A new expansion around mean field for the quantum Ising model

F. de Pasquale and S.M. Giampaolo

1Departement of Physics University of Rome "La Sapienza", P-le A.Moro 2, 00185 Rome Italy
2b INFN Rome

(Dated: Nov. 23 2001)

Abstract

We show that an high temperature expansion at fixed order parameter can be derived for the quantum Ising model. The basic point is to consider a statistical generating functional associated to the local spin state. The probability at thermal equilibrium of this state reflects directly the occurrence of a spontaneous symmetry breaking. It is possible to recover the expansion around the mean field in the system dimensionality if the “direction” in the Hilbert space of local spin states is suitably chosen. Results for the free energy at the critical temperature, as a function of the transverse field, in first order approximation in the inverse system dimensionality are compared with those of the standard approach.
The recent interest in decoherence\[1\] phenomena in connection with quantum computing leads naturally to the study of a local spin state interacting with an environment. It has been shown that quantum computation can be performed acting on a nuclear spin at thermal equilibrium\[2\]. In this perspective it is interesting to study the simplest quantum spin model, i.e the Ising model in a transverse field. This model has an exact solution in one dimension\[3\], and approximate techniques, such as the random phase approximation \[4\] and exact cumulant series expansion\[5, 6\] have also be applied for higher order. The main result is due to Suzuki’s work\[7\] who showed the correspondence with a classical model in d+1 dimensions. A systematic expansion around the mean field result is however still lacking. As we shall see such an expansion can be introduced if the phase transition is characterized by a statistical generating functional associated to the local spin state. The probability of finding the spin in the i-th site in the general state $|s_i\rangle = \cos \frac{\theta_i}{2} |\uparrow_i\rangle + e^{i\varphi_i} \sin \frac{\theta_i}{2} |\downarrow_i\rangle$ when the system is in thermal equilibrium is

$$\rho_i(\theta_i, \varphi_i) = \frac{\text{Tr}[e^{-\beta H}|s_i\rangle\langle s_i|]}{\text{Tr}(e^{-\beta H})}$$

(1)

It is convenient to express the projection operators in terms of the Pauli spin operators

$$|s_i\rangle\langle s_i| = \frac{1}{2} + S_i \cdot n_i$$

(2)

Here $n_i (\sin \theta_i \cos \varphi_i, \sin \theta_i \sin \varphi_i, \cos \theta_i)$ and $S_i (S_i^x, S_i^y, S_i^z)$ are respectively the unitary vector which defines the symmetry breaking direction, and the spin - $\frac{1}{2}$ vector operator. Taking into account Eq. (2), the local spin state probability becomes

$$\rho_i(\theta_i, \varphi_i) = \frac{1}{2} + \frac{\text{Tr}[\exp(-\beta H)S_i \cdot n_i]}{\text{Tr}[\exp(-\beta H)]}$$

(3)

Note that the non trivial local spin probability $\rho_i - \frac{1}{2}$ corresponds to the magnetization in the symmetry breaking direction. It is immediately seen that $\rho_i$ is directly related to the symmetry breakdown. In the quantum Ising model

$$H = -\sum_{i,j} J_{i,j} S_i^z S_j^z - \sum_i h_i S_i^x$$

(4)

the only symmetry is the spin inversion $S_i^z \rightarrow -S_i^z$. Above the critical temperature $T_c$, the magnetization is directed along the transverse field direction, while in the ordered phase a non vanishing component in the z direction appears. The local state probability of the
symmetrical phase (above $T_c$) is

$$\rho_i^S(\theta_i, \varphi_i) = \frac{1}{2} + \frac{Tr [\exp(-\beta H) S_i \cdot n_{i\perp}]}{Tr [\exp(-\beta H)]}$$  \hspace{1cm} (5) $$

where $n_{i\perp}$ is the unitary vector orthogonal to the $z$ direction. When the symmetry is broken (below $T_c$)

$$\rho_i^{SB}(\theta_i, \varphi_i) = \rho_i^S(\theta_i, \varphi_i) + \frac{Tr [\exp(-\beta H) S_i^z \cos \theta_i]}{Tr [\exp(-\beta H)]}$$  \hspace{1cm} (6) $$

We see that the qualitative change of the local probability is directly related, as expected, to a non vanishing statistical average of $S_i^z$. The non trivial part of the local spin state probability is the first moment of the statistical generating function $G$ in the limit of vanishing source field $\lambda_i$.

$$G = \ln \left\{ Tr \left[ e^{-\beta H} \exp \left( \sum_i \lambda_i S_i \cdot n_i \right) \right] \right\}$$  \hspace{1cm} (7) $$

We see that for vanishing $\lambda_i$, $G$ becomes the free energy. Moreover in the absence of a transverse field and for $\theta_i = 0$ the statistical functional $G$ reduced to that of the Ising model in the presence of a symmetry breaking field along the z - direction $h_i = \frac{\lambda_i}{\beta}$.

