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EVIDENCE FOR VORTEX FORMATION IN MONTE CARLO STUDIES OF THE TWO-DIMENSIONAL XY-MODEL

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Monte Carlo studies of the classical XY-model on 20 x 20 and 30 x 30 square lattices with periodic boundary conditions and nearest neighbor interactions are presented. At low temperatures vortex pair formation is clearly seen as was suggested by Kosterlitz and Thouless. Preliminary results on the temperature-dependence of the pair correlation functions, susceptibility and specific heat are given.

IT IS NOW WELL ESTABLISHED that the two-dimensional XY-model has a phase transition at a non-zero critical temperature T_c where the susceptibility diverges [1–5], although no long-range ferro- or antiferromagnetic order exists for $0 < T < T_c$ [6]. Kosterlitz and Thouless [7, 8] suggested to interpret the physical nature of this transition in terms of the behavior of "vortices", low-temperature excitations which may occur below T_c pairwise only. Some renormalization group treatments [9] lead to the conclusion that this interpretation was inappropriate, however, Zittartz [5] has shown this phase transition not to be of second order but of "continuous order" without using the concept of vortices. In view of this situation, it seems very interesting to clarify the role of the vortices in the XY-models, and it is the intention of the present note to deal with this question.

While Monte Carlo studies of phase transitions in Ising and Heisenberg models have been made for years [10], the present work is the first investigation of the classical XY-model, whose Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) \qquad (1)$$

where $\mathbf{S}_i$ is a unit vector in the direction of the spin at site i, and the summation goes over nearest neighbor pairs only. 20 x 20 and 30 x 30 square lattices with periodic boundary conditions were treated, making runs over 1000 Monte Carlo steps per spin and using various initial conditions. For technical details of the simulation we refer to reference [11], since the program of the present study was obtained by simple generalization [12].

According to Kosterlitz and Thouless [7], the vorticity q of a given region is defined by

$$q = \frac{1}{2\pi} \oint d\phi(\mathbf{r}), \qquad (2)$$

where the integral is taken over the boundary of that region and $\phi(\mathbf{r})$ is the angle a spin situated at $\mathbf{r}$ makes with the x-axis. Before one tries to apply a discrete version of equation (2) to obtain quantitative information, it is advisable to study the qualitative behavior by producing printouts of the spin configurations [13]. Figure 1 shows the time evolution of the system [14], where one starts with all spins aligned in the $+z$ axis at $t = 0$. It is seen that after a few Monte Carlo steps per spin one obtains a rather random arrangement, while later on the spins lie in the xy-plane nearly completely and form quite well-developed vortices. The lower the temperature falls, the better these vortices develop (Fig. 2), and while they become rather diffuse at higher temperatures (e.g. at $k_B T/J = 0.4, 0.5$) one can hardly identify well-defined vortices. Figure 3 shows that roughly at that temperature region the specific heat has its maximum and the susceptibility increases strongly. Due to finite size-effects one cannot expect to see a sharp transition in systems of such small linear dimension, of course [10, 11]; in addition there is a considerable statistical error due to time-correlation effects [10, 11] which becomes very large at low temperatures and thus leads to considerable scatter of the data points. In Fig. 3, we have included the high temperature series for χ [3] which includes terms up to $(J/k_B T)^{10}$, while for the specific heat only the leading term of order $(J/k_B T)^2$ was available (dashed curves). For $k_B T/J \lesssim 1$, it even becomes difficult to

