MONTE CARLO SIMULATIONS OF THE TWO-DIMENSIONAL QUANTAL AND CLASSICAL SPIN SYSTEMS – A NEW TYPE OF PHASE TRANSITION WITH VORTICES

Masuo SUZUKI, Seiji MIYASHITA, Akira KURODA[1]
Department of Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo, Japan

and

Chikao KAWABATA
Okayama University Computer Center, Okayama, Japan

Received 16 December 1976

A new type of phase transition has been found in the two-dimensional XY-model using Monte Carlo simulations, which show a divergence of susceptibility, but no divergence of specific heat. Vortices appear below T_c as was predicted by Kosterlitz and Thouless.

A critical behavior of the two-dimensional quantal and classical XY-model [1] has been very fascinating to study since Stanley and Kaplan [2] proposed a phase transition without ordinary long-range order. The purpose of our paper is to clarify the truth of confusing situations on the above problem, by using the Monte Carlo method and to give definite foundations to theoretical work past and also in future, together with some conceptual proposals on our numerical results. Our Hamiltonian is described by

$$\mathcal{H} = -J \sum_{(i,j)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \mu H \sum_j \sigma_j^x \qquad (1)$$

where $\{\sigma_j^x\}$ denote Pauli matrices for the quantal case and $\boldsymbol{\sigma}_j$ a unit vector for the classical case $((\sigma_j^x)^2 + (\sigma_j^y)^2 + (\sigma_j^z)^2 = 1)$.

Using the Monte Carlo method of quantal systems proposed by one of the present authors (M.S.) [3], we have calculated the energy, specific heat and susceptibility of the periodic 15×15 square quantal lattice for $n = 1$ in Trotter's formula [3]. The results [4] are shown in figs. 1–3, which indicate no divergence of specific heat (although a possibility of cusp is not excluded at present), but indicate divergence of susceptibility around $k_B T_c \approx 2J$ or less. These confirm a conjecture by Betts et al. [1] based on high temperature expansions. From spin configurations obtained in our simulation, we find that there appear a number of *very large* ferromagnetic clusters below T_c for $J > 0$. This may correspond to the appearance of "vortices" in the classical XY-model to be presented below.

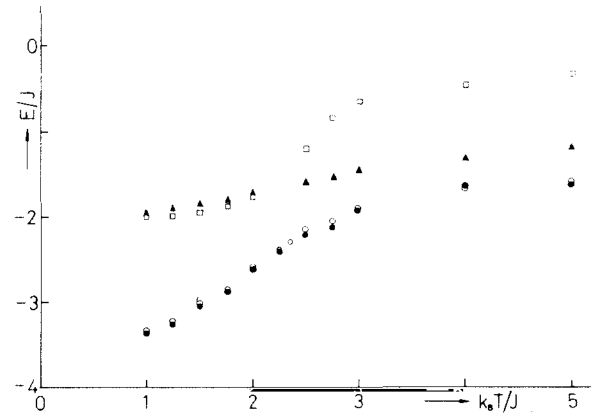


Fig. 1. Temperature-dependence of energy per spin for the two-dimensional quantal systems (15×15): □, △ and ○ (or ●) denote Ising model, Heisenberg model and XY-model, respectively.

In order to study more explicitly the structure of phase below T_c, it is convenient to simulate the *classical* XY-model by using the ordinary Monte Carlo method [5, 6]. Figs. 4 and 5 show the specific heat and typical spin configurations at low temperatures ($k_B T = 0.2J$ and $k_B T = 0.01J$), respectively, for a

[1] Permanent address: Faculty of Agriculture, Yamagata University, Tsuruoka, Yamagata.

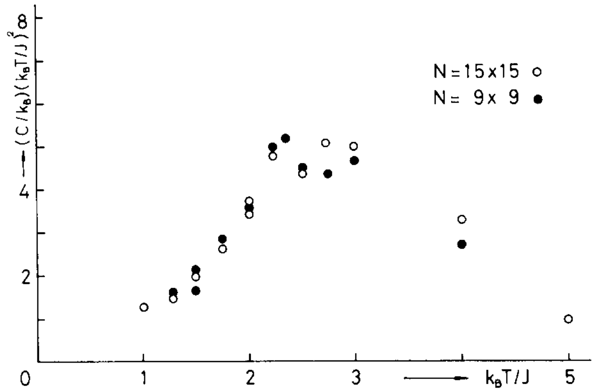


Fig. 2. Temperature-dependence of energy-correlation (i.e. specific heat per spin) for the quantal XY-models.