Expansion around the mean field are usually derived by introducing a generalization of the free energy in the presence of symmetry breaking fields and then by Legendre transform which makes the order parameter the independent variable of the problem. This generalization is usually accomplished introducing symmetry breaking fields as perturbation in the system Hamiltonian. We consider here an alternative generalization considering the generating function of Eq. (7). The main advantage of the present approach is the possibility of a straightforward expansion in the inverse temperature. At infinite temperature there is a complete degeneracy of the local spin state, which is removed only for the presence of the symmetry breaking fields. At finite temperature, the correction due to spin - spin interaction and the transverse field compete each other to determine the local spin state probability and the local magnetization.

Let us to introduce the Legendre transform of the generating function $W(m) = G(\lambda) - \sum_i \lambda_i m_i$. Here $m_i = < S_i \cdot n_i >$ and angular brackets stand for

$$< \hat{O} >= \frac{Tr \left[ e^{-\beta H} \hat{O} \exp \left( \sum_i \lambda_i(\beta)(S_i \cdot n_i) \right) \right]}{Tr \left[ e^{-\beta H} \exp \left( \sum_i \lambda_i(\beta)(S_i \cdot n_i) \right) \right]}$$  \hspace{1cm} (8) $$

Note that $m_i$, as a consequence of the relation between $m_i$ and the generating function $m_i = \frac{\partial G}{\partial \lambda_i}$, become the independent variables of $W$. On the other hand, the source field $\lambda_i$
depends on $m_i$ and $\beta$

$$\lambda_i = -\frac{\partial W}{\partial m_i}$$  \hspace{1cm} (9)

The free energy in the limit of vanishing source field is given by $W$ calculated for the “magnetization” which satisfies extremum condition $\frac{\partial W}{\partial m_i} = 0$. This is the same procedure which applies to the free energy of the Ising model. Following reference (2), we exploit the limit of vanishing $\beta$ to fix the relation between $m_i$ and $\lambda_i(0)$

$$m_i = \frac{1}{2} \tanh \left( \frac{\lambda_i(0)}{2} \right)$$  \hspace{1cm} (10)

The next step is to derive the high temperature expansion of $W$. The expansion up to the second order in $\beta$ is related to the following quantities.

$$W|_{\beta=0} = \sum_i \ln \left[ 2 \cosh \left( \frac{\lambda_i(0)}{2} \right) \right] - \lambda_i(0)m_i$$

$$\left. \frac{\partial W}{\partial \beta} \right|_{\beta=0} = < H >_0$$

$$\left. \frac{\partial^2 W}{\partial \beta^2} \right|_{\beta=0} = < H^2 >_0 - ( < H >_0)^2 - 2 \sum_i \left. \frac{\partial \lambda_i}{\partial \beta} \right|_{\beta=0} < H (S_i \cdot n_i - m_i) >_0 +$$

$$\sum_{i,j} \left. \frac{\partial \lambda_i}{\partial \beta} \right|_{\beta=0} \left. \frac{\partial \lambda_j}{\partial \beta} \right|_{\beta=0} < (S_i \cdot n_i - m_i)(S_j \cdot n_j - m_j) >_0$$

There the symbol $<>_0$ stands for the statistical average defined in Eq. (8) evaluated at $\beta = 0$, and the derivative of $\lambda_i$ with respect to $\beta$ are obtained from Eq. (9)

$$\left. \frac{\partial \lambda_i}{\partial \beta} \right|_{\beta=0} = - \left. \frac{\partial^2 W}{\partial \beta \partial m_i} \right|_{\beta=0}$$  \hspace{1cm} (12)

A straightforward calculation gives

$$W \approx - \sum_i \left( \frac{1}{2} + m_i \right) \ln \left( \frac{1}{2} + m_i \right) + \left( \frac{1}{2} - m_i \right) \ln \left( \frac{1}{2} - m_i \right)$$

$$+ \beta \sum_{i,j} J_{i,j} m_i m_j \cos \theta_i \cos \theta_j + \beta \sum_i h_i m_i \sin \theta_i \cos \varphi_i$$

$$+ \frac{\beta^2}{8} \sum_{i,j,k} (J_{i,j} + J_{j,i})(J_{i,k} + J_{k,i}) m_j m_k \cos \theta_k \cos \theta_j \sin^2 \theta_i + \frac{\beta^2}{8} \sum_i h_i^2 (1 - \sin^2 \theta_i \cos^2 \varphi_i)$$

$$- \frac{\beta^2}{4} \sum_{i,j} (J_{i,j} + J_{j,i}) h_i m_j \cos \theta_j \sin \theta_i \cos \theta_i \cos \varphi_i - \frac{\beta^2}{4} \sum_{i,j} (J_{i,j} + J_{j,i})^2 m_j^2 \cos^2 \theta_j \sin^2 \theta_i$$