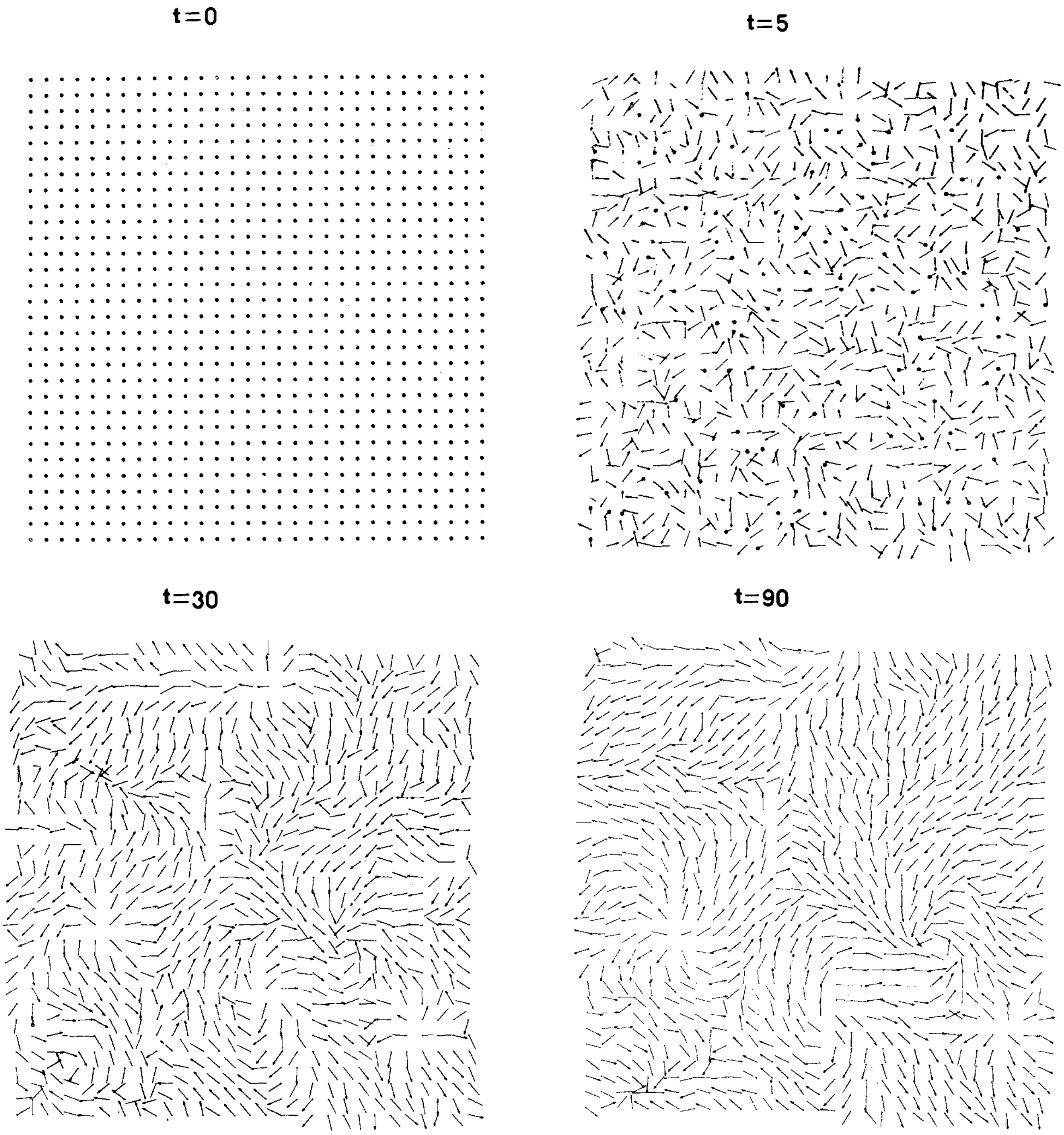

Fig. 1. Spin configurations of the classical XY-model on a 30×30 lattice at $k_B T/J = 0.2$ at various times (in units Monte Carlo step/spin). Plotted length of a spin denotes the magnitude of the projection on the xy plane. Spins with arrows have a positive z-component, spins without arrows a negative z-component.

obtain the order of magnitude of χ correctly! A similar breakdown of accuracy was observed in simulations of the two-dimensional classical Heisenberg model [15], too. In any case we are unable to make any statements about the nature of the critical singularities whatsoever on the basis of the present data.

