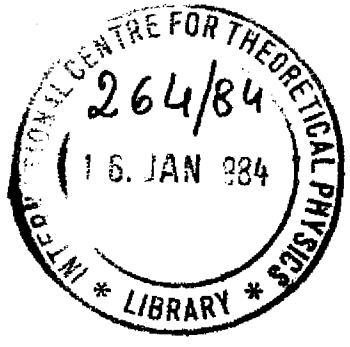

IC/83/171

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

EFFECTIVE HAMILTONIAN FOR 2-DIMENSIONAL ARBITRARY SPIN ISING MODEL

J. Sznajd

INTERNATIONAL ATOMIC ENERGY AGENCY

UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

1983 MIRAMARE-TRIESTE

IC/83/171

International Atomic Energy Agency

and

United Nations Educational Scientific and Cultural Organization

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

EFFECTIVE HAMILTONIAN FOR 2-DIMENSIONAL ARBITRARY SPIN ISING MODEL *

J. Sznajd

International Centre for Theoretical Physics, Trieste, Italy

and

Institute for Low Temperature and Structure Research, Polish Academy of Sciences,

50-329 Wroclaw, Poland.

ABSTRACT

The method of the reduction of the generalized arbitrary spin 2-dimensional Ising model to spin-half Ising model is presented. The method is demonstrated in detail by calculating the effective interaction constants to the third order in cumulant expansion for the triangular spin - 1 Ising model(the Blume-Emery-Griffiths model).

MIRAMARE-TRIESTE

August 1983

* To be submitted for publication

I. INTRODUCTION

The Hamiltonians describing a considerable number of magnetic systems, besides the linear terms, have the higher-order terms in powers of the spin variables. The existence of such terms can be caused, for example, by crystal field or coupling of the spin and elastic degrees of freedom. As for the crystal field, due to single-ion interactions, they can be easily considered by the standard methods, the higher-order interactions between various spins need some additional assumptions or rather approximations even in the molecular field theory (MFA). In order to avoid these difficulties we have proposed a simple method which allows us to reduce the arbitrary spin Ising model to spin-half Ising model. It is obvious that after such a reduction the higher-order interaction constants may only renormalize the bi-linear interaction constants and create the many-site interactions.

The most general Hamiltonian describing an arbitrary spin Ising model, with nearest-neighbour two-spin and single-ion interactions, can be written in the form

$$\mathcal{H} = \sum_{\langle ij \rangle} \sum_{nn'} K_{nn'} S_i^n S_j^{n'} \qquad (1)$$

where the powers n and n' run from 0 to 2S, and the spins have values -2S, -2(S-1), ..., 2S. The usual factor $-\beta = -1/kT$ has already been absorbed in the Hamiltonian.

Specific examples of the model (1) were studied by several methods from MFA to renormalization group approach (RG) in real space. In the MFA one has to introduce 2S parameters (molecular fields) which described 2S kinds of ordering (dipolar $\sim \langle S_i \rangle$, quadrupolar $\sim \langle S_i^2 \rangle$ etc.) and assume that each of these parameters is independent of the others [1].

The Monte Carlo RG method was used to study the model (1) with S = 1-Blume, Emery, Griffiths model (BEG), by Emery and Swendsen [2], who proposed the modified form of Migdal's recursion formula appropriate for higher spin Ising models. They wrote the Hamiltonian in the form

$$\mathcal{H} = \sum_{ij} \mathcal{J}(S_i, S_j) + \sum_k G(S_k^2) \qquad (2)$$

and chose $\mathcal{J}(S_i, S_j)$ so that it vanishes if $S_i = S_j$. Then the two-spin interactions, that ought to be small quantities, are left out, while one retains the single-ion interactions $G(S_k^2)$. Using this procedure, according to the authors, is relatively easy for S = 1. However, it is much more complicated for higher-spin models and, of course, this method is charged by all disadvantages of the Migdal-Kadanoff renormalization procedure.

