Mean Field critical behaviour for a Fully Frustrated Blume-Emery-Griffiths Model

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Abstract

We present a mean field analysis of a fully frustrated Ising spin model on an Ising lattice gas. This is equivalent to a degenerate Blume-Emery-Griffiths model with frustration, which we analyze for different values of the quadrupolar interaction. This model might be useful in the study of structural glasses and related systems with disorder.

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1 Introduction

In the last two decades the physics of complex systems, ranging from dilute magnets to structural glasses has been captured by models which couple Ising variables with lattice gas or Potts variables [1]-[6], i.e. models with this type of Hamiltonian:

\[- \beta \mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j n_i n_j + \sum_{\langle ij \rangle} K n_i n_j + \mu \sum_i n_i, \]  

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where $\varepsilon_{ij} = \pm 1$ are quenched variables associated to pairs of nearest neighbour sites, $J > 0$ is the interaction between the Ising spin variables ($S = \pm 1$), $K$ is the interaction between the particles, $n_i = 0, 1$ are the lattice gas variables, $\mu$ is the chemical potential. The spins can interact each other ferromagnetically ($\varepsilon_{ij} = 1$) or antiferromagnetically ($\varepsilon_{ij} = -1$).

For $\varepsilon_{ij} = 1$ everywhere, this model concides with the original Blume-Emery-Griffiths model (BEG) \[7\]-\[17\] with an extra degeneracy 2 at each empty site. $J\varepsilon_{ij}$ is the bilinear interaction, $K$ the quadrupolar interaction, and $\mu$ the crystal field. In the last few years the disordered BEG model has been studied for random values of the $\varepsilon_{ij} = \pm 1$ \[18, 19\]. Recently the Degenerate BEG (DBEG) \[20, 21\] has been found suitable to describe the martensitic trasformation.

It may be useful to write the Hamiltonian of Eq. (1) in the following way:

$$-\beta \mathcal{H} = \sum_{\langle ij \rangle} [J(\varepsilon_{ij}S_iS_j - 1)n_in_j + \eta Jn_in_j] + \mu \sum_i n_i,$$

(2)

where $\eta = K/J + 1$. For $\eta = 0$ and $J = \infty$, this model has been extensively studied in the last few years to study glassy systems and granular materials in the disordered case (i.e. when the $\varepsilon_{ij}$ variables are randomly distributed on the lattice ) \[6\], \[22\]-\[29\]. This model can be considered as a model of particles with an internal degree of freedom ($S = \pm 1$) that interact with an effective coupling $J(\varepsilon_{ij}S_iS_j - 1)$ which is zero for spin configurations that satisfy the interactions (i.e. $\varepsilon_{ij}S_iS_j = 1$) and gives an infinite repulsion, for those that do not satisfy the interaction (i.e. $\varepsilon_{ij}S_iS_j \neq 1$). So these last configurations are forbidden for $J = \infty$.

Here we analyze the model for $J$ finite and $\eta \geq 0$. For $\eta \neq 0$ there is an extra interaction between a pair of n.n. particles, while finite values of $J$ correspond to softening the hard core potential between the spin variables.

In particular we present a mean field analysis of the Hamiltonian of Eq. (1) in the fully frustrated (FF) case on the square lattice. In this case the $\varepsilon_{ij}$ variables are choosen in such a way that every plaquette (i.e. elementary cell of the lattice) is frustrated. In other terms every plaquette has an odd number of $\varepsilon_{ij} = -1$, so that the four spins of the plaquette cannot completely satisfy the interactions. In Fig. 1 we show the Villain \[30\] scheme for the 2D FF model, highlighting the differences between the A and B sublattices. For this FF lattice we have recently \[31\] made a mean field analysis of the frustrated Percolation problem \[32\]-\[43\].

In Sec. 3 and Sec. 4 we write down the equations for site magnetizations ($m_A$ and $m_B$) and site densities ($D_A$ and $D_B$) and these enable us to find the critical lines for the order-disorder transitions in our model for the FF case.
For $K/J > -1$ (i.e. $\eta > 0$) there is a tricritical point which separates the critical line in two branches, respectively characterized by first-order and second-order transitions. On the other hand for $K/J = -1$ (i.e. $\eta = 0$) the transitions are second-order for any $\mu$.

