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1983 J. Phys. A: Math. Gen. 16 4423

(http://iopscience.iop.org/0305-4470/16/18/041)

J. Phys. A: Math. Gen. **16** (1983) 4423–4426. Printed in Great Britain

COMMENT

Heat capacity of two-dimensional O(n) spin systems by the Monte Carlo method

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Received 8 August 1983

Abstract. Monte Carlo estimates of the heat capacity of the two-dimensional O(n) spin systems with $n = 3$, 4 and 5 are compared to the results given by the spherical model ($n \to \infty$). The values of the maxima of the heat capacity are approximately equal to $\frac{1}{2}n$, when the temperature is $2n^{-1}$. The C/n against nT curves of the estimates come close to the curve of the spherical model for $nT \geq 4$.

1. Introduction

The role of the heat capacity in the understanding of the two-dimensional O(n) spin systems has been emphasised in recent papers by Brout *et al* (1983*a*, *b*) and Brout and Silovy (1983). Maxima in the heat capacity, as shown on the O(3) energy curves in terms of the temperature (Watson *et al* 1970, Shenker and Tobochnik 1980), are reminiscent of an ordering transition. In the corresponding region of temperature, the fluctuation regime of the spins differs qualitatively from the low-temperature regime where one degree of freedom is inactivated for the short length scales. The application of the spherical model to the analysis of this fluctuation regime provides a guide for a better understanding of the mechanism which foils a true transition in those two-dimensional systems (Brout *et al* 1983a, b), and in the systems of lattice gauge theory to which they are related (Polyakov 1975). This comment makes a quantitative comparison of the heat capacity of the two-dimensional O(n) systems for small n(3, 4 and 5) with that of the limit case $n \to \infty$, the spherical model. The computations were made using the Monte Carlo method.

2. The method

The algorithm of Metropolis (Binder 1979) determines the transition process of the n-dimensional spins for an energy defined by the expression

$$E = -(2T)^{-1} \sum_{i,j} \boldsymbol{S}_i \boldsymbol{S}_j$$

where T is the temperature and i, j are neighbouring sites of the lattice. A convenient transition rate is obtained by using as new spin vector, the normalisation of the sum of its most recent value with a random vector selected out of a sphere (Landau and Binder 1981). For convenience and computational efficency in the APL language which

has been used, the algorithm is vectorised. The lattice 32×33 is split into two sublattices A and B so that the nearest neighbours of the sublattice A be located on the sublattice B, and vice versa. The transition process is applied globally to the spins of a sublattice. Quasi-periodic boundary conditions are used (Watson *et al* 1969). In this scheme, the spins may be labelled by a single index, and the indices of the nearest neighbours are easily computed by adding a constant to the site index (modulo the number of the sublattice sites).

The first 20 percent of each run have been systematically disregarded. If necessary, more have been skipped until no significant difference was found between the runs corresponding to the ordered and the random initial configurations.

The standard deviation of the energy is estimated from the expression

$$\sigma^2(E_g) = N^{-1}(N-1)^{-1} \sum_g (E_g - \langle E_g \rangle)^2$$

for the variance of the energy E_g of N groups of 40 approximately independent configurations. The averages are taken once every eight passes through the lattice, and sometimes four. The heat capacity C is estimated from the fluctuation of the energy

$$C = N_s T^{-2} \sum (E - \langle E \rangle)^2$$

where N_s is the number of the lattice sites. The corresponding standard deviation is given in the same way by the variance of C across groups of 40 configurations. The

