Does the Quantum Compass Model in Three Dimensions have a Phase Transition?

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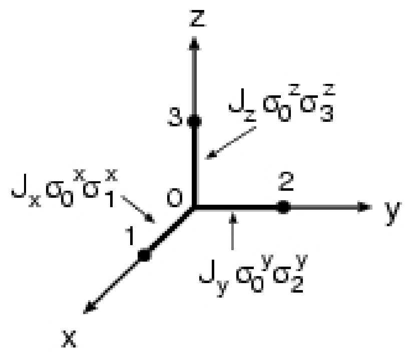
We investigate the existence of a phase transition to a low-temperature orientational or nematic phase in the Quantum Compass model on the simple cubic lattice. We conjecture, on the basis of our results, that there is no such finite temperature transition. This is in contrast to the square lattice, where such a transition has been found.

1. Introduction

'Quantum Compass' models are spin models in which the nearest-neighbour exchange coupling has the form $J^\alpha S_i^\alpha S_j^\alpha$ where $\alpha = (x,y,z)$ depends on the direction of the particular link or bond, as shown in Fig. 1. This then implies a coupling between the spin space and the physical space of the lattice. Such models were first introduced and used to describe orbital ordering in transition metal compounds [1]. They are also of interest in quantum information theory, as models of $p + ip$ superconducting arrays [2].

In the present work we consider the isotropic (all J's equal) spin-½ model on the square and simple cubic lattices, and examine the existence of a phase transition between the high-temperature disordered phase and a low-temperature phase with orientational or 'nematic' order. Such a transition has been found for the square lattice, using Quantum Monte Carlo methods [3] but there has been no previous study of the three-dimensional (3D) case.

We employ a standard method of high-temperature series expansions [4], where long series are computed in powers of $x = J/k_BT$ for thermodynamic quantities, and analysed via Padé approximant and other methods to identify a singular point x_c corresponding to the expected phase transition. Special features of this model allow rather long series to be obtained (up to x^{20} for the 3D case). Details of the calculation are given in a forthcoming paper [5].



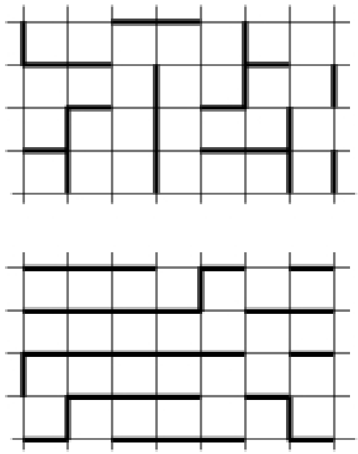


Fig. 1. (Left) The exchange couplings of the model; (Right) A schematic of the orientational or 'nematic' phase. The solid bonds have lower than average energy.

2. Method and Results

The Hamiltonian of the model, in standard notation, is

$$H = J_x \sum_{<ij>}^{(x)} \sigma_i^x \sigma_j^x + J_y \sum_{<ij>}^{(y)} \sigma_i^y \sigma_j^y + J_z \sum_{<ij>}^{(z)} \sigma_i^z \sigma_j^z$$

where the σ_i^α are Pauli spin operators ($\alpha = x,y,z$; $\sigma_i^\alpha = 2S_i^\alpha$). By expanding the Boltzmann factor $e^{-\beta H}$ in powers of $\beta = 1/k_B T$, and evaluating the resulting traces of spin operators, we obtain a conventional high-temperature expansion for the free energy

$$-\beta f = \ln 2 + \sum_r a_r (J_x, J_y, J_z) \beta^r$$

From the free energy expansion we can compute the specific heat. However, this is usually not the best quantity for identifying a phase transition, as it has only a weak singularity. For magnetic phase transitions the existence and/or location of a critical point is usually determined from the susceptibility, which has a much stronger singularity. In the present model, including a field term in the Hamiltonian $H = H_0 - hD$ where D is the nematic order parameter:

$$D = 2J_z \sum_{<ij>}^{(z)} \sigma_i^z \sigma_j^z - J_x \sum_{<ij>}^{(x)} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>}^{(y)} \sigma_i^y \sigma_j^y$$

We obtain a similar high-temperature expansion for the generalized susceptibility

$$\beta\chi = \lim_{h \to 0} \partial^2/\partial h^2 (\ln Z/N) = \sum_{r=2}^{\infty} c_r (J_x, J_y, J_z) \beta^r$$

We have derived the series to order β^{16} for the isotropic model (all J's equal). The series for the susceptibility, which contains only even powers of β, is:

$$\beta\chi = 6 - 6\beta^2 + 20\beta^4 - 81.0476190476\ldots \beta^6 + 367.149206349\ldots \beta^8 - 1787.51576719\ldots \beta^{10} + 9155.75874989\ldots \beta^{12} - 48688.4786086\ldots \beta^{14} + 266451.000791\ldots \beta^{16} + \ldots$$

As is apparent, the terms are of alternating sign, indicating that the dominant singularity lies on the negative β^2 i.e., the imaginary β axis. Thus we need to use Padé approximants or similar methods to analyse the series beyond its radius of convergence. The series have proved difficult to analyse, because of the complex singularity structure. However, for the two-dimensional (2D) case we do find a critical point, consistent with the Monte Carlo result [3]. On the other hand, we find no evidence for a critical point in the 3D case.

