry breaking operator is fixed along the $z$ axis. Consequently, the Legendre transformation introduces a dependence on only one parameter, i.e., the $z$ component of the magnetization. The result for the free energy can be, actually, recovered developing the expansion of (9) and then taking into account the substitutions summarized in Table II.

It is possible to compare results for the free energies of the two approaches as function of the temperature for different values of the external field $h$ (Fig. 2). The two approaches have the same limit for vanishing $h$, i.e., the free energy of the Ising model and thus, for small value of $h$ the difference is very small and grows when the amplitude of the external field increases. It is worth to note that, for any values of $h$, the corrections become larger when the temperature is close to $T_c$.

All these features are a consequence of the existence, in our method, of a second parameter which allows, via a variational calculation, a resummation of the $1/z$ expansion both for the $z$ and $x$ component of the magnetization. In our approach, the resummation on the $x$ axis, due to the

**Table II. Substitutions Needed to Recover from the Expansion of Eq. (2) the Stratt's Expansion**[14]

| This work | Stratt[14] |
|---|---|
| $\beta\lambda(0)$ | $\Gamma$ |
| $m\cos\theta$ | $m_z$ |
| $m$ | $\tanh\Gamma$ |
| $\sin\theta$ | $\beta K/\Gamma$ |
| $\cos\theta$ | $\gamma/\Gamma$ |

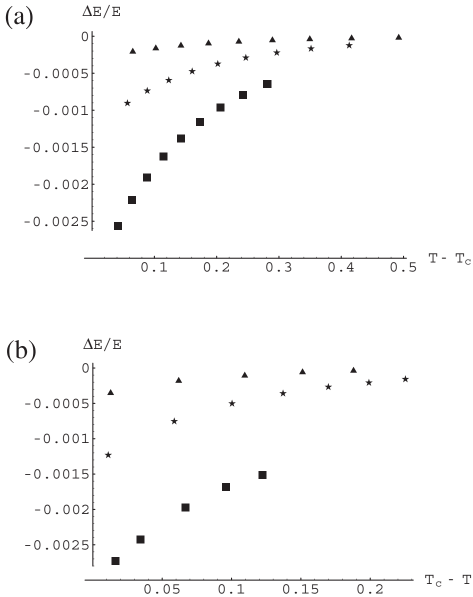


Fig. 2. Comparison between the free energies at different temperature of our approach and the free energy evaluated by Stratt[14] for an hypercubic lattice with $z=6$. In Fig. 2(a) is represented the comparison above $T_c$ and in Fig. 2(b) the comparison below this temperature. The triangles corresponds to $h/J=0.2$, the stars corresponds to $h/J=0.4$, and the grey boxes to $h/J=0.6$. $T_c$ is the critical temperature evaluated in our approach.

Eq. (29) holds even in the "normal," i.e., disordered, phase, where the direction is fixed by $\theta=\pi/2$. On the other hand the Stratt's approach has no resummation above the critical temperature but only an expansion in power of $1/z$. It is then expected that results, for fixed external field amplitude, are quite different between the two approaches, and this difference increases when the temperature is lowered toward $T_c$. Below this temperature the competition between the $x$ and the $z$ components of the magnetization decreases the role of the $x$ component of the magnetization and the differences are lowered. On the other hand, at any temperature, the difference is enhanced when the role of $m_x$ is increased enhancing the amplitude of the external field $h$. (See Fig. 3.)

We have made the same kind of comparison between our approach and the one derived form Eq. (9) for this model. The comparison shows that this third approach is an improvement of the evaluation of the free energy made by Stratt, at least close to $T_c$, but it is worse then our approach according to the same comparison made for the XY model.

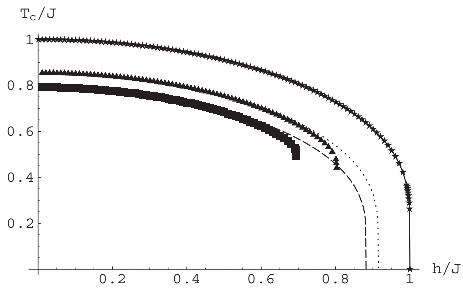


Fig. 3. The critical temperature as function of external field for different coordination numbers compared with the same results obtained by Stratt in ref. 14. Boxes and triangles refer to our's result while dashed and dot lines refer to Stratt's result respectively for $z = 6$ and $z = 8$. The upper line is the mean field result.

## 5. CONCLUSION

We obtain the magnetization amplitude and direction in the ordered phase for the quantum magnetic system from extremum conditions of the statistical functional related to the LSSP. This quantity is different from the free energy defined in the presence of the symmetry breaking fields in the case of quantum system where the symmetry breaking operators does not commute with the hamiltonian. We derive an expansion in the inverse coordination number which is valid even in the presence of quantum fluctuations. This expansion avoids the divergency in the number of "diagrams" corresponding to the same order which seems to be a draw-back of a direct $1/k_B T$ expansion in the case of quantum magnetic system.[4] Moreover the characterization of the ordered phase in terms of thermodynamics functionals based on a quantum information concept like LSSP allows to define an expansion which is uniform in the magnetization amplitude while the standard approach based on generalization of the free energy in the presence of a symmetry breaking perturbation is affected by divergencies in the $m = 1$ limit. It is, however, expected that both expansion are asymptotic with a zero radius of convergence Results for XY and quantum Ising model compare favorably with those of other approaches. In the latter case the improvement is also due to the new variational scheme which takes into account both the magnetization and the direction in the Hilbert space, and then, allows a meaningful resummation of the $1/z$ expansion valid both above and below the critical temperature.

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