Evidence for the phase transition is also seen in the pair correlation function, Fig. 4. We define the correlation function by $G(X) = \langle S_i^x S_j^x \rangle + \langle S_i^y S_j^x \rangle$, with $i \equiv (K, L), j \equiv (K + X, L)$, the point $i \equiv (K, L)$ being averaged over the lattice. At higher temperatures $G(X)$ decreases quickly as X increases (note that $G(X) = G(\sqrt{N} - X)$ because of the periodic boundary condition). But clearly it would be very difficult to check the prediction of Berezinski [7] that $G(X) \propto X^{-k_B T/\pi J}$ from data of the present kind reliably.

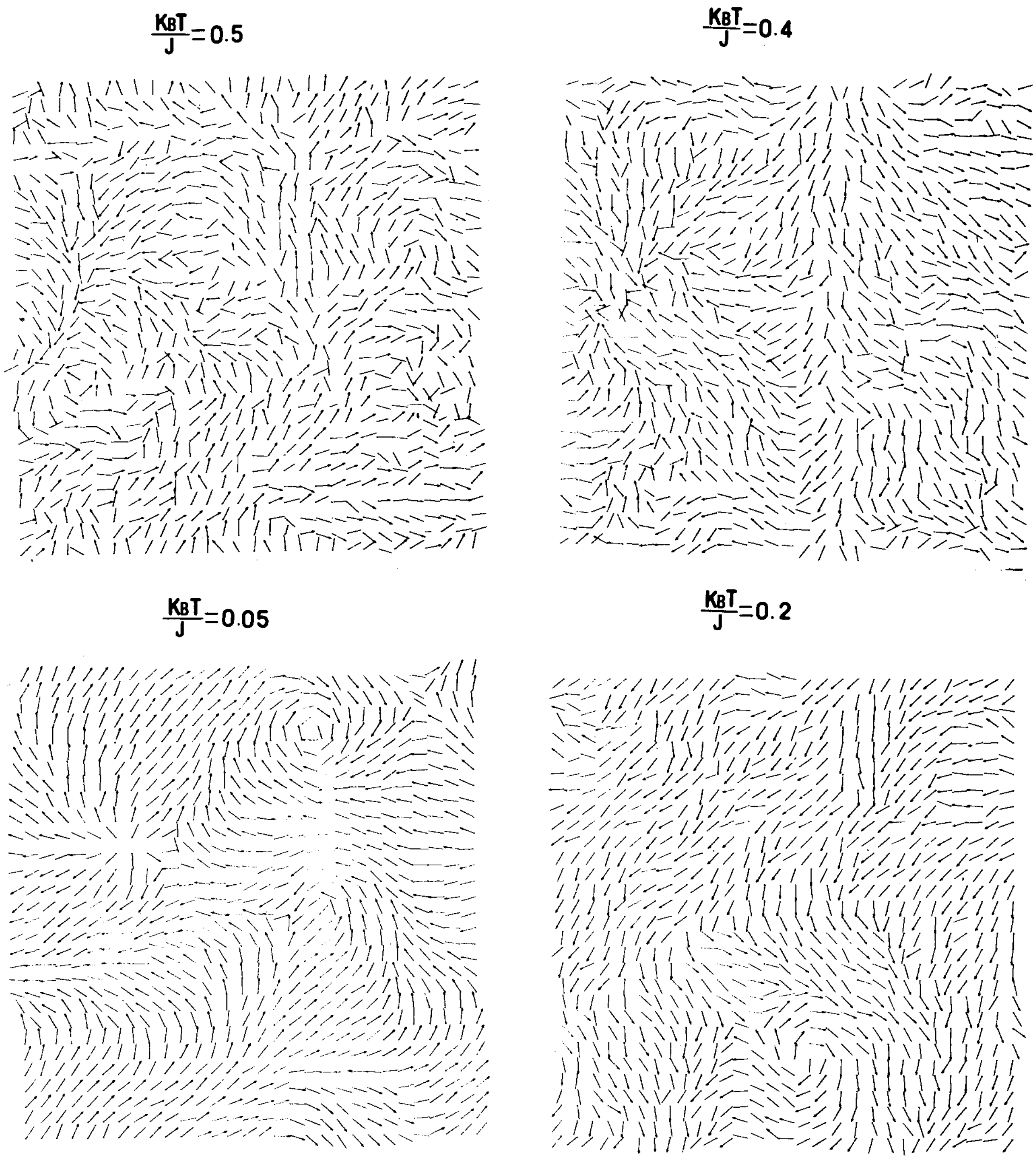

Fig. 2. Spin configurations at $t = 1000$ Monte Carlo steps/spin at various temperatures for explanations cf. Fig. 1.

