*Helium*, edited by K. H. Bennemann and J. B. Ketterson (Wiley, New York, 1976).
[2]A. C. Anderson, M. Kuchnir, and J. C. Wheatley, Phys. Rev. 168, 261 (1968).
[3]M. Kuchnir, P. R. Roach, and J. B. Ketterson, Phys. Rev. A 2, 262 (1970).
[4]Paul D. Roach, J. B. Ketterson, and Pat R. Roach, in Proceedings of the International Symposium on Quantum Fluids and Solids, Sanibel Island, Florida, January 1977 (to be published).
[5]B. D. Josephson and J. Lekner, Phys. Rev. Lett. 23, 111 (1969).
[6]M. Kuchnir, J. B. Ketterson, and P. R. Roach, J. Low Temp. Phys. 19, 531 (1975).
[7]C. N. Barber, P. V. E. McClintock, I. E. Miller, and G. R. Pickett, Phys. Lett. 54A, 241 (1975).
[8]A. I. Ahonen, J. Kokko, O. V. Lounasmaa, M. A. Paalanen, R. C. Richardson, W. Schoepe, and Y. Takano, Phys. Rev. Lett. 37, 511 (1976), and to be published.
[9]J. C. Wheatley, Rev. Mod. Phys. 47, 415 (1975), Appendix *A*.
[10]T. Soda, in *Proceedings of the Fourteenth International Conference on Low Temperature Physics, Otaniemi, Finland, 1975*, edited by M. Krusius and M. Vuorio (North-Holland, Amsterdam, 1975), Vol. 1, p. 13.
[11]R. M. Bowley, J. Phys. C 9, L151 (1976).
[12]G. Baym, C. J. Pethick, and M. Salomaa, Phys. Rev. Lett. 38, 845 (1977).
[13]A. L. Fetter and J. Kurkijärvi, in Proceedings of the International Symposium on Quantum Fluids and Solids, Sanibel Island, Florida, January 1977 (to be published).
[14]C. J. Pethick, private communication.

# Fluctuation-Induced First-Order Phase Transitions Studied by the Monte Carlo Technique

O. G. Mouritsen and S. J. Knak Jensen
*Department of Physical Chemistry, Chemical Institute, Aarhus University, DK-8000 Aarhus C, Denmark*

and

Per Bak
*Nordita, 17 Blegdamsvej, DK-2100 Copenhagen Ø, Denmark*
(Received 30 June 1977)

The critical behavior of a three-dimensional antiferromagnet described by a six-dimensional order parameter has been investigated by the Monte Carlo technique. A *first-order phase transition* is observed. This result is in agreement with the prediction of renormalization-group calculations in $4-\epsilon$ dimensions and with neutron scattering experiments on $UO_2$, but in contrast to the mean-field theory, which leads to a second-order phase transition.

Recently it was shown by Bak and co-workers[1] and simultaneously by Brazovsky and co-workers[2] that fluctuations may change a possible second-order phase transition into a first-order phase transition. The calculations were carried out within the framework of Wilson's renormalization-group theory in $4-\epsilon$ dimensions.[3] The theoretical derivation is based on symmetry arguments only and does not depend on the actual physical mechanisms involved. The first-order phase transitions are associated with a lack of stable fixed points of the Ginzburg-Landau-Wilson Hamiltonians corresponding to the actual systems. The nonexistence of stable fixed points is restricted to systems described by order parameters with $n \geq 4$ components. The first-order phase transition takes place when the correlation length exceeds a certain limit, where fluctuations in the order parameter make a discontinuous phase transition energetically favorable. These so called fluctuation-induced first-order phase transitions should take place even in cases where the mean-field theory predicts second-order phase transitions. The theoretical analysis was used to explain the observed first-order phase transitions in the antiferromagnets MnO, $UO_2$, Eu, and Cr.[1]

The validity of the hypothesis that absence of stable fixed points within the $\epsilon$ expansion leads to a first-order phase transition in *three dimensions* may be investigated by calculations on precisely defined three-dimensional models. In this Letter, we shall report a Monte Carlo calculation on a model defined in terms of a microscopic spin Hamiltonian which at low temperatures yields a magnetic structure similar to the magnetic structures of $UO_2$[4] and $NdSn_3$.[5] For a real spin system like $UO_2$, we very seldom know the details of the microscopic Hamiltonian governing the physical behavior. It is therefore virtually impossible to prove rigorously that an appropriate mean-field theory taking into account the actual physi-

cal mechanisms (such as coupling of the spins to the lattice[6]) might not eventually lead to a first-order phase transition. If that were the case the above-mentioned experimental results could not be taken as supporting the renormalization-group theory. In contrast, for our completely specified Hamiltonian it is a trivial matter to check whether or not the mean-field theory leads to a first-order phase transition.