periodic 30 × 30 lattice. The specific heat shows no anomaly, corresponding to the quantal case. However, it is quite interesting that there appear many vortices and more general disclinations (sinks and sources), for $k_BT \lesssim 0.5J$, as was partly suggested phenomenologically by Kosterlitz and Thouless [7]. The transition point is smaller than the value predicted by them, partly because the classical spins in our model can assume three degrees of freedom while the exchange interaction is anisotropic and confined in the xy-plane. It should be also noted that there are several large ferromagnetic regions (domains or clusters) among "vortices". These large ferromagnetic clusters are considered to be responsible to the divergence of susceptibility. In fact, a small applied magnetic field in the xy-plane has been found in our simulation to produce spin configurations well ordered to the direction of the field. This means the singularity of response with respect to the magnetic field. On the other hand, the development of short-range order is very gradual, which corresponds to the smooth specific heat.

Vortices and disclinations appear even for non-periodic boundary conditions. The energy of a disclination with pure divergence is calculated to be $E \approx \pi J \log(R/a_0)$ for a radius R with a lattice spacing a_0, which is equal to that of pure vortices [7]. Thus, the zeroth approximation for our system with various kinds of disclinations gives a transition point $k_BT_c \approx \frac{1}{2}\pi J$, just corresponding to the theory in [7]. This is rather higher than the numerical results. Interaction effect between disclinations will be important for more precise treatments. The number and size of disclinations depend on temperature. Details of temperature-dependence will be published elsewhere. As our calculations are based on the kinetic XY-model, a microscopic explanation of our results will be also given in the future in the framework of the kinetic XY-model or equivalently of the TDGL-model with two components.

The above results suggest a *similarity* between the present critical behaviour and that of spin-glasses [8] or magnetic models with random bonds, in which there exists a phase without ordinary long-range order and yet with singularity of response function or susceptibility. The physical reasoning of this similarity may be the appearance of large clusters in both systems in a certain sense, below the transition point. Here are suggested two types of order parameters to describe the above new type of phase transition: one is the number of "vortices" or disclinations and the

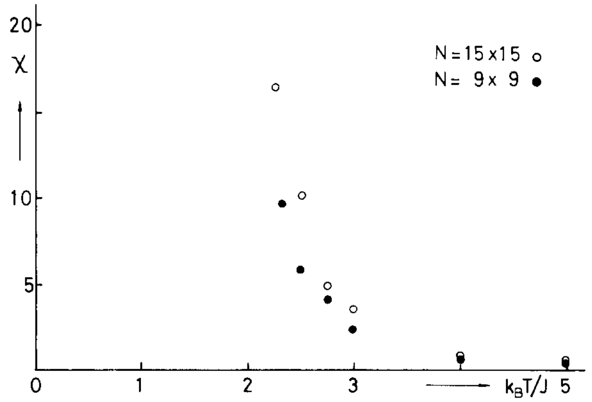


Fig. 3. Susceptibility in the xy-plane for the quantal XY-model.

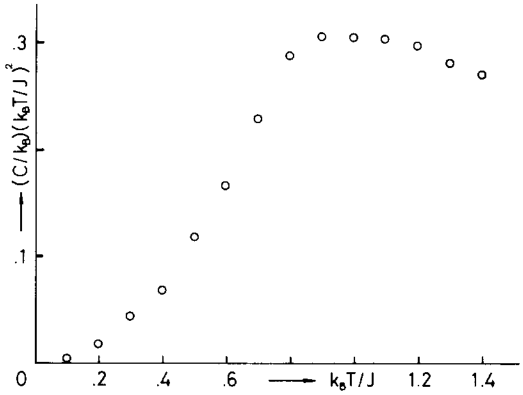
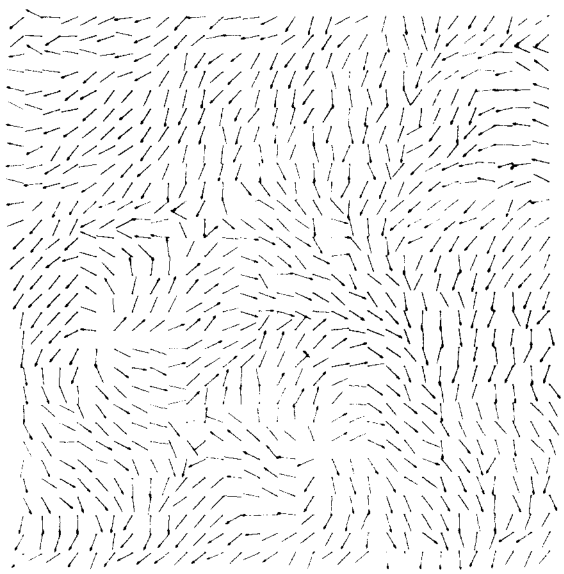
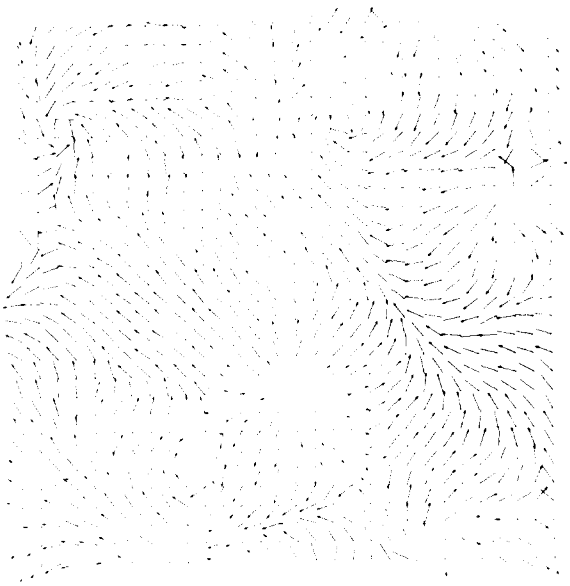