According to universality the critical singularities are independent the value of S or, in other words, of the number of the spin states. Thus we propose [3] the alternative method to study the critical behaviour of the generalized Ising model by reducing the Hamiltonian (1) which describes the (2S+1)- state Ising model to two-state Ising model. Such a reduction ought to lead to the effective Hamiltonian which not only describes, in a proper way the critical behaviour of the original system (which is obvious because all Ising models with given d belong to the same universality class) but predicts the critical temperature and an eventual tricritical point as well.

II. TRANSFORMATION

We consider a triangular lattice with a spin $S_i = -2S, \ldots, 2S$ on every site. Let us substitute, in thought, 2S elementary spins $S_i^\alpha = \pm 1$ ($\alpha = 1,2,\ldots,2S$) for each original spin S_i. The original spin S_i takes, of course, each value -2S, ..., 2S with the same probability whereas the state with given value of the sum $\sum_\alpha S_i^\alpha$ n times occurs, where

$$n^{-1} = c\left(\sum_\alpha s_i^\alpha, S\right) = \binom{S}{\frac{1}{2}\sum_\alpha s_i^\alpha} . \qquad (3)$$

These imaginational elementary spins create the site-cell with 2S internal states. Now we can treat this upgrowth as the cell in the Niemeyer-Van Leeuwen sense [4] and find the effective site Hamiltonian $\mathcal{H}'(\tilde{S}_i)$ by summing over the internal states, taking into account two weight factors,

$$C(s, S) = \prod_i c\left(\sum_\alpha s_i^\alpha, S\right), \qquad (4)$$

which depend on the original spin S and site-cell spin configurations $\{S\}$ and $P(\tilde{S}, S)$ (see [4])

$$P(\tilde{s},s) = \prod_i \frac{1}{2}\left[1 + \tilde{s}_i\, t(\{s_i\})\right], \qquad (5)$$

which depend on the effective site spin and site-cell spin configurations $\{\tilde{s}\}$ and $\{S\}$ respectively.

Then the transformation is defined by

$$\exp \mathcal{H}'(\tilde{s}) = \sum_{\{s\}} P(\tilde{s},s)\, C(s,S) \exp \mathcal{H}\left(S_i \to \sum_\alpha s_i^\alpha\right). \qquad (6)$$

Thus, the transformation (6) is composed of two operations: substitution of the original spins S_i by the set of the elementary spins $\{s_i^\alpha\}$ (splitting)and summation over the internal configurations (reduction).

The similar mapping of the spin-S Ising model onto a spin - 1/2 Ising model was proposed by Berker[5], who considered the models with many-site interactions described by the Hamiltonian

$$\mathcal{H}(\{\mu_i\}) = \sum_a K_a \mu_a, \quad \mu_a = \prod_i^a \mu_i \qquad (7)$$

The author defined a new variable σ_i at each lattice site

$$\sigma_i = \mathrm{sgn}\,(\mu_i) \quad \text{for} \quad \mu_i \neq 0 \qquad (8)$$

and found the effective Hamiltonian $\mathcal{H}'(\sigma_i)$ after the summation over all configurations (μ_i) of the spin-S variables which are in accordance with the specified configuration $\{\sigma_i\}$ of the spin - 1/2 variables, with the added provision that for integer S, $\mu_i = 0$ is to contribute equally to $\sigma_i = +1$ and to $\sigma_i = -1$,

$$\exp \mathcal{H}'(\sigma_i) = \sum_{\{\mu_i\}\ \text{fixed}\ \{\sigma_i\}} \exp \mathcal{H}(\{\mu_i\}). \qquad (9)$$

For the models under consideration in this paper, that include only the nearest-neighbour two-spin interactions, Berker's procedure is equivalent to ours when $K_{nn'} = 0$ unless $n = n' = 1$ (1), i.e., when only bilinear terms

are taken into account. However we are, first of all, interested in the influence of the higher-order terms on the critical behaviour.