Finally we compare the FF behaviour with that of the original Ferromagnetic BEG with and without degeneracy.

2 Mean field analysis

We will study the model defined by the Hamiltonian (1) by evaluating its free energy in a mean field approximation. For convenience we will set $\kappa = K/J$.

At each site $i$ of the lattice we have to consider the variables $S_i = \pm 1$ and $n_i = 0,1$. For notation purposes it is useful to introduce a new 4-state variable $\nu_i$ such that $\{\nu_i\} = \{n_i\} \otimes \{S_i\} = \{1 \uparrow, 1 \downarrow, 0 \uparrow, 0 \downarrow\} \equiv \{1, 2, 3, 4\}$. We can express the old variables in terms of this new variable by means of the relations: $n_iS_i = \delta_{\nu_i,1} - \delta_{\nu_i,2}$ and $n_i = \delta_{\nu_i,1} + \delta_{\nu_i,2}$.

Moreover, using the index $r$ to denote one of the four states of $\nu_i$, we can define $p_i^r = \langle \delta_{\nu_i,r} \rangle$, i.e. the probability that the site $i$ will be found in the state $\nu_i = r$. Here the angular brackets represent, as usual, the average done with the Hamiltonian of Eq. (1).

To obtain the free energy we evaluate first the internal energy of the system, which is the expectation value of our Hamiltonian:

$$-\beta U \equiv \langle -\beta H \rangle = -\beta \sum_{\langle ij \rangle} \langle H_{ij} \rangle - \beta \sum_i \langle H_i \rangle =$$

$$= J \sum_{\langle ij \rangle} \varepsilon_{ij} \langle (\delta_{\nu_i,1} - \delta_{\nu_i,2})(\delta_{\nu_j,1} - \delta_{\nu_j,2}) \rangle +$$

$$+ \kappa \sum_{\langle ij \rangle} \langle (\delta_{\nu_i,1} + \delta_{\nu_i,2})(\delta_{\nu_j,1} + \delta_{\nu_j,2}) \rangle + \mu \sum_i \langle \delta_{\nu_i,1} + \delta_{\nu_i,2} \rangle.$$

In the MF context we neglect the fluctuations and can simply put

$$\langle \delta_{\nu_i,r} \delta_{\nu_i,s} \rangle = \langle \delta_{\nu_i,r} \rangle \langle \delta_{\nu_i,s} \rangle,$$

so relation (4) implies

$$\langle -\beta H_{ij} \rangle = J \left[ \varepsilon_{ij} (p_i^1 - p_i^2) (p_j^1 - p_j^2) + \kappa (p_i^1 + p_i^2) (p_j^1 + p_j^2) \right],$$

$$\langle -\beta H_i \rangle = \mu (p_i^1 + p_i^2).$$

3
The order parameters we will use in the following are the site magnetization \( m_i \) and the lattice gas particle density \( D_i \) expressed by

\[
\begin{align*}
m_i &= \langle S_i n_i \rangle = \langle \delta_{\nu_i,1} - \delta_{\nu_i,2} \rangle = p_1^i - p_2^i, \\
D_i &= \langle n_i \rangle = \langle \delta_{\nu_i,1} + \delta_{\nu_i,2} \rangle = p_1^i + p_2^i,
\end{align*}
\]

from which we have:

\[
\begin{align*}
p_1^i &= \frac{1}{2}(D_i + m_i) \\
p_2^i &= \frac{1}{2}(D_i - m_i).
\end{align*}
\]

These relations and the equivalence condition \( p_3^i = p_4^i \), together with the normalization \( \sum_{r=1}^{4} p_r^i = 1 \), imply:

\[
p_3^i = p_4^i = \frac{1}{2}(1 - D_i).
\]

Moreover we invoke the typical translation invariance requirement of the MF approximation, taken separately on the two sublattices. Then we look for a solution in which all the sites of sublattice A (B) have the same probabilities, i.e. \( p_r^i = p_r^A \) \( \forall \ i \in A \) and \( p_r^i = p_r^B \) \( \forall \ i \in B \). This solution is one of the many occurring in the degenerate ground state.

