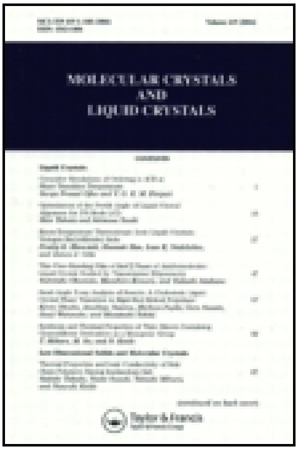


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# Quadrupole Analog of the Ising Model Spin-S : Bragg-Williams Approximation

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# QUADRUPOLE ANALOG OF THE ISING MODEL SPIN-S:BRAGG-WILLIAMS APPROXIMATION



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ABSTRACT: An analog of the spin-S Ising Model with quadrupolar interaction has been solved in the Bragg-Williams Approximation. We got a first order phase transition for special values of the parameters. We compare with results obtained by other authors and we recover the same results given by Maier-Saupe Theory for Nematic Liquid Crystals when the spin-S becomes infinite.

## Introduction

Recently Tareeva[1] proposed an analog of the Ising Model with spin-1 and quadrupolar interaction which is supposed to be useful for Liquid Crystals and Molecular Crystals solutions. His Hamiltonian is represented by

$$v_{ij} = -\alpha\,|(3s_i^2 - 2)(3s_j^2 - 2)| \qquad (1)$$

where s=1,0,-1. He found a first order phase transition using the Bragg-Williams Approximation.[2]

On the other side the Hamiltonian proposed for Liquid Crystals to describe the Nematic Phase is represented by[3]

$$v_{ij} = -\frac{\alpha}{4}\{(3\cos^2\theta_i -1)(3\cos^2\theta_j -1)\} \qquad (2)$$

where $\theta_i$ is the angle the molecule has with a prefered direction.

In this paper we discuss the solution, in the Bragg-Williams Approximation, for a spin-S Ising Model, with quadrupolar interaction, represented by

$$v_{ij} = -\frac{\alpha}{4}\ \{3(s_i/S)^2 - \lambda_s\}\ \{3(s_j/S)^2 - \lambda_s\} \quad (3)$$

where $\lambda_s = S(S+1)/S^2$

When $S=1$ and $\lambda_s=2$ we recover Tareeva's Model and $S=\infty$ with $\lambda_s=1$ gives Maier-Saupe Theory Model for Nematic Liquid Crystals.

## THEORETICAL CONSIDERATIONS

Let's consider a rectangular periodic lattice to each of whose sites a spin variable is assigned which can take one of the 2S+1 numerical values $S, S-1, \ldots -(S-1), -S$. We consider that the interaction is not zero only for nearest neighbours and is of the quadrupole type

$$v_{ij} = \frac{\alpha}{4}\ \{3(s_i/S)^2 - \lambda_s\}\ \{3(s_j/S)^2 - \lambda_s\} \quad (4)$$

The system configuration is determined by the set of numbers $\{s_i\}$ and the system energy in the configuration is

$$E(s_i) = -\frac{\alpha}{4}\sum_{<i,j>}\{3(s_i/S)^2-\lambda_s\}\ \{3(s_j/S)^2-\lambda_s\} \quad (5)$$

where the symbol <i,j> denotes the pair of nearest neighbours and the sum in (5) contains $\gamma N/2$ terms where $\gamma$ is the number of nearest neighbours of each site.

The statistical sum is

$$Q_N = \sum_{s_1}\sum_{s_2}\ldots\sum_{s_N} e^{-\beta\{s_i\}} \quad ; \quad \beta = 1/k_BT \qquad (6)$$

Here the variable s takes values -S,...S, independently of the others. The thermodynamic functions are obtained as usual from the free energy

$$A_N = -k_BT \ln Q_N$$

Let the numbers $N_s$ denote the total number of sites with a value s for the spin and $N_{ss'}$ the number of pairs of nearest neighbours with spin s and s'. Using equation (5) the energy for a certain configuration of pairs will be

$$E = -\frac{\alpha}{4}\sum_{s=-S}^{S}\ \sum_{s'\geq s}^{S} N_{ss'}\ \{3(s_i/S)^2-\lambda_s\}\ \{3(s_j/S^2-\lambda_s\} \qquad (7)$$

In the Bragg-Williams Approximation we suppose that the probability of finding a pair, $N_{ss'}/(\gamma N/2)$ is equal to the product of the probabilities of finding a lattice site with spin s and a nearest neighbour with spin s' plus the probability of finding a lattice site with spin s' and a nearest neighbour with spin s, or

$$N_{ss'}/(1/2)\gamma\ N = 2(N_s/N)(N_{s'}/N) \tag{8}$$

If s=s' the factor 2 is not necessary and

$$N_{ss}/(1/2)\gamma N=(N_s/N)^2$$

In this approximation the energy becomes a function of the long range order parameter and we can write eqs. (6) and (7) as

$$\frac{E}{N}=-\sum_{s=-S}^{+S}\ \sum_{s'=-S}^{+S}(N_s/N)(N_{s'}/N)\{3(s/S)^2-\lambda_s\}\{3(s'/S)^2-\lambda_s\}$$

$$Q_N=\sum_{N_s}\ \sum_{N_{s'}}\ g(N_s)\ \exp\{-\beta E(N_s)\} \tag{9}$$

where $g(N_s)$ is the number of different configuration with the same $N_s, N_{s-1},\ldots N_{-(s-1)}, N_{-s}$ that we can get when the lattice has N sites. Equation (9) will stay

$$Q_N=\sum_{s,s'}\frac{N!}{\prod_{-S}^{+S}N_s!}\quad \exp\{-\beta E(N_s)\} \tag{10}$$