$$+ \frac{\beta^2}{4} \sum_{i,j} \left[ \left( \frac{1}{4} - m_i^2 \right) \left( \frac{1}{4} - m_j^2 \right) \cos^2 \theta_i \cos^2 \theta_j + \frac{1}{16} (1 - \cos^2 \theta_i \cos^2 \theta_j) \right]$$  \hspace{1cm} (13)
Eq. (10) has been used to eliminate the dependence from $\lambda_i(0)$. Note that the first line of the left hand side of Eq. (13) corresponds to the mean field approximation. In the limit of vanishing transverse field, i.e. when the symmetry for rotation around the z axis is recovered, the dependence on $\varphi_i$ disappears as expected. Moreover if the symmetry breaking fields is fixed along the z - axis, we recover the free energy expansion of the Ising model[8]. This direction is however selected from the extremum condition on the free energy which corresponds to a minimum in mean field approximation. In such a case it is easily shown that, considering a constant interaction among next neighbors sites, which scales with the system dimensionality ($J_{i,j} + J_{j,i} = J/D$), the high temperature expansion becomes an expansion in $\frac{\beta J}{D}$. This result is actually a consequence of the compensation of contributions which are of second order in $\beta$ and zero order in $\frac{1}{D}$. As we shall see this compensation is valid also in the presence of transverse field with a suitable choice of the symmetry breaking fields direction.

Let us consider for simplicity the case of an homogeneous symmetry breaking $m_i = m$, $\theta_i = \theta$ and $\varphi_i = \varphi$. The minimum of the free energy in $\varphi$ gives, as expected $\varphi = 0$. The probabilistic functional becomes

$$W(m, \theta) = N \left\{ - \left[ \left( \frac{1}{2} + m \right) \ln \left( \frac{1}{2} + m \right) + \left( \frac{1}{2} - m \right) \ln \left( \frac{1}{2} - m \right) \right] + \beta \left( \frac{J}{2} m^2 \cos^2 \theta + hm \sin \theta \right) + \frac{\beta^2}{8} \cos^2 \theta \left[ (Jm \sin \theta - h)^2 - \frac{J^2 m^2}{D} \sin^2 \theta \right] + \frac{\beta^2 J^2}{4D} \left[ \left( \frac{1}{4} - m^2 \right)^2 \cos^4 \theta + \frac{1}{16} (1 - \cos^4 \theta) \right] \right\} \tag{14}$$

Considering only contributions in $\beta$ up to the first order we recover the well known results of the mean field approximation, by an extremum condition in $m$ and $\theta$. The first condition $\frac{\partial W}{\partial m} = 0$ gives

$$m = \frac{1}{2} \tanh \left[ \frac{\beta}{2} \left( Jm \cos^2 \theta + h \sin \theta \right) \right] \tag{15}$$

corresponds to the vanishing of the symmetry breaking fields, i.e. to the limit in which the probabilistic generating function $W$ reduces to the free energy. The second corresponds to the selection of the direction of the symmetry breaking field corresponding to an extremum
of free energy $\frac{\partial A}{\partial \theta} = 0$.

$$\cos \theta (Jm\sin \theta - h) = 0$$  \hspace{1cm} (16)

It is important to note that the first order expansion in $\beta$ plus the minimum condition in $\theta, \varphi$ gives the exact solution associated to the mean field Hamiltonian. It means that the rotation in the $\theta$ and $\varphi$ space that diagonalizes the mean field Hamiltonian coincides with the choice of $\theta$ and $\varphi$ which minimize the first order correction to the energy.

As far as the second order terms in $\beta$ are concerned, we note that the “spurious” term which does not scale with the inverse dimensionality $D$, can be neglected close to the magnetization directions selected in the first order approximation ($\sin \theta = \frac{h}{Jm}$ under the critical temperature, and, $\cos \theta = 0$ above). The solution for the extremum condition, below the critical temperature for $\theta$ and $m$ modifies as follows:

$$\sin \theta = \frac{h}{Jm} + \frac{\beta h}{4mJ^2D} \left( 4h^2 + J^2(1 - 4m^2) \right)$$  \hspace{1cm} (17)

$$m = \frac{1}{2} \tanh \left\{ \frac{\beta}{2} Jm - \frac{\beta^2 m}{8D} \left( 4h^2 + J^2(1 - 4m^2) \right) \right\}$$  \hspace{1cm} (18)

Within this approximation we find an expansion in $\frac{\beta J}{D}$ which is the generalization of the Ising model results[8]. In the limit of vanishing transverse field we obtain, as expected, the Ising model results.

