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LETTER TO THE EDITOR

A discrete vector spin model

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Abstract. A modification of the classical Heisenberg model is proposed in which the continuously rotating spin variables are replaced by spins which are only allowed an isotropically distributed discrete set of directions. The change is motivated by a need to simplify the calculations associated with Monte Carlo simulation of vector spin systems, a goal accomplished by the present model. An efficient table-based simulation technique is described and preliminary results for the critical region presented; various extensions of the model are discussed.

The Ising model, because of its computational simplicity, has been extensively studied by Monte Carlo simulation with a view to understanding a variety of magnetic phenomena. A companion system, the classical Heisenberg model, despite its capacity for emulating a wider range of behavioural possibilities due to the additional freedom provided by the vector spins, has not been subject to the same degree of attention, principally because of its increased computational complexity. Evidence for the continued interest in spin-model simulations derives from the appearance of a number of improved algorithms for Ising Monte Carlo computation (e.g. Jacobs and Rebbi 1981, Williams and Kalos 1984) and the construction of special-purpose processors (Hoogland *et al* 1983, Pearson *et al* 1983); equivalent developments for the Heisenberg model have not occurred.

The purpose of this letter is to introduce a new vector spin model having a great deal in common with the classical Heisenberg model, yet which is nevertheless only marginally more complex than the Ising model from the simulation point of view. In addition to describing the model, presenting results of a preliminary Monte Carlo analysis and comparing the efficiency of the computations required for the new model with those of the old, we outline the directions in which the model can be extended for use in studying other systems of current interest.

The key step in simplifying the calculations associated with Monte Carlo simulation of the classical Heisenberg model is the replacement of the freely oriented spin vectors by vectors allowed a relatively large but finite set of directions: large so as to maintain the similarity with the continuous spin system, finite in order to facilitate replacement of the relatively heavy computations by references to tabulated values. In a sense the model is related to the original Heisenberg system in the same way that the two-dimensional clock model (e.g. José *et al* 1977, Tobochnik 1982) is related to the planar rotator (or classical XY) model.

The precise number of allowed spin directions is a matter of choice, the only requirement being that each direction is equivalent in the sense of having an identical

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set of neighbour directions. The value 30 is used in the present work, the directions being those of the midpoints of the edges of the regular icosahedron (or, equivalently, the dodecahedron) from the middle of the polyhedron. Given the vertex coordinates of either of these Platonic solids (Coxeter 1963), the unit vectors to the edge midpoints are readily found to be $(0, 0, \pm 1)$, $(\pm\frac{1}{2}, \pm\tau/2, \pm 1/2\tau)$ and their cyclic permutations, where $\tau = 2\cos(\pi/5) = \frac{1}{2}(5^{1/2}+1)$ is the familiar golden ratio. Each of the directions defined in this way has four equivalent adjacent directions.

The simplest Hamiltonian based on this finite vector set is the analogue of the isotropic Heisenberg Hamiltonian, namely

$$E = -J\sum_{\langle ij\rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j - \boldsymbol{H}\cdot\sum_i \boldsymbol{s}_i \qquad |\boldsymbol{s}_i| = 1 \tag{1}$$

with the first sum being over all nearest-neighbour site pairs on the lattice; J is the exchange interaction parameter and $\boldsymbol{H}$ the applied field. Now both the spin product $\boldsymbol{s}_i \cdot \boldsymbol{s}_j$ and the component of $\boldsymbol{s}_i$ parallel to $\boldsymbol{H}$ (assuming $\boldsymbol{H}$ to lie along one of the 30 spin directions) can take only nine possible values $\{0, \pm\frac{1}{2}, \pm 1, \pm\tau/2, \pm 1/2\tau\}$, and it is this feature that leads to the greatly simplified Monte Carlo computations.

Applied to a particular spin $\boldsymbol{s}_i$ the steps of the typical Monte Carlo process are: (i) a random selection of a new trial spin direction $\boldsymbol{s}_i'$; (ii) computing the energy change

$$\Delta E = -J(\boldsymbol{s}_i' - \boldsymbol{s}_i)\cdot\sum \boldsymbol{s}_j - \boldsymbol{H}\cdot(\boldsymbol{s}_i' - \boldsymbol{s}_i) \tag{2}$$

where the sum is over the neighbours of site i; (iii) computing the quantity $\omega = 1/(\lambda+1)$ where

$$\lambda = \exp(\beta\Delta E) = \eta^{(\boldsymbol{s}_i'-\boldsymbol{s}_i)\cdot\sum \boldsymbol{s}_j}\zeta^{\hat{\boldsymbol{H}}\cdot(\boldsymbol{s}_i'-\boldsymbol{s}_i)} \tag{3}$$

and $\eta = \exp(\beta J)$, $\zeta = \exp(\beta H)$ $(\beta = 1/k_B T)$; (iv) selection of a random number $R \in (0, 1)$ and replacement of $\boldsymbol{s}_i$ by $\boldsymbol{s}_i'$ on condition (Yang 1963) that $R \leqslant \omega$. Each spin is considered in turn, and a complete simulation run consists of many such passes over the entire lattice.