III. APPLICATION TO S = 1 MODEL

As an example of the use of the transformation (6) consider the spin-1 BEG model for which the Hamiltonian (1) can be written in the well-known form

$$\mathcal{H} = \tilde{K} \sum_{\langle ij\rangle} S_i S_j + \tilde{A} \sum_{\langle ij\rangle} S_i^2 S_j^2 + \tilde{D} \sum_i S_i^2. \qquad (10)$$

Inserting, according to our prescription, $(S_i^1 + S_j^2)$ instead of S_i into (10) we have

$$\mathcal{H}(s) = \tilde{K} \sum_{ij} \sum_{\alpha\beta} s_i^\alpha s_j^\beta + A \sum_{ij} s_i^1 s_i^2 s_j^1 s_j^2 + D \sum_i s_i^1 s_i^2, \qquad (11)$$

where

$$A = 4\tilde{A}, \quad D = 2(12\tilde{A} + \tilde{D}), \quad \alpha,\beta = 1,2. \qquad (12)$$

In order to find the effective Hamiltonian $\mathcal{H}'(\tilde{s})$ one can use one of the standard methods, say the cumulant approximation. Splitting of the Hamiltonian (12) into a zeroth part

$$\mathcal{H}_0 = D \sum_i s_i^1 s_i^2 \qquad (13)$$

and perturbation

$$V = \sum V_{ij} = \sum \left(\tilde{K} s_i^\alpha s_j^\beta + A\, s_i^1 s_i^2 s_j^1 s_j^2\right) \qquad (14)$$

we adapt to this problem, the Niemeyer-Van Leeuwen method [4], defining, in our case, the zeroth average as

$$\langle B\rangle_0 = \sum_{\{s\}} P(\tilde{s},s)\, C(s,S)\, B \exp \mathcal{H}_0 . \qquad (15)$$

It is easy to find that

$$\sum_{\{S\}} \exp \mathcal{H}_0 = Z_0^N , \quad Z_0 = e^D + \frac{1}{2} e^{-D} \tag{16}$$

and for the calculation of $\langle V_{ij} V_{k\ell} \ldots \rangle$ we use the following averages:

$$\langle S_i^1 \rangle = \tilde{S}_i , \quad \langle S_i^2 \rangle = f \tilde{S}_i , \quad \langle S_i^1 S_i^2 \rangle = f$$

$$f = Z_0^{-1} \left(e^D - \frac{1}{2} e^{-D} \right) . \tag{17}$$

With these rules we find

$$\langle V_{ij} \rangle_0 = (1+f)^2 \tilde{K} \tilde{S}_i \tilde{S}_j + A f^2 . \tag{18}$$

Thus to first order in cumulant expansion the effective Hamiltonian of the BEG model has the form

$$\mathcal{H}'(\tilde{S}) = N \ln Z_0 + 6 N f^2 A + (1+f)^2 \tilde{K} \sum_{\langle ij \rangle} \tilde{S}_i \tilde{S}_j . \tag{19}$$

It is easy to see that for $\tilde{D} = 0$ and $\tilde{A} = 0$ $f = 1/3$ and we get for the effective interaction constant $K_1^{(2)} = 16/9 \, \tilde{K}$, hence Berker's result [5]. Note the different definition of the Hamiltonians, which in paper [5] are normalized so that the maximum interaction between two parallel spins remains constant for each value of spin $(\tilde{K} \to \tilde{K}/(2S)^2)$. For D large and negative $f \to -1$ and $K_1^{(2)} \to 0$ (all original spins are in the state 0) and for D large and positive $f \to 1$ and $K_1^{(2)} \to 4\tilde{K}$ (all original spins are in states ± 1). For the spin 3/2 (half-integer) the result is, of course, quiet different [3] and $K_1^{(2)}$ can change only from $4\tilde{K}$ (for $D \to -\infty$) to $9\tilde{K}$ (for $D \to \infty$).

Similarly as was done in paper [5] we can, in the case under consideration, calculate the critical interaction K^c using the results of Niemeyer and Van Leeuwen [4]. From the first order cumulated expansion they lead to the following equation for K^c:

$$\left(1 + \frac{e^{dK^c} - \frac{1}{2} e^{-dK^c}}{e^{dK^c} + \frac{1}{2} e^{-dK^c}} \right)^2 K^c = 1.0968 \tag{20}$$

where $K^c = 1/4K^c$ (for comparison to Berker's result [5]) and $d = D/\tilde{K}$. As mentioned above for $d = 0$ the relation (20) gives for K^c the same value as was found by Berker, $K = 0.617$, whereas for large and positive D $K^c \to 0.274$.