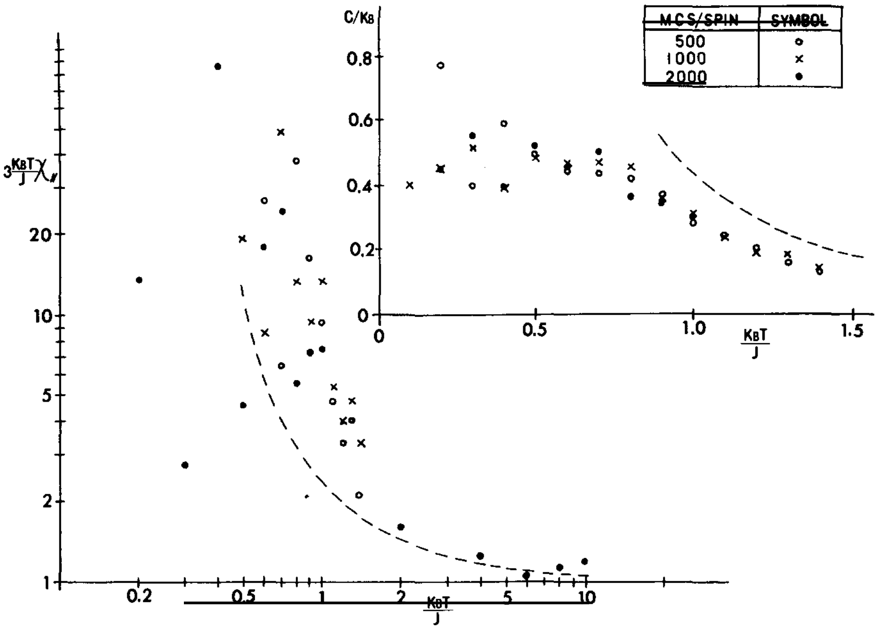

Fig. 3. (a) Susceptibility $\chi_{xx} = (\langle M_x^2\rangle - \langle M_x\rangle^2)N J/k_B T$ plotted vs temperature, where M_x denotes the x-component of the magnetization/spin at a particular observation, and the brackets denote time averages over 2000 Monte Carlo steps/spin for $N = 30 \times 30$. For $k_B T/J < 0.5$ we could not even get the order of magnitude of χ reliably. (b) Specific heat $C = (\langle E^2\rangle - \langle E\rangle^2)N(J/k_B T)^2$ plotted vs temperature, where E denotes the energy/spin of a particular observation. The arrow shows the theoretical value of C at $T = 0$. Dashed lines indicate high temperature behavior (cf. text).