Using the translation invariance we can write

\[-\beta \mathcal{H}_{AB} = J [m_A m_B + \kappa D_A D_B]\]

for the expectation value \( \langle -\beta \mathcal{H}_{ij} \rangle \) of the partial Hamiltonian relative to any AB ferromagnetic bond, i.e. any ferromagnetic bond \( \langle ij \rangle \) such that \( i \in A \) and \( j \in B \). A similar relation holds for all the partial Hamiltonians relative to any AA ferromagnetic bond. On the other hand, the expectation value of the partial Hamiltonian relative to any BB antiferromagnetic bond (\( \varepsilon_{ij} = -1 \)) is given by

\[-\beta \mathcal{H}_{BB} = J [-m_B^2 + \kappa D_B^2].\]

Therefore, for \( N \) sites, since the number of A sites and the number of B sites are both \( N/2 \), the internal energy is

\[
\frac{-\beta \mathcal{U}}{N} = \frac{1}{N} \sum_{i=1}^{N} \left[ \frac{1}{2} \sum_{j: \exists \langle ij \rangle} \langle -\beta \mathcal{H}_{ij} \rangle + \mu D_i \right]
\]

\[
= \frac{1}{N} \sum_{i \in A} \left[ \frac{1}{2} \left\{ \frac{z}{2} \langle -\beta \mathcal{H}_{AA} \rangle + \frac{z}{2} \langle -\beta \mathcal{H}_{AB} \rangle + \mu D_A \right\} \right]
\]
\[ + \frac{1}{N} \sum_{i \in B} \left\{ \frac{z}{2} \langle -\beta \mathcal{H}_{BA} \rangle + \frac{z}{2} \langle -\beta \mathcal{H}_{BB} \rangle + \mu D_B \right\} \]
\[ = \frac{Jz}{8} \left[ m_A^2 + 2m_Am_B - m_B^2 + \kappa (D_A + D_B)^2 \right] + \frac{1}{2} \mu (D_A + D_B). \]

(8)

For the evaluation of the MF entropic term we use the factorization property of the probability distribution \( P(\nu_1, \ldots, \nu_N) \) and therefore get

\[ S \equiv -k \sum_{\{\nu\}} P \ln P = -k \sum_{i=1}^N \sum_{r=1}^4 p_i^r \ln p_i^r. \]

Using the translation invariance, this can be written in the form

\[ \frac{S}{kN} = -\frac{1}{2} \sum_{r=1}^4 (p_A^r \ln p_A^r + p_B^r \ln p_B^r). \]

(9)

Using Eqs. (8) and (9) we can finally write the MF free energy per site of the lattice:

\[ \beta f \equiv \frac{\beta F}{N} \equiv \frac{\beta U}{N} - \frac{S}{kN}, \]

(10)

where the probabilities \( p_A^r \) and \( p_B^r \) have to be expressed in terms of the local order parameters \( m_A, m_B, D_A \) and \( D_B \) through Eq (7).

### 3 Equations for the site Magnetizations and Densities

The knowledge of the free energy allows us to write down easily the MF equations that must be satisfied by the order parameters \( m_A, m_B, D_A \) and \( D_B \).

From the stationary relations \( \partial f/\partial m_A = 0 \) and \( \partial f/\partial m_B = 0 \) it follows that

\[ m_A = D_A \tanh \left( \frac{\lambda}{2} (m_A + m_B) \right), \quad m_B = D_B \tanh \left( \frac{\lambda}{2} (m_A - m_B) \right). \]

(11)

Here \( \lambda = 4J = 4J_0/kT = T_c/T \) where \( T_c \equiv 4J_0/k \) is the mean field critical temperature of the isotropic Ising model recovered by the isotropic version of the Hamiltonian (1) in the \( \mu \rightarrow \infty \) limit.