The critical temperature is identified as the temperature at which the symmetry breaking direction coincides with that of the transverse field, i.e $\sin \theta = 1$. Solving for the extremum conditions we obtain a self consistent equation for the critical temperature.

$$\beta_c = \frac{2}{h} \text{arctanh} \left( \frac{2h}{J \left( 1 - \frac{J \beta}{4D} \right)} \right)$$  \hspace{1cm} (19)

The solution for Eq. (19) is defined in a limited range of dimensionality and transverse field amplitude. The lowest critical temperature and highest transverse field are given by

$$\frac{2h}{J \left( 1 - \frac{\beta J}{4D} \right)} = \tanh \left[ \frac{2h}{J} \left( 1 - 2 \sqrt{\frac{h^2}{J^2} + \frac{1}{4D}} \right) \right]$$

$$\beta = \frac{4D}{J} \left( 1 - 2 \sqrt{\frac{h^2}{J^2} + \frac{1}{4D}} \right)$$  \hspace{1cm} (20)

In order to compare our results with those derived in reference (9), we must take into account that this model is the same of Eq. (4) with spin operators substituted by Pauli operators. This implies the following scaling in the Eqs. (14), (19): $m \rightarrow \frac{m}{2}, J \rightarrow 4J, h \rightarrow 2h$. 

6
FIG. 1: The free energy for site at critical temperature as function of transverse field

FIG. 2: The critical temperature as function of transverse field. The lower curve gives the temperature and the corresponding transverse field which determines the limit of our approximation.

In Fig. (1) the free energy at critical temperature obtained in the framework of the standard approach of reference (9) is compared with our results. We find an improvement for \( h \neq 0 \). The same comparison for the critical temperature as function of the transverse magnetic field is performed for dimensionality greater than four in Fig. (2). It is easily seen that the free energy is lowered because of corrections of order \( \frac{1}{D} \) in the direction \( \theta \) of the magnetization. The presence of this extra variational parameter seems to be the main advantage of the present approach. As a concluding remark we would like to comment about possible extensions of this approach to other quantum system. We think about system defined on a lattice where in the energy there is a “local” term, which depends only on the
degrees of freedom associated to a single site, plus an interaction which takes into account the
coupling between degrees of freedom of different lattice sites. If for a particular choice of the
system parameters there is a symmetry in the local energy operator we can treat interaction
and symmetry breaking part of the local Hamiltonian as a perturbation. The degeneracy of
the system in the limit of vanishing perturbation, can be removed by the introduction of the
source field, which determines the ”orientation” in the Hilbert space of the system ground
state. In the case of the quantum Ising system the local energy is zero and then any local
spin state is allowed. The source field $\lambda$ determines the local state. The expansion parameter
is associated to the inverse temperature $\beta$. Taking into account the perturbation we can
develop an expansion whose first term is the mean field approximation. The convergence
of this expansion can be improved if a direction selection mechanism, analogous to that
discussed previously applies. It means that the minimum of the first order approximation
of the free energy (mean field) determines a direction in the degenerate state Hilbert space
and next order contributions give only small correction to that direction. We are referring
to lattice models where the local energy is determined by the site particle occupation and
particle - particle interaction on the same site, and the interaction among sites is associated
to hopping of particles from on site to next neighbors site (Hubbard model). For particular
values of the chemical potential there is a degeneracy of the statistical weight of the two
lowest energy states of the local Hamiltonian. We use the subspace associated to these
states to introduce a general local state as a superposition of the two independent ground
states. The spontaneous symmetry breakdown will be discussed in terms of the probability
of a local ground state at thermal equilibrium. Application to repulsive Hubbard model for
bosons on a lattice, and attractive Hubbard model for fermions are in progress. Preliminary
results concerning the boson system can be found in reference\textsuperscript{10}.

[1] W. H. Zurek, Phys. Today, 36, 44, (1991)
[2] J. A. Jones Prog. NMR Spectrosc, 325, 38, (2001).
[3] D. C. Mattis in “The Theory of Magnetism II: Thermodynamics and statistical Mechanics”,
Springer Series in Solid - State Science, 55 (Springer - Verlag, Berlin, 1985)
[4] Y. L. Wang and B. R. Cooper Phys. Rev. 696 185 (1969)
[5] P. Pfeuty and R. J. Elliot, J Phys C, 2370 4, (1971)
[6] Z. Weihong, J. Oitmaa and C. J. Hamer, J. Phis. A, 5425, 27, (1994)
[7] M. Suzuki, Prog.Theor.Phys., 1454, 56, (1976)
[8] A. Georges and J.S Yedidia, J.Phys.A:Math.Gen., 2173, 24, (1991)
[9] R.M. Stratt Phys.Rev.B., 1921, 33, (1986)
[10] F. De Pasquale, S.M. Giampaolo cond-mat/0103293