The Monte Carlo technique, on which our results are based, has proven particularly valuable in the study of the behavior of spin systems,[7,8] even near second-order phase transitions, where the correlation length becomes comparable to the size of the system. For example, it is possible to calculate critical exponents with reasonable accuracy.

We consider a three-dimensional simple-cubic lattice with $N$ lattice points. A classical spin, $\vec{S}_i$, of unit length is placed at each lattice point and the interaction between the spins is given by the following Hamiltonian:

$$H = J_1 \sum_{j,k(\neq j)}^{(nn)} \vec{S}_j \cdot \vec{S}_k + K \sum_{j,k(\neq j)}^{(nn)} (\vec{r}_{jk} \cdot \vec{S}_j)(\vec{r}_{jk} \cdot \vec{S}_k)/r_0^2 + J_2 \sum_{j,k(\neq j)}^{(nnn)} \vec{S}_j \cdot \vec{S}_k + P \sum_j (S_{jx}^4 + S_{jy}^4 + S_{jz}^4), \quad (1)$$

where (nn) and (nnn) indicate that the summations are extended over six nearest neighbors and twelve next-nearest neighbors, respectively. $\vec{r}_{jk}$ is the vector connecting the $j$th and the $k$th spin, and $r_0$ is the lattice parameter of the cubic unit cell. $J_1$, $J_2$, $K$, and $P$ are model parameters, which in our calculations were chosen in the following way: $P = \frac{1}{5}K = -2J_2 = J_1 \equiv J < 0$. At low temperatures, this choice leads to an antiferromagnetic structure characterized by a propagation vector $\vec{k}_1 = (2\pi/r_0)(\frac{1}{2}, 0, 0)$. The star of $\vec{k}_1$ consists of the three vectors $\vec{k}_1$, $\vec{k}_2 = (2\pi/r_0)(0, \frac{1}{2}, 0)$, and $\vec{k}_3 = (2\pi/r_0)(0, 0, \frac{1}{2})$. For each propagation vector, $\vec{k}_j$, the sublattice magnetization is along one of the two principal axes of the simple-cubic unit cell, which are orthogonal to $\vec{k}_j$. Accordingly, the dimension $n$ of the order parameter is six, corresponding to the six possible equivalent domains existing in the ordered phase. We note that the magnetic structure of $UO_2$ is similar to the structure just described except that the magnetic moments are situated in a face-centered-cubic lattice.[9] However, it turns out that the fourth-order invariants which can be formed from the six components of the order parameter are the same for $UO_2$ as for $NdSn_3$ and for the model studied here. This implies that they all belong to the same universality class and that the theory in Ref. 1 applies to all three equally well.

A conventional Monte Carlo importance-sampling technique was employed to generate a canonical ensemble of spin systems corresponding to the Hamiltonian in Eq. (1). For each chosen temperature, we constructed the ensemble by going sequentially through the lattice flipping each spin randomly. The limit distribution of the generated systems will represent an equilibrium ensemble provided that appropriate transition probabilities are used. Details of the applied criteria of convergence will be described elsewhere.[8] All computations were performed on the CDC 6400 computer at the computing center at Aarhus University.

The Monte Carlo experiment was performed on a fairly large lattice consisting of $N = 14^3 = 2744$ spins in order to obtain results close to the thermodynamic limit. Periodic-boundary conditions were applied to reduce finite-size effects. We performed calculations for both a decreasing and an increasing series of temperatures in order to detect possible metastable states. As the initial system in the ensemble at a given temperature, $T$, we used a spin configuration representative of the preceding temperature. The increasing temperature series was started from a completely ordered spin system, while the decreasing temperature series was started from a spin system where the orientations of the spins were random. From the ensemble we have calculated the average value of the internal energy, $E(T)$, as well as the six components of the order parameter, which are defined as

$$\Phi(T) = \Phi_{jq}(T) = \frac{1}{N}\left\langle \sum_{r \in \omega(j,1)}^{N/2} S_{rq} - \sum_{r \in \omega(j,2)}^{N/2} S_{rq} \right\rangle, \quad (2)$$

where $\omega(j, 2)$ are the two sublattices corresponding to the propagation vector, $\vec{k}_j$. In Eq. (2) $q$ denotes the direction of the two principal vectors of the simple-cubic unit cell, which are orthogonal to $\vec{k}_j$. In addition, we have calculated the distribution functions of the internal energy and the order parameter. These functions are very helpful in the determination of energy and order parameter near the phase transition. In the critical region a small change in the temperature may cause the systems to evolve into transient states, which may persist for several thousands of spin flips per spin but eventually they dampen out and disappear. This behavior necessitates a very large