The difference is seen more strikingly in Fig. 2, which shows estimates of the inverse susceptibility, obtained from Padé approximants, versus temperature T.

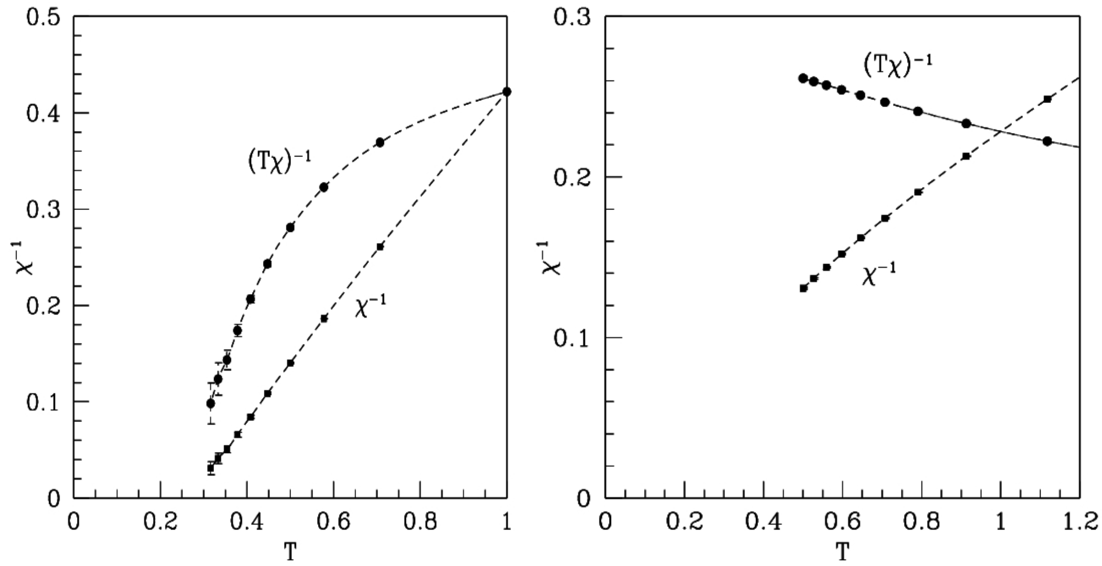


Fig.2. Inverse susceptibility versus temperature for the (a) 2D and (b) 3D models. The lines are guides for the eye.

In the 2D case the inverse susceptibility clearly approaches zero, heralding a phase transition, at a temperature $k_BT/J \sim 0.25$. This is consistent with, albeit less precise than the Quantum Monte Carlo result [3]. This clearly demonstrates that the method works. On the other hand, for the 3D case, χ^{-1} appears to approach zero, if at all, very close to or at $T = 0$. The $(\beta\chi)^{-1}$ points are, in fact, monotonically increasing, indicating that χ is increasing less rapidly than $1/T$ with decreasing temperature.

3. Discussion

The question of the existence of a thermodynamic phase transition in the Quantum Compass model in 3D models remains an important and open question. The present work is, to our knowledge, the first attempt to address this problem using the technique of high-temperature series expansions, a well established method in other contexts.

We have found a striking qualitative difference between the previously studied 2D Quantum Compass model, which has been shown to have a phase transition to a low-temperature phase with orientational or nematic order, and the 3D model. Our results lead us to conjecture that there is no finite T transition in the 3D model. At first sight this seems surprising, since for normal magnetic phase transitions an increase in spatial dimensionality reduces the effect of thermal fluctuations and thereby leads to an increase in critical temperature. In the present model the bond interactions along different spatial directions compete with each other in ‘pulling’ the spins in different directions, and the additional direction in going from two- to three dimensions leads to an increase in the tendency to disorder.

The series have proved difficult to analyse, as they are dominated by singularities on the imaginary temperature axis. This is, perhaps, a reflection of the peculiar ‘one-dimensional’ nature of the couplings in the model. Further insight into this complex singularity structure may suggest other, more effective, ways of analysing the series.

Acknowledgments

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