It is clear that the first order cumulated expansion cannot be successful in predicting the critical behaviour of the original system not only quantitatively but even qualitatively. The effective Hamiltonian contains, in this order, only nearest-neighbour two spin -1/2 interactions then for arbitrary finite values of $\tilde{D}$ and $\tilde{A}$ one finds a critical point - in contradiction to the well-known result for the BEG model that for some relations between the interaction constants a discontinuous phase transition ought to be observed. In order to study the tricritical behaviour described by the Hamiltonian (10) one must, probably, use the third order cumulant expansion, at least.

It is obvious that the transformation (6) introduces to the effective Hamiltonian further neighbour and many-site interactions even though there have been only nearest-neighbour two-spin interactions in the original Hamiltonian. Generally the new effective interaction constants, for the model under consideration, can be written in the form

$$K_i^{(r)} = \sum_{n m} \tilde{K}^n A^m \sum_k a_{nmk}^{(r)} \, c_{nmk}^{i(r)} , \tag{21}$$

where r denotes number of interacting spins (two-spin, fourth-spin, ... interactions) and i-neighbourhood.

The second order term of the cumulant expansion has the form

$$\frac{1}{2} \left[\langle V_{ij} V_{k\ell} \rangle - \langle V_{ij} \rangle \langle V_{k\ell} \rangle \right] . \tag{22}$$

It is easy to see that the relevant contributions to the effective Hamiltonian are given only by the following terms:

$$\frac{1}{2} \tilde{K}^2 \sum_{\alpha\beta\gamma\delta} \left[\langle S_i^\alpha S_k^\beta S_k^\gamma S_j^\delta \rangle - \langle S_i^\alpha S_k^\beta \rangle \langle S_k^\gamma S_j^\delta \rangle \right] = \tilde{K}^2 (1+f)^2 (1-f^2) \tilde{S}_i \tilde{S}_j \tag{23}$$

and

$$\tilde{K}A \sum_{\alpha\beta} \left[\langle s_i^\alpha s_k^\beta s_k^1 s_k^2 s_j^1 s_j^2 \rangle - \langle s_i^\alpha s_k^\beta \rangle \langle s_k^1 s_k^2 s_j^1 s_j^2 \rangle \right] = \tilde{K}A f(1-f)(1+f)^2 \tilde{S}_i \tilde{S}_j$$

where the rules (17) were used. The first term contributes to the nearest-, next-nearest- and third-neighbour two-spin interactions $K_1^{(2)}$, $K_2^{(2)}$ and $K_3^{(2)}$ with factors 2, 2 and 1 respectively, whereas the second term only to the nearest-neighbour two-spin interaction with the factor 10.

In the third order seven interaction parameters come into play, five 2-spin coupling parameters from nearest-to fifth-neighbour and two 4-spin parameters (for eight types of interactions). The typical figures which lead to these latter ones are presented in Fig. 1.

The coefficients $a_{nmk}^{(r)}$ and $c_{nmk}^{i(r)}$ for the third-order cumulant expansion are presented in Tables I and II respectively. Note that some of the coefficients $a_{nmk}^{(r)}$ change signs for certain values of f(D). And so $a_{nmk}^{(4)}$ is negative for $f > 0$ ($D > 1/4 \ln 2$) and positive for $D < 1/4 \ln 2$. The dependence of the coefficients $a_{100}^{(2)}$, $a_{200}^{(2)}$ and $a_{300}^{(4)}$ on D is presented in Fig. 2.