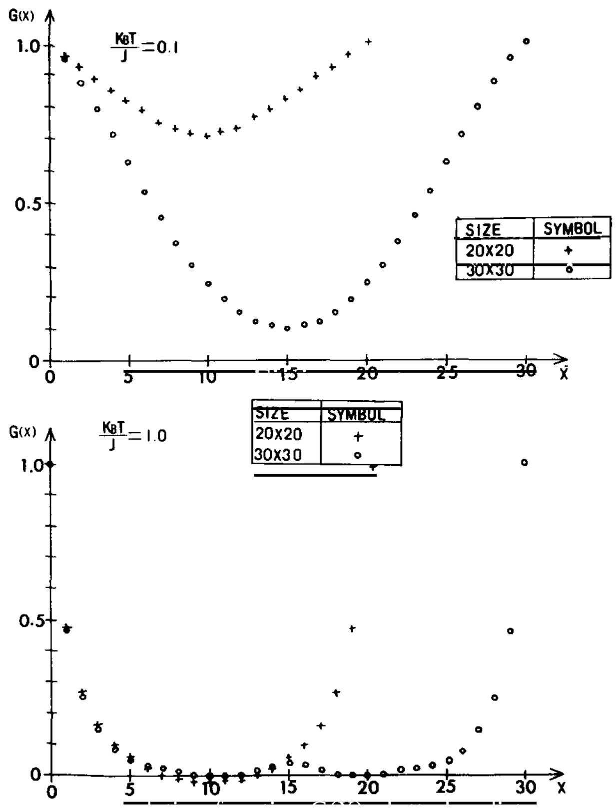

Fig. 4. Correlation function $G(X)$ plotted vs distance X between the spins along the x-direction of the lattice. Two values of N and two temperatures are shown.

The difficulty of obtaining more quantitative results is illustrated in Fig. 5, where data for $k_B T/J = 0.01$ are shown. In the upper part the starting state was a random spin configuration, all spins being aligned in the XY-plane. After 1000 Monte Carlo steps/spin a state with only one vortex pair was obtained. The lower part of Fig. 5 shows that a much higher vortex density is obtained, if one uses a ferromagnetic state (like in Fig. 1) as an initial condition. A comparison of states at times $t = 500$ and $t = 1000$ clearly shows that the resulting vortex configuration is "frozen-in". Clearly such frozen-in vortex configurations are metastable only: Since formation of a vortex pair requires a non-zero excitation energy ΔU, one expects that the vortex pair density vanishes as $\exp(-\Delta U/k_B T)$ at low enough temperatures. Thus vortex observations at $k_B T/J \lesssim 3 \cdot 10^{-1}$ do not contain information relevant for thermal equilibrium properties.

In conclusion, these results can be summarized as follows: (i) the Monte Carlo studies suggest the existence of a phase transition in the two dimensional XY-model, where χ becomes strongly divergent, and C probably much less singular (the specific heat exponent is probably negative, perhaps even $\alpha = -\infty$). (ii) Below T_c no long range order occurs, but one observes vortex pair formation. The vortices seem to become rather diffuse as T approaches the critical region. (iii) The relaxation time of the stochastic XY-model (defined