Fig. 4. Temperature-dependence of energy-correlation (i.e. specific heat per spin) for the classical XY-model (30 × 30)).



(a)



(b)

Fig. 5. Typical spin configurations of the classical XY-model (a) at $k_BT = 0.2J$ and (b) at $k_BT = 0.01J$ for 500 and 1000 Monte Carlo steps per spin, respectively. Spins with arrows are directed slightly upward above the plane and spins without arrows downward. Plotted lengths of spins denote magnitude of unit spin vectors projected on the xy-plane.

other is the long-range order in the time coordinate in a certain physical sense.

The above fact that the systems both quantal and classical show similar critical behavior even in the marginal dimensions ($d = 2$) is quite natural, because the quantal spin system can be transformed into the corresponding classical system *asymptotically*, by using Trotter's formula and Stratonovich–Hubbard transformation. The proof of this asymptotic equivalence will be reported in detail elsewhere.

A simulation of the classical XY-model with spin vectors restricted in the xy-plane will be performed in future to confirm the universality of critical phenomena. This model has been discussed by Kosterlitz and Thouless. Simulations of the two-dimensional quantal Heisenberg model have been made for the periodic 9×9 lattice, which show no singularity both in specific heat and susceptibility.

Detailed calculations of various physical quantities of the two-dimensional quantal and classical XY-models will be published elsewhere together with some theoretical considerations on numerical results.

The authors would like to thank Professors R. Kubo, H. Suzuki, T. Ninomiya, and K. Hirakawa for useful discussions. The simulation of the classical XY-model was performed due to the kind suggestion to C.K. by Professor K. Binder, who kindly supplied C.K. at Saarbrücken with program listings on the classical Heisenberg model, and also informed C.K. on the relevance of vortices mentioning ref. [7].

[1] For a review of the XY-model, see D.D. Betts, in: Phase transitions and critical phenomena, vol. 3, eds. C. Domb and M.S. Green (Academic Press, Ne York);
see also C. Kawabata, J. Phys. Soc. Japan 28 (1970) 1396;
J. Rogiers and R. Dekeyser, Phys. Rev. B13 (1976) 4886.
[2] H.E. Stanley and T.A. Kaplan, Phys. Rev. Lett. 17 (1966) 913.
[3] M. Suzuki, Prog. Theor. Phys. 56 (1976) 1454; Commun. Math. Phys. 51 (1976) 183.
[4] The results for quantal spin systems have been partially reported by M. Suzuki, at Banff Summer School on Phase transition (August, 1976).
[5] K. Binder and H. Rauch, Phys. Lett. 27A (1968) 247;
R.E. Watson, M. Blume and G.H. Vineyard, Phys. Rev. B2 (1970) 684.
[6] K. Binder and D.P. Landau, Phys. Rev. B13 (1976) 1140.
[7] J.M. Kosterlitz and D.J. Thouless, J. Phys. C: Solid State Phys. 6 (1973) 1181;
J.M. Kosterlitz, J. Phys. C: Solid State Phys. 7 (1974) 1046;
V.L. Berezinskii, Soviet Phys. JETP 32 (1971) 493;
J. Zittartz, Z. Physik B23 (1976) 55, 63.
[8] S.F. Edwards and P.W. Anderson, J. Phys. F: Metal Phys. 5 (1975) 965.