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STATISTICAL MECHANICS OF ISING MODELS WITH $S > 1$ HAVING BIQUADRATIC EXCHANGE AND UNIAXIAL ANISOTROPY

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Abstract. - Ising ferromagnets having spins greater than unity, with the inclusion of biquadratic exchange and single-ion anisotropy, are studied by the cluster variational method. The critical temperature, the magnetization curves, and the thermal variation of the quadrupolar moment, are studied for a range of interaction parameters where anomalous behaviour occurs.

1. Introduction

For a spin-one Ising model on a Bethe lattice, anomalous behaviour in the magnetization curves when the ratio of the biquadratic and bilinear exchange interactions is negative, was reported [1, 2]. Identical results were obtained for the same Ising model on a regular periodic lattice when treated within the generalised constant coupling approximation. More recently, we have shown that this approximation is equivalent to the use of the generalised cluster variational method within the pair approximation, and we have applied the latter method to a study of Ising models having higher spin values [3]. In that reference, the critical temperature and magnetisation curves were studied in the regime where anomalous behaviour was expected. Although the single-ion anisotropy was fully accounted for in the theory, only detailed results in the absence of single-ion anisotropy were reported in that paper where the emphasis was to high light the differences in the results to those of the Oguchi pair model approximation. In the present paper we report additional results of our study that show clearly the competing roles played by the biquadratic exchange and single-ion anisotropy in determining the shape of the magnetization curves. Some results for the quadrupolar moment are also reported. The nomenclature of this paper is that of reference [3], where the Hamiltonian studied and the theory used is fully described.

2. The critical temperature

In figures 1-3 we show the critical temperature as a function of $\alpha \equiv J'/J$ (the ratio of biquadratic to bilinear exchange interactions) for $S = 3/2, 2$ and $5/2$ for several values of the single-ion anisotropy parameter $\alpha' = D/J_z$. The results are for a lattice with coordination number, $z = 6$. For a fixed value of $\alpha$ it is seen that the Curie temperature shifts to higher temperatures as the strength of the single-ion anisotropy is made more negative. There is, however, an unexpected feature for spin 2 in the region where the solutions become double-valued. It is seen that curves a, b and c, for the smaller negative values of single-ion anisotropy, cross in the vicinity of their bulges. Thus the lower solutions for the critical temperature do not decrease monotonically to lower temperatures for some values of $\alpha$.
the shape of the magnetization curves is shown in figure 5. In that figure curves of the same type (full, dashed or dash-dotted lines) belong to the same value of \( \alpha \). We refer first to the curves for \( \alpha = -0.15 \). Curve a corresponding to the absence of single-ion anisotropy, has a downwards convex shape in the vicinity of \( k_B T/J \approx 1 \). It is seen that this anomalous behaviour is progressively removed (curves b, c) as the single-ion anisotropy is increased negatively, and the magnetization curve assumes a more conventional concave form. A more striking effect occurs in the case when \( \alpha = -0.18 \). Comparison of curves d, e and f show that the magnetization in the low temperature limit switches from \( m = 3/2 \) to \( m = 2 \) when a negative single-ion anisotropy above a certain strength is present. An even greater switch is possible from \( m = 1 \) to \( m = 2 \) for some values of the parameters, see for example, curves g and h corresponding to \( \alpha = -0.4 \).

3. The quadrupolar moment

In figure 4 we present typical results for the temperature variation of the quadrupolar moment \( q \) in the case of spin 2 for the simple cubic lattice. The chosen values of \( \alpha \) are those used in figure 6 of reference [3] to enable a comparison with the magnetization curves to be made.

4. The magnetization curves

The effect of the competition between the biquadratic exchange and the single-ion anisotropy on the shape of the magnetization curves is shown in figure 5. In that figure curves of the same type (full, dashed or dash-dotted lines) belong to the same value of \( \alpha \). We refer first to the curves for \( \alpha = -0.15 \). Curve a corresponding to the absence of single-ion anisotropy, has a downwards convex shape in the vicinity of \( k_B T/J \approx 1 \). It is seen that this anomalous behaviour is progressively removed (curves b, c) as the single-ion anisotropy is increased negatively, and the magnetization curve assumes a more conventional concave form. A more striking effect occurs in the case when \( \alpha = -0.18 \). Comparison of curves d, e and f show that the magnetization in the low temperature limit switches from \( m = 3/2 \) to \( m = 2 \) when a negative single-ion anisotropy above a certain strength is present. An even greater switch is possible from \( m = 1 \) to \( m = 2 \) for some values of the parameters, see for example, curves g and h corresponding to \( \alpha = -0.4 \).

Fig. 4. – The thermal variation of the quadrupolar moment, \( q \), for spin 2 (with \( \alpha' = 0, \alpha = 6 \)). Curves a-h correspond to \( \alpha = 0, -0.1, -0.15, -0.18, -0.2, -0.3, -0.4 \) and \( -0.5 \) respectively.

Fig. 5. – The magnetization, \( m \), for spin 2 (with \( \alpha = 6 \)). The solid curves are for \( \alpha = -0.15 \) with curves a-c having \( \alpha' = 0, -0.1, -0.2 \) respectively. The dashed curves belong to \( \alpha = -0.18 \) with curves d-f having \( \alpha' = 0, -0.03 \) and \( -0.1 \) respectively. The dash-dotted curves, g and h, are for \( \alpha = -0.4 \) with \( \alpha' = 0 \) and \( -1.2 \) respectively.