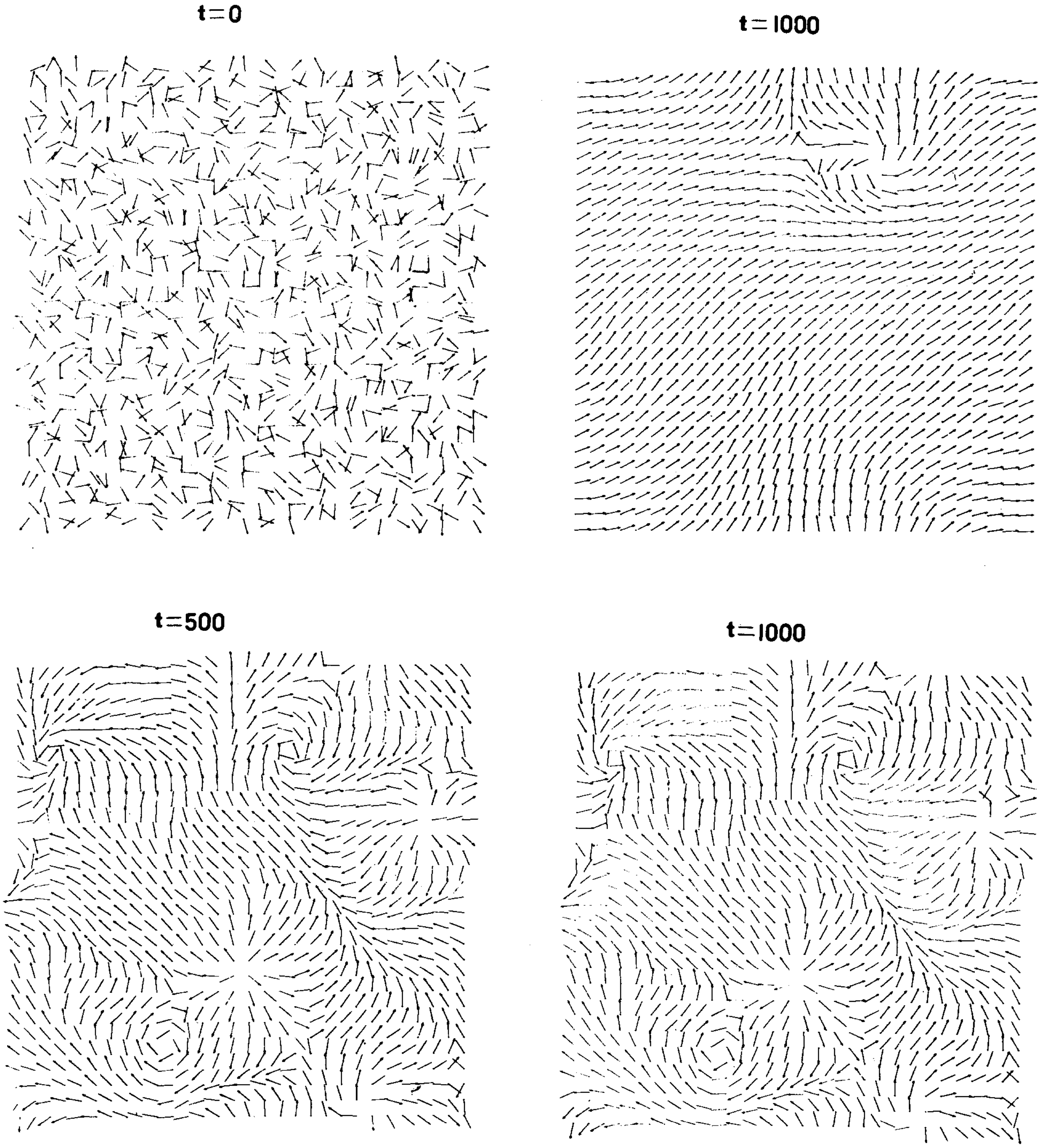

Fig. 5. Spin configurations at $k_B T/J = 0.01$. For explanations cf. text.

in terms of a master equation analogous to the kinetic Ising model [10]) is also strongly divergent at T_c. Probably the relaxation functions decay non-exponentially with time below T_c, similarly to that the pair correlation function does as a function of distance. All these results are in accord with theoretical expectations [5, 7, 8]. Property (iii) make more accurate Monte Carlo studies of the XY-model extremely difficult, however.

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12. Note that the Hamiltonian $\mathcal{H} = -J' \Sigma\ [(1-\Delta)(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z]$ studied in reference [11] reduces to equation (1) in the limit $\Delta \to -\infty, J' \to 0, |J'\Delta| \to J \neq 0, \infty$.
13. Some of our results have been mentioned very briefly in the context of simulations of the quantum-mechanical $S = 1/2$ XY-model by SUZUKI M., MIYASHITA S., KURODA A. & KAWABATA C. (to be published in *Phys. Lett. A*).
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