Moreover from the stationary relations \( \partial f/\partial D_A = 0 \) and \( \partial f/\partial D_B = 0 \) we deduce that

\[ e^{\kappa \lambda (D_A + D_B) + 2\mu} = \frac{D_A^2 - m_A^2}{(1 - D_A)^2}, \]
\[ e^{\kappa \lambda (D_A + D_B) + 2\mu} = \frac{D_B^2 - m_B^2}{(1 - D_B)^2}. \]  

These relations give in implicit form \( D_A \) and \( D_B \) for every \( m_A \) and \( m_B \).

Now, replacing Eqs. (11) into Eqs. (12) we get stationarity in the four order parameters \( m_A, m_B, D_A \) and \( D_B \). After straightforward calculations we find:

\[
D_A = \frac{\cosh[(\lambda/2)(m_A + m_B)]}{e^{-\kappa \lambda/2(D_A + D_B)} \mu + \cosh[(\lambda/2)(m_A + m_B)]},
\]

\[
m_A = \frac{\sinh[(\lambda/2)(m_A + m_B)]}{e^{-\kappa \lambda/2(D_A + D_B)} \mu + \cosh[(\lambda/2)(m_A + m_B)]},
\]

\[
D_B = \frac{\cosh[(\lambda/2)(m_A - m_B)]}{e^{-\kappa \lambda/2(D_A + D_B)} \mu + \cosh[(\lambda/2)(m_A - m_B)]},
\]

\[
m_B = \frac{\sinh[(\lambda/2)(m_A - m_B)]}{e^{-\kappa \lambda/2(D_A + D_B)} \mu + \cosh[(\lambda/2)(m_A - m_B)]}.
\]

These equations can be studied numerically for different values of \( \kappa \) in order to find the fixed points for every \( \lambda \) and \( \mu \). This analysis, together with the values of the free energy (10) for each fixed point, has enabled us to find for every \( \mu \) the critical value \( \lambda_c \) where the order parameters \( m_A, m_B, D_A \) and \( D_B \) undergo a first-order or second-order transition.

4 Critical lines and Results

We have done our analysis for a number of values of the \( \kappa \) parameter, but report here, for convenience, only the most interesting cases in the range \( \kappa \geq -1 \) (i.e. \( \eta \geq 0 \)). Note that the antiquadrupolar phase that generally appears in the BEG model for \( \kappa < 0 \) does not appear here because our sublattice partition is intrinsically different from the usual BEG sublattice partition. The critical behaviours are reported in Fig. 2–6 respectively for \( \eta = 1.16, 1, .84, .5, 0 \). To appreciate the differences between the FF model and the Ferromagnetic model (i.e. \( \varepsilon_{ij} = 1 \) for all bonds), each figure contains the (a)-section in which we report the behaviour of the Degenerate FF BEG model and the (b)-section relative to behaviour of Degenerate Ferromagnetic BEG model. In the (a)-section for each \( T/T_c \) we give the field \( -\mu/\lambda \) were the transition from the high-field disordered phase (\( m_A = m_B = 0 \) and \( D_A = D_B \)) to the low-field ordered phase (\( m_A > m_B \neq 0 \) and \( D_A > D_B \)) takes place. Bold (dotted) lines represents second-order (first-order) transitions. Dashed
lines represent the spinodals, i.e. the boundaries of areas of metastability that surround any first-order transition line. Below the first-order transition line, the metastable phase is the disordered phase, above this line the metastable phase is the ordered phase. In the (b)-section for each \( T/T_c \) we give the field \(-\mu/\lambda\) were the transition from the high-field disordered phase \((m = 0\) and \(D \leq 1/2)\) to the low-field ordered phase \((m > 0\) and \(D \geq 1/2)\) takes place. As for the (a)-section, bold (dotted) lines represents second-order (first-order) transitions; dashed lines represent the spinodals. Fig. 2-6 is relative to decreasing values of the extra-interaction \(\eta = \kappa + 1\). The overall feature is that decreasing \(\eta\) we obtain a smaller ordered region. This is expected if we look at the Hamiltonian since \(\eta\) is the extra interaction among the particles. In the insert of Fig. 3b and Fig. 4b we report also the behaviour of the original BEG.