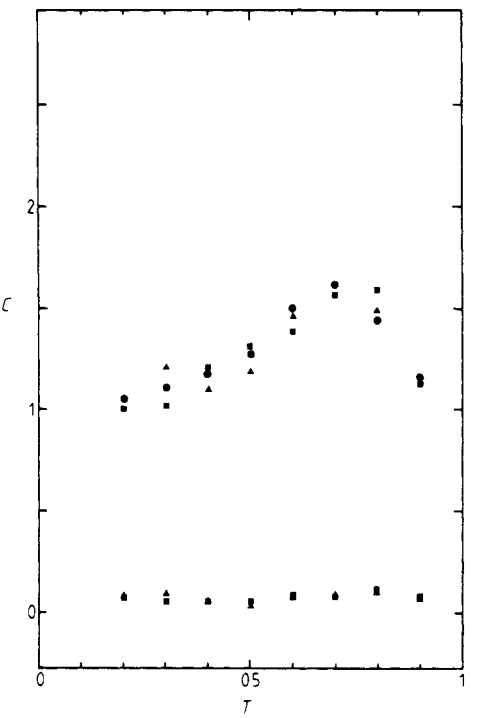

Figure 1. Heat capacity of O(3) in terms of the temperature. Estimates from the energy fluctuations are shown for (▲) ordered and (■) random initial configurations. The lower graph indicates standard deviations of these quantities.

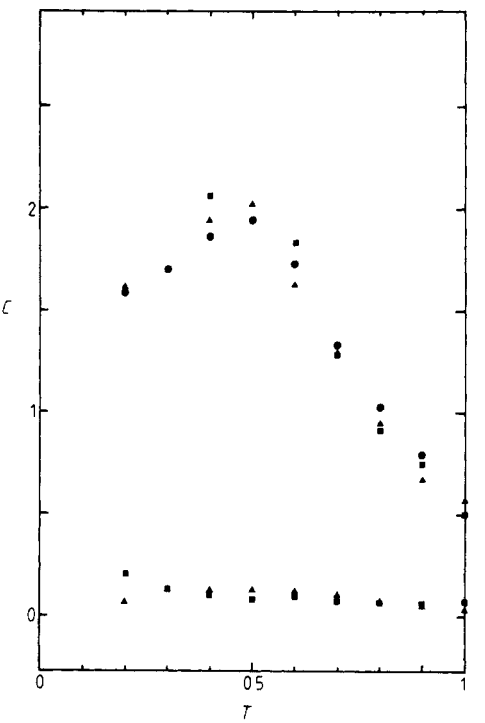

Figure 2. Heat capacity of O(4) in terms of the temperature. Symbols as for figure 1.

heat capacity is also computed by derving the energy by means of the expression

$$[E(T+0.1)-E(T-0.1)]/0.2.$$

The statistical error is measured in this case by

$$\{\sigma[E(T+0.1)]+\sigma[E(T-0.1)]\}/0.2.$$

Typically 6000 Monte Carlo passes through the crystal have been calculated for the temperatures where the heat capacity reaches the maximum. This was needed in order to get satisfactory $\sigma(C)$. $\sigma(E)$ is then lower than 0.0025, and the estimates of the energy for runs with ordered and random initial configurations differ by less than the statistical inaccuracy. The ordered initial configuration is taken with equal spin components.

3. Results

The heat capacity per spin is shown in figures 1, 2 and 3 for O(3), O(4) and O(5) respectively. The estimates obtained from the energy fluctuations are denoted respectively for ordered and random initial configurations by triangles and squares. In the lower part of the graph, the same symbols are used for the standard deviations of these quantities. The values related to the energy differences are indicated by circles for both ordered and random initial configurations as they are close. The statistical

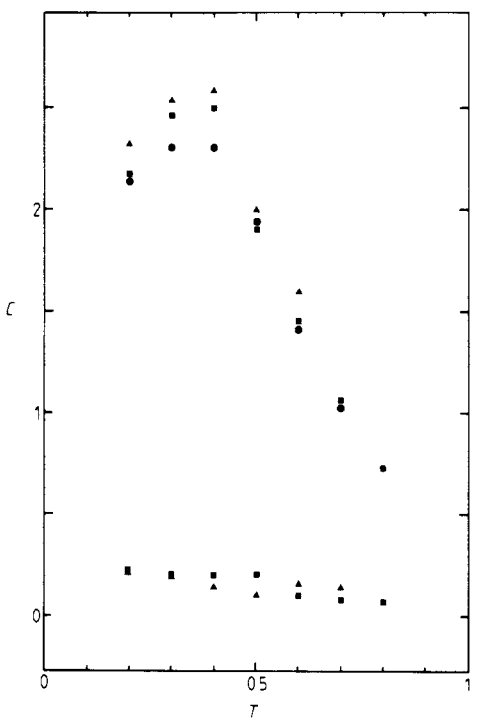

Figure 3. Heat capacity of O(5) in terms of the temperature. Symbols as for figures 1 and 2.