The fact that $\boldsymbol{s}_i \cdot \boldsymbol{s}_j$ has only nine possible values allows the spin term in (3) to be rewritten as

$$(\boldsymbol{s}_i' - \boldsymbol{s}_i)\cdot\sum \boldsymbol{s}_j = \sum_{k=1}^{9} n_k v_k \qquad \sum_{k=1}^{9} n_k = 12 \tag{4}$$

for the simple cubic lattice, where $\{v_k\}$ are the values of $\boldsymbol{s}_i \cdot \boldsymbol{s}_j$ and $\{n_k\}$ is the number of times each appears in the spin-product sum. The possible values of this sum are of the form $m_1/2 + m_2/2\tau$, where $|m_1| \leqslant 24$ and $|m_2| \leqslant 12$; there are a total of 1225 such values that can be indexed by means of the expression $25m_1 + m_2$, but because the $\{n_k\}$ are constrained (equation (4)), not all will be realised. It follows from (3) that for $\boldsymbol{H} = 0$ there will be a similar number of possible values of ω, while in a non-zero field there will be nine times as many. All that is needed in order to be able to use a table of precomputed values of ω in the Monte Carlo process is a suitable indexing scheme based on the spin values; this we now describe.

The spin vectors $\boldsymbol{s}_i$ are replaced by numbers g_i, $1 \leqslant g_i \leqslant 30$, that uniquely identify the spin directions. To enable the system to evolve gradually, the trial spin vector $\boldsymbol{s}_i'$ is selected at random from among the four directions adjacent to $\boldsymbol{s}_i$ and the corresponding number is g_i'; this selection employs a table giving the four allowed g_n' for each g_n. (The limitation to adjacent directions is not essential, and a slightly different approach allows an unrestricted choice among the 30 directions.) Now there are just 3600 possible combinations of spin directions that go to make up the term $(\boldsymbol{s}_i' - \boldsymbol{s}_i)\cdot\boldsymbol{s}_j$

which itself has only nine possible values $\{0, \pm(\frac{1}{2}-1/2\tau), \pm 1/2\tau, \pm\frac{1}{2}, \pm 1/\tau\}$; note that these values are all of the form $m_1/2+m_2/2\tau$. It is therefore possible to combine g_i, g_i' and g_j to select a value ν_j from a table of 3600 entries; there are only nine distinct values in this table, each of the form $25m_1+m_2$, and the selected ν_j corresponds to the term's contribution to the sum $\Sigma\, n_k v_k$. For the case of zero field the sum of six such ν_j for the neighbours of site i is used as an index for accessing the appropriate value of ω, while for non-zero field an additional ν_j is included to account for the field contribution. In this manner, the not inconsiderable computation implicit in (3) is replaced by a few simple operations supporting the table lookup; a similar approach can also be used for evaluating the spin correlation functions.

Justification for introducing the discrete vector model follows from a comparison of the computation speeds with that of the classical Heisenberg model simulated in the usual way (Binder 1976). Tests conducted using an IBM 3081 computer give a rate of approximately 60 μs per spin for the Heisenberg case, while for the new model the value falls to 6 μs, an order of magnitude improvement. Another comparison of interest is with a Heisenberg simulation on the ICL Distributed Array Processor (DAP) (Parkinson 1983), a set of 4096 parallel processing elements which has proved especially well adapted for Ising model studies (Reddaway *et al* 1985). When the simulation is reorganised for DAP efficiency a value of 2 μs per spin is obtained, with scope remaining for further optimisation; the DAP however is unable to take advantage of the table-based approach for the discrete model. The DAP therefore also remains the ideal choice of computer for the vector model, but it suffers from limited availability. Another possibility that merits consideration is the development of a special-purpose processor to handle the discrete model; the use of tables means that the implementation ought not to be significantly more complicated than for the Ising model.