For the Ferromagnetic Degenerate BEG we find that the degeneracy reduces the area of the ordered region and increases the area of the region of first-order transitions, in agreement with recent results [20, 21].

On the other hand it is known that the frustration has the conflicting effect of reducing this region both for the original BEG with random bonds [12] and for the DBEG with random field [21]. Here we find that the frustration reduces the ordered region and moves the tricritical point toward low temperatures, i.e. the frustration in the Fully-Frustrated model (in spite of the small degeneracy present) reduces the first order region.

These results may be useful to study the effects of the softening of the hard core potential and the effect of the attraction between particles for systems described by Hamiltonian (2) such as for example glasses and granular material.

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Figure captions

Figure 1 2d FF model on the square lattice. Straight (wavy) lines represent ferromagnetic (antiferromagnetic) interactions. \( z = 4 \) ferromagnetic interactions start from each site of the sublattice \( A \) (open circles); \( z/2 \) ferromagnetic interactions and \( z/2 \) antiferromagnetic interactions start from each site of the sublattice \( B \) (closed circles).

Figure 2 (a) Critical lines for the FF lattice for \( \kappa = +.16 \) (i.e. \( \eta = 1.16 \)). Bold (dotted) lines represent second-order (first-order) transitions. Dashed lines represent the spinodals. (b) Corresponding critical lines for the ferromagnetic model (i.e. \( \varepsilon_{ij} = 1 \) for all bonds).

Figure 3 (a) Critical lines for the FF lattice for \( \kappa = 0 \) (\( \eta = 1 \)). The tricritical point is located at \( T/T_c \approx 0.233 \) and \( -\mu/\lambda = (1/\lambda) \ln(-1 + \lambda/\sqrt{2}) \approx .166 \). (b) Corresponding critical lines for the ferromagnetic model. The insert reports the critical lines for the original BEG [7].

Figure 4 (a) Critical lines for the FF lattice for \( \kappa = -.16 \) (\( \eta = .84 \)). (b) Corresponding critical lines for the ferromagnetic model. In the insert we report the corresponding critical lines for the original BEG [4].

Figure 5 (a) Critical lines for the FF lattice for \( \kappa = -.5 \) (\( \eta = +.5 \)). (b) Corresponding critical lines for the ferromagnetic model. Observe that both in the ferromagnetic and fully-frustrated case the first-order transition line continues in the ordered phase, below the tricritical point, similarly to the corresponding behaviour of the original BEG [14, 15].

Figure 6 (a) Critical lines for the FF lattice for \( \kappa = -1 \) (\( \eta = 0 \)). (b) Corresponding critical lines for the ferromagnetic model. Observe that the first-order transition line now disappears, differently from what happens in the spin glass case [18, 19].
DBEG (FF) $\kappa=+.16$
i.e. $\eta=1.16$

\[-\frac{\mu}{\lambda}\]

$\frac{1}{\lambda}=\frac{T}{T_c}$
DBEG (Ferromag.) $\kappa = +.16$

i.e. $\eta = 1.16$
DBEG (FF)_{\kappa=0}

i.e. $\eta = 1$

$\frac{-\mu}{\lambda}$

$\frac{1}{\lambda} = \frac{T}{T_c}$
DBEG (Ferromag.) $\kappa=0$

i.e. $\eta=1$
DBEG (FF) $\kappa = -0.16$

i.e. $\eta = 0.84$
DBEG (Ferromag.) $\kappa = -0.16$

i.e. $\eta = 0.84$
$$\kappa = -0.5$$

i.e. \( \eta = 0.5 \)
DBEG (Ferromag.) $\kappa = -0.5$

i.e. $\eta = +0.5$
DBEG (FF) $\kappa = -1$

i.e. $\eta = 0$
DBEG (Ferromag.) $\kappa = -1$
i.e. $\eta = 0$