IV. CONCLUSION

We have demonstrated how a simple Niemeyer-Van Leeuwen type transformation can be used to reduce the Hamiltonian appropriate for the generalized arbitrary spin Ising model with nearest-neighbour two-site interactions to effective spin-half Hamiltonian. As an example we have considered the Hamiltonian of the well known BEG model with single-ion, bilinear and biquadratic interactions on the triangular lattice. By using the third order cumulant expansion this Hamiltonian was reduced to the spin-half effective Hamiltonian with two-spin from nearest-to fifth-neighbour and four-spin interactions. In the first order cumulant expansion both single-ion ($\tilde{D}$) and biquadratic ($\tilde{A}$) terms affect, in the same way , the critical temperature which depends only on $D = 2(12\tilde{A} + \tilde{D})/\tilde{K}$. In the higher-order expansions the dependence is more complicated but the critical temperature as a function of $\tilde{D}$ and $\tilde{A}$ can, of course, be found by numerical calculations.

It is straightforward to apply our method to the Hamiltonian with higher spin interactions although the calculations become more tedious.

The open question is the possibility of the description, by the effective Hamiltonian, of the tricritical behaviour of the original system. It is obvious that in a subspace of our two-and four-spin interaction parameters (which can change sign for some values of $\tilde{D}$ and $\tilde{A}$) some first-order phase transitions can occur [6] and we will consider this problem in future.

ACKNOWLEDGMENTS

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.

REFERENCES

[1] M. Blume, V.J. Emery and R.B. Griffiths, Phys. Rev. A4, 1071 (1971), J.Sivardiere and M. Blume, Phys. Rev. B5, 1126 (1972).

[2] V.J. Emery and R.H. Swendsen, Phys. Lett. A, 64A, 325 (1977).

[3] J. Sznajd, in press.

[4] Th. Niemeyer and J.M.J. Van Leeuwen, Physica 71, 17 (1974).

[5] A. Nihat Berker, Phys. Rev. B12, 2752 (1975).
I wish to thank P. Rujan who called my attention to Berker's paper and I apologize to A.Nihat Berker for not mentioning his work in my previous paper.

[6] B. Ninhuis and M. Nauenberg , Phys. Rev. Lett. 35, 477 (1975).

TABLE I

nmk	$a^{(r)}_{nmk}$
r = 2	
100	$(1 + f)^2$
200	$(1 + f)^2(1 - f)^2$
110	$f(1 + f)^2(1-f)$
300	$(1 + f)^2 (f^2- 1)^2$
301	$(1 + f)^2 (f^2- 1) (f^2 + 2f - 1)$
302	$1/3 (1 + f) (f^2- 1) (f^3 - 5f^2 + 5f - 3)$
210	$(1 + f)^3 (f^2 - 1) (2f - 1)$
211	$2f^2(1 + f)^2 (f^2 - 1)$
212	$2(1 + f)^2 (f^2 - 1)^2$
213	$f(1 + f) (f^2 - 1)^2$
121	$1/2 (1 + f)^2$
122	$(f^2 - 1)^2$
123	$f^2(f^2- 1)^2$
r = 4	
301	$2f(1 + f)^3 (f^2 - 1)$
210	$(1 + f)^2 (f^2 - 1)^2$

Coefficients $a^{(r)}_{nmk}$ to the third order in the cumulant expansion for the BEG model.

TABLE II

	r = 2					r = 4			
i / nmk	1	2	3	4	5	 1'	 2'	 3'	 4'
100	1								
200	2	2	1						
110	10								
300	4	6	6	3	1	2	1	1	
301	10								
302	1								
210	4	4	2			6			1
211	8	8	4						
212	2								
213	8	10	10						
121	10								
122	2								
123	23								

Coefficients $c^{i(r)}_{nmk}$ - number of ways leading to given coupling of the Ising 1/2-spins for BEG model. In the column 4' are contained all the fourth-order interactions in the form $S_i S_{i+\delta_i} S_{i+\delta_i+\delta_j} S_{i+\delta_i+\delta_j+\delta_k}$, where δ_i denotes one of the nearest-neighbour sites of the site i, δ_j one of the nearest-neighbours of the site $i + \delta_i$ excluding i, etc.