Several Monte Carlo runs were carried out for the discrete model at $\boldsymbol{H}=0$ and results for an $N=30^3$ system are described below. The results are based on 26 000 passes through the lattice at each of a sequence of decreasing temperatures, excluding the first 2000 passes to allows equilibration at each temperature. Due to the 30-fold ground-state degeneracy the direction of the usual order parameter (the magnetisation) $\Sigma\, \boldsymbol{s}_i$ tends to drift at finite temperature, and this leads to a configuration average $\langle \Sigma\, \boldsymbol{s}_i \rangle = 0$ even though the spins may be aligned to a significant extent. A quantity which does reflect the presence of long-range order independent of the directional instability is the averaged magnitude of the magnetisation $\langle |\Sigma\, \boldsymbol{s}_i| \rangle$, and it is this quantity that is studied here; the susceptibility is computed from the fluctuations.

Figures 1 and 2 show the magnetisation (M) and susceptibility (χ) per spin over the temperature range considered. There is clear evidence in support of the expected second-order transition which occurs at a critical temperature $T_c \approx 1.5$ (units of J). While the results for χ are too scattered to permit meaningful exponent estimation, the graph of M is sufficiently smooth to warrant an examination of the exponent β defined by $M \propto (1-T/T_c)^{\beta}$, $T \leqslant T_c$. A graph of $\log M$ against $\log(1-T/T_c)$ should be linear near T_c with gradient β. Since T_c is not available to the required accuracy, a series of trial values increasing in steps of 0.005 were used; the best (i.e. the most linear) results were obtained for $T_c = 1.455$, corresponding to $\beta = 0.32$. These values, while still subject to further refinement, are satisfyingly close to those of the classical Heisenberg model: series analysis of χ (McKenzie *et al* 1982) yields $T_c = 1.44$, while the Monte Carlo estimate of β is ≈ 0.32 (Watson *et al* 1969).

A more detailed study of the model would, in addition to probing the critical region, consider the field dependence and examine the longitudinal and transverse

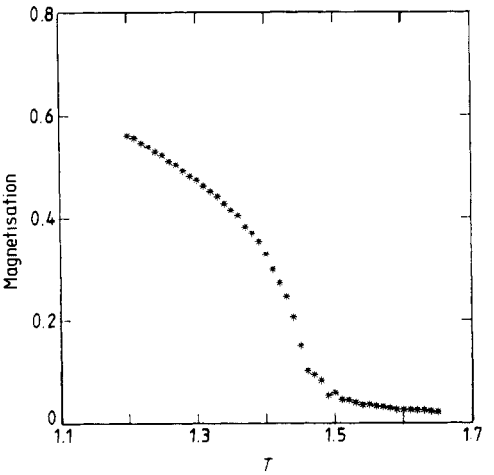

Figure 1. Magnetisation (as defined in the text) plotted as a function of temperature for the discrete vector model on a 30^3 lattice.

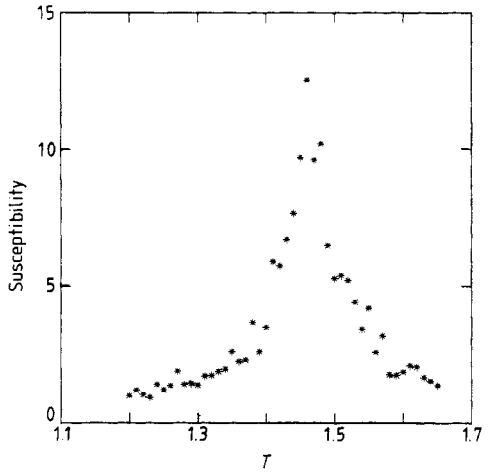

Figure 2. A plot of susceptibility as a function of temperature.

spin correlations. Critical behaviour can also be studied by series methods (see Domb and Green 1974). High-temperature expansions can be developed using well known techniques; the susceptibility in particular can be treated by means of the χ^{-1} star expansion (Rapaport 1974). Low-temperature expansions should also be feasible given the discrete nature of the excitations from the ground state.

The model presented here is the simplest member of a family capable, in principle, of efficiently modelling a range of effects that are of considerable interest. Several examples and the necessary modifications follow. A random field model is obtained by replacing the constant applied field $\boldsymbol{H}$ by a local field variable $\boldsymbol{h}_i$ at each site, where $|\boldsymbol{h}_i|$ is fixed and the direction picked at random from among the allowed spin directions. Essentially no changes to the algorithm are needed to handle this model. Directional anisotropy of the form $(\boldsymbol{L}\cdot\boldsymbol{s}_i)^2$ can be included together with the field term ($\boldsymbol{L}$ is

assumed to be parallel to one of the allowed spin directions) by simply altering the tables. Spin glasses and dilute magnets can also be treated; for example, a random $\pm J$ interaction can be incorporated through additional manipulation of the table indices that adds little to the computational effort.

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