Ground-State Entropy of $\pm J$ Ising Lattices by Monte Carlo Simulations

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An accurate numerical calculation of the ground-state entropy associated to two-dimensional $\pm J$ Ising lattices is presented. The method is based on the use of the thermodynamic integration method. Total energy is calculated by means of the Monte Carlo method. Then the entropy (or degeneracy) of a state of interest is obtained by using thermodynamic integration starting at a known reference state. Results for small sizes are compared to exact values obtained by exhaustive scanning of the entire ground-state manifold, which serves as a test for the reliability of the simulation model developed here. The close agreement between simulated and exact results for energy and remnant entropy supports the validity of the technique used for describing the properties of $\pm J$ Ising lattices at the fundamental level. Finally, the results are extrapolated in order to estimate tendencies for larger systems.

KEY WORDS: Remnant entropy; thermodynamic integration; Monte Carlo method; $\pm J$ Hamiltonian; frustration.

1. INTRODUCTION

In many complex systems, evaluation of thermodynamic properties is a difficult matter. In the case of $\pm J$ Ising lattices it is even more so, due to the highly degenerate fundamental level as a consequence of two factors: (i) frustration and (ii) randomness. An analytic exact solution yielding the low-energy portion of the density of states (to mention just one example) is nearly impossible. Then it is necessary to shift to precise numerical calculations in order to calculate thermodynamic quantities such as energy and entropy.
as free energy and entropy. However, the difficulty of reaching solutions of desired accuracy increases with lattice size. In the present paper, we aim to apply a method that leads to accurate descriptions of the just-mentioned thermodynamic variables for square lattices, even when temperature approaches zero and only states of the ground manifold (GM) are populated. For this extreme case, we have at our disposal exact results for small samples, which can be used for comparison to establish criteria to reach results of prescribed precision.

In fact, one difficult task in this work is to characterize the GM to calculate properties of these systems at extremely low temperatures. So far this has been done following two lines of thought: on one hand, exact calculations based on exhaustive scanning of the whole GM (3–7) and on the other hand, numerical techniques based on the analysis of a representative set of states belonging to the GM. (8–15) The number of states of the GM at the thermodynamic limit constitutes a very severe limitation for both descriptions. In fact, upon increasing the size of the system, the degeneracy of the GM grows exponentially. Thus, the huge computer time needed in either case makes these approaches nearly impossible.

Several authors have discussed the applicability of numerical algorithms for determining thermodynamic properties such as entropy. Without attempting a complete review of the field, let us mention here the attempt by S. Kirkpatrick (16) (among others) using Monte Carlo (MC) simulation techniques. Then, J. Vannimenus and G. Toulouse (17) made progress in the field taking advantage of the topological properties of the system. Some other authors, such as I. Morgenstern and K. Binder, (18) H.-F. Cheung and W. L. McMillan, (19) and A. J. Kolan and R. G. Palmer, (20) made important contributions using transfer matrix calculations. More recently, A. K. Hartmann (21) has explored the configuration space of these systems by means of a ballistic-search algorithm and genetic cluster-exact approximation (CEA). These diverse approaches have obtained different representative values for the entropy of the GM in the thermodynamic limit. In particular, in ref. 16 the evaluation of the remnant entropy has been determined via numerical implementation of the well-known "thermodynamic integration method" (TIM). (22) This pioneering work was one of the first reliable calculations of entropy associated to the GM. The disagreement between the numerical value proposed in that early work and those reported in more recent contributions can be attributed to the limited observation times used in the early work in comparison with the characteristic relaxation time scale of the phenomenon.

In this context, the main aim of the present work is to reformulate the use of the TIM and to show that it is able to determine accurate values for thermodynamic quantities associated to the GM of $\pm J$ Ising lattices. This