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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 Tareeva¹ 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

$$v_{ij} = -\alpha \frac{1}{2} (3s_i^2 - 2)(3s_j^2 - 2) \quad (1)$$

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 by³

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

where θ_i is the angle the molecule has with a preferred 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 $S, S-1, \dots, -(S-1), -S$. 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

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

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

The statistical sum is

$$Q_N = \sum_{s_1} \sum_{s_2} \dots \sum_{s_N} e^{-\beta \{s_i\}} \quad ; \quad \beta = 1/k_B T \quad (6)$$

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

$$A_N = -k_B T \ln Q_N$$

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} (1/N) \ln Q_N = & (\alpha \sqrt{4}) \sum_{s,s'} (N_s/N)(N_{s'}/N) \{3(s/S)^2 - \lambda_s\} \\ & \{3(s'/S)^2 - \lambda_{s'}\} - \sum_s (N_s/N) \ln(N_s/N) \end{aligned} \quad (11)$$

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

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

where the order parameter is defined by

$$\eta = \frac{1}{N} \sum_{k=-S}^{+S} (N_k/N) \{3(k/S)^2 - \lambda_S\}$$

When $S=1$ eq. (3) gives $\lambda_1=2$ and we get Tareeva's¹ results. If S goes to infinity eq. (3) gives $\lambda_\infty=1$ and we recover Maier Saupe³ solution for Nematic Liquid Crystals which is

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

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 ∞ . where we can see the first order phase transition.

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 λ_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 Lajzcrowicz⁴ theory for spin $S=1$.

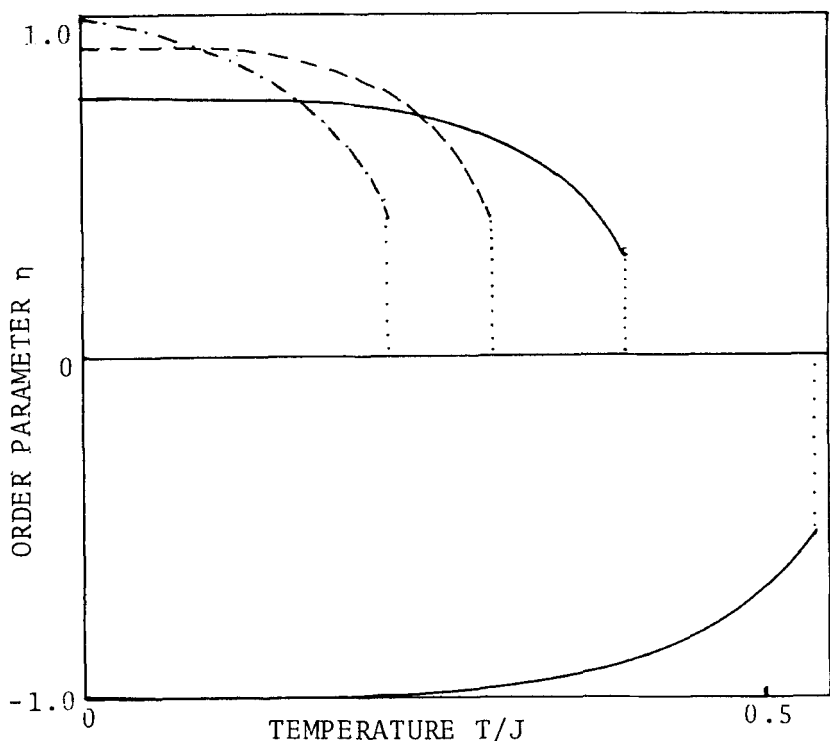


FIGURE 1 Calculated values of the order parameter as a function of the reduced temperature ($J=\alpha\gamma/k_B$) Lower line for $S=1$, upper solid line for $S=2$, dashed line for $S=5$ and dashed-dotted line for $S=\infty$.

REFERENCES:

1. E. E. TAREEVA, Soviet. Phys. Dk1.22256 (1977).
2. W. L. BRAGG and E. J. WILLIAMS, proc. R. Soc .
A 145699 (1934).
3. W. MAIER and A. SAUPE, Z. Naturforschg.14a882
(1959) and 15a287 (1960).
4. J. LAJZEROWICZ, Phys. Rev. A, 112079 (1975).