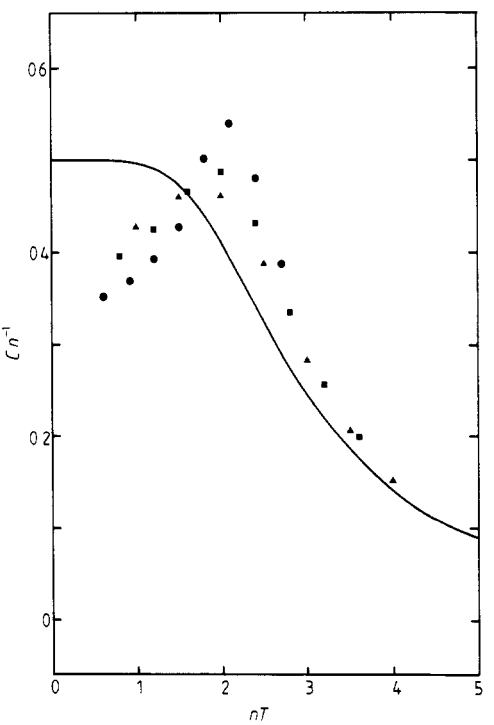

Figure 4. Comparison between the heat capacity of O(n) spin system. The heat capacity divided by n is plotted in terms of the temperature multiplied by n for: ●, O(3); ■, O(4) and ▲, O(5).

errors previously defined are less than the diameter of the circles. One sees that the two estimates of the heat capacity are coherent.

For low temperatures, the curves are compatible with the spin wave theory $C = \frac{1}{2}(n-1)$. In the intermediate region ($T \sim 2n^{-1}$), the heat capacity shows a maximum approximately equal to $\frac{1}{2}n$. More precisely, the values of nT are 2.07, 2 and 1.75 for $n = 3$, 4 and 5 respectively, while the maxima of the curves become less sharp. From the extrapolation of these values (and including in addition O(1), the Ising model ($nT_c \sim 2.269$), and O(2), the XY model ($nT \sim 2.17$)), we speculate that the maxima will disappear for $n \geqslant 7$. The curves for different values of n are compared in figure 4. The heat capacity (estimated by deriving the energy) divided by n is plotted in terms of the temperature multiplied by n for O(3) (circles), O(4) (squares) and O(5) (triangles). The limit $n \to \infty$ (the continuous curve) is approached when the temperature is higher than $4n^{-1}$.

Additional computations, for the estimate of the derivative of the energy with temperature differences of 0.1, and for samples of 14×15 O(3) spins, show no significant deviations from these results.

Acknowledgments

I wish to express my gratitude to Professor R Brout for introducing me to the problem and for helpful discussions. I wish also to thank A Silovy for useful remarks about his work.

Note added in proof. For the case of O(3), we have further analysed the data in an attempt to interpret the maximum in heat capacity. Our tentative conclusion is the following. At low temperature where our sample are effectively magnetised, we divide the Hamiltonian into three pieces

$$\langle H \rangle = -(2T)^{-1} \sum_{i,j} \{\langle S_i^+ S_j^- \rangle + \langle S_i'' \rangle \langle S_j'' \rangle + [\langle S_i'' S_j'' \rangle - \langle S_i'' \rangle \langle S_j'' \rangle]\}$$

$\langle S_i'' \rangle$ the magnetisation and $\perp$ denotes the $n-1$ directions transverse to it. In the vicinity of the maximum, it is the term in $\langle S_i'' \rangle \langle S_j'' \rangle$ which varies the most rapidly with T. Therefore, it appears that the maximum is due to the break-up of short range order, i.e. a remnant of the heat capacity singularity of the Ising model which is due to the break-up (on the low T side) or establishment (on the high T side) of global order. We intend to publish a more detailed report of these aspects in a future publication.

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