As $N\to\infty$ the logarithm of $Q_N$ equals the logarithm of the greatest member in the sum. Using Stirling's approximation for N! we find

$$(1/N)\ \ln Q_N=(\alpha\beta\nu/4)\sum_{s,s'}(N_s/N)(N_{s'}/N)\{3(s/S)^2-\lambda_s\}$$

$$\{3(s'/S)^2-\lambda_s\}-\sum_s(N_s/N)\ \ln(N_s/N) \tag{11}$$

Considering the constraint over the $N_s$ which is $\Sigma N_s = N$ we can use the Lagrange multipliers and minimize eq.(11) to get a self consistent equation for the order parameter

$$\eta = \frac{\sum_{k=-S}^{+S} (1/2)\{3(k/S)^2 - \lambda_s\} \exp\{(\alpha\beta\gamma\eta/2)\{3(k/S)^2 - \lambda_s\}}{\sum_{k=-S}^{+S} \exp\{(\alpha\beta\gamma\eta/2)|3(k/S)^2 - \lambda_s|\}} \tag{12}$$

where the order parameter is defined by

$$\eta = \sum_{k=-S}^{+S} (N_k/N)\{3(k/S)^2 - \lambda_s\}$$

When S=1 eq. (3) gives $\lambda_1 = 2$ and we get Tareeva's[1] results. If S goes to infinity eq. (3) gives $\lambda_\infty = 1$ and we recover Maier Saupe[3] solution for Nematic Liquid Crystals wich is

$$\eta = \frac{\int_{-1}^{+1} P_2(\cos\theta)\exp\{\alpha\beta\gamma\eta P_2(\cos\theta)\}\sin\theta d\theta}{\int_{-1}^{+1} \exp\{\alpha\beta\gamma\eta P_2(\cos\theta)\}\sin\theta d\theta} \tag{13}$$

where $P_2(\cos\theta) = (3\cos^2\theta - 1)/2$.

Next we show some numerical calculations for the order parameter as a function of temperature for values of the spin S=1,2,5 and $\infty$. where we can see the first order phase tansition.

## Conclusions:

We have shown that an Ising Spin Model with quadrupole interaction similar to the one proposed for Nematic Liquid Crystals can be solved for any value of the spin S in the Bragg-Williams approximation. We find a first order phase transition for special values of the spin dependent parameter $\lambda_S$. When the spin value goes to infinity the Bragg-Williams Approximation gives for our model a solution equivalent to the Maier-Saupe molecular field approximation for nematic liquid crystals. These results are also in agreement with those we obtain from Lajzcrowicz[4] theory for spin S=1.

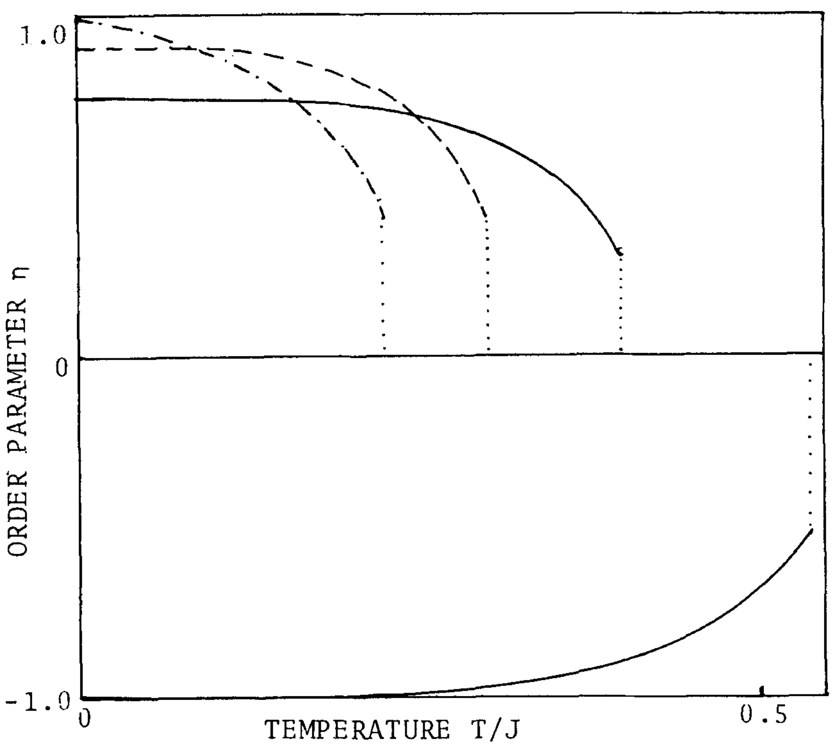


FIGURE 1 Calculated values of the order parameter as a function of the reduced temperature ($J=\alpha\gamma/k_B$) Lower line for S=1, upper solid line for S=2, dashed line for S=5 and dashed-dotted line for S=∞.

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