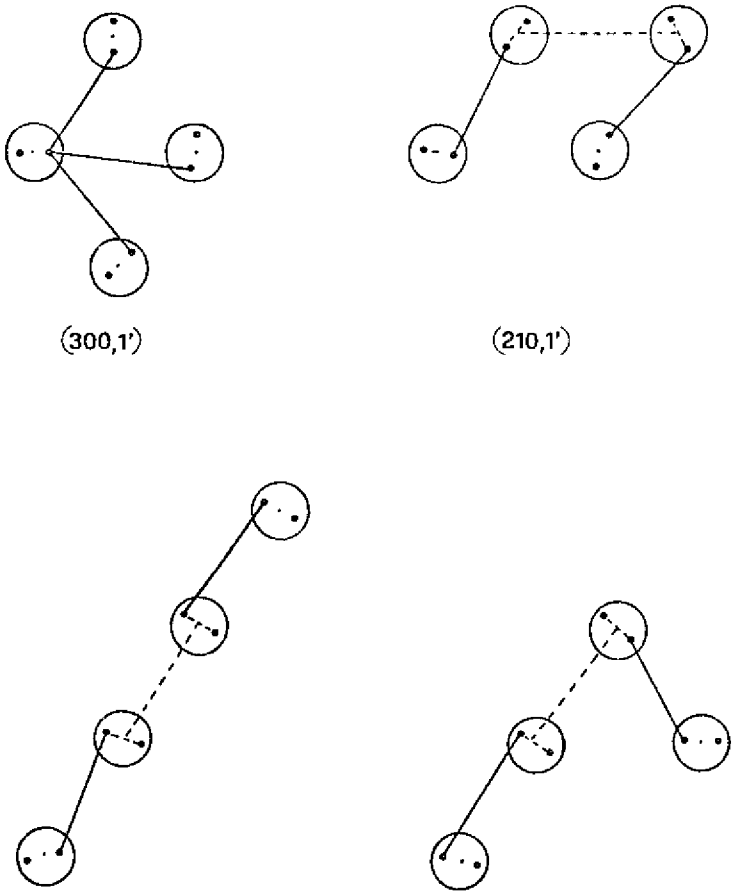

Fig.1

Some graphs which lead to the fourth-spin interactions in third order cumulant expansion. Solid and dashed lines represent the interactions $\tilde{K}$ and A respectivley. The dots in the circles represent the imaginational elementary spins $S_i^{\alpha} = \pm 1$.

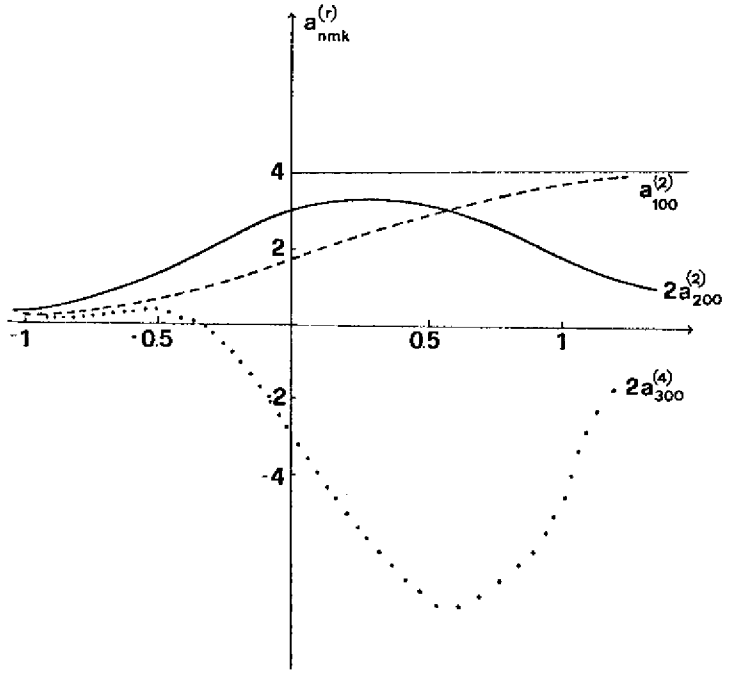

Fig.2

Coefficients $a^{(1)}_{100}$ (dashed line), $a^{(2)}_{100}$ (solid) and $a^{(4)}_{300}$ (dotted) as function of D for BEG model with $\tilde{A} = 0$.