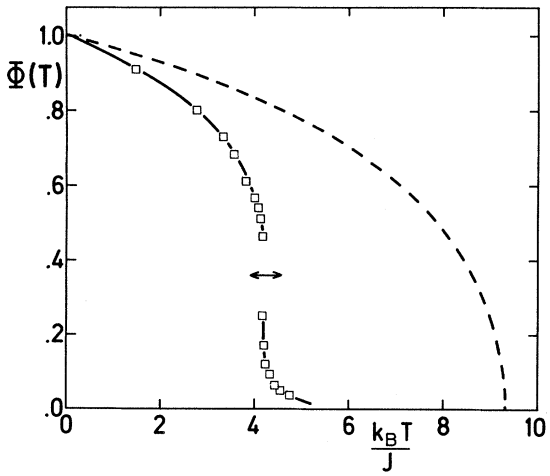


FIG. 1. Temperature dependence of the order parameter for the spin system defined Eq. (1). Full line: Monte Carlo calculations; dashed line: prediction of the mean-field theory. The horizontal arrow indicates the temperature region displayed in Fig. 2.

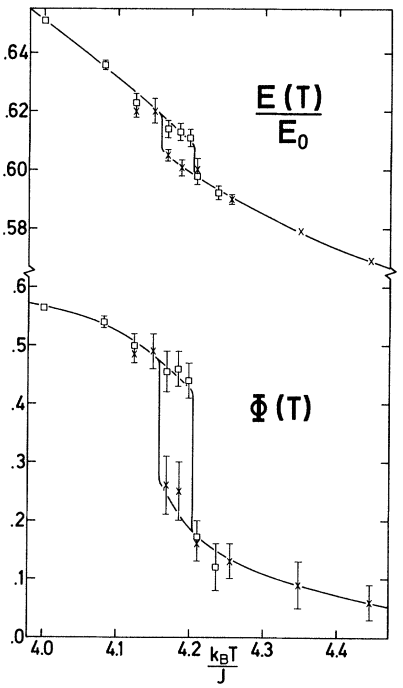


FIG. 2. Temperature dependence of the normalized internal energy and the order parameter in the critical region for the spin system defined in Eq. (1). $E_0$ is the energy in the completely ordered state. × indicates data calculated at decreasing temperatures. □ indicates data calculated at increasing temperatures. The full line is drawn as a guide to the eye and has no further meaning.

number of systems and for several temperatures each spin was flipped more than $10^4$ times. The averaging process leading to the energy and order parameter did not include these initial states.

The data obtained for the order parameter are shown in Fig. 1. We notice a discontinuous change in the order parameter, demonstrating that the phase transition is of first order. The tail above the critical region is due to finite-size effects similar to those observed in Monte Carlo calculations of second-order phase transitions.[7,8] Figure 1 also includes the order parameter as calculated from the mean-field theory. The disagreement is striking. The mean-field theory predicts a second-order phase transition appearing at a temperature more than twice that of the observed first-order transition temperature. Figure 2 shows the detailed temperature dependence of the internal energy and the order parameter in the critical region. The results obtained from the increasing and decreasing temperature series are the same, except for a narrow temperature region, $4.16 < k_B T/J < 4.20$. In this region, both the internal energy and the order parameter exhibit hysteresis, which is consistent with the first-order nature of the phase transition. The rather large "error bars" on the order-parameter data in the critical region indicate the fluctuations of the order parameter, which tends to shift between the various components. This seems to be related to finite-size effects and to indicate —like the large tail above the transition—the appearance of rather long-ranged correlations in the systems near the phase transitions. This is consistent with the renormalization-group calculations, which require a certain critical, but finite, correlation length before the phase transition takes place.

In conclusion, we have shown that the Hamiltonian in Eq. (1) leads to a first-order phase transition in contrast to the prediction of the mean-field theory, but in agreement with the result of the renormalization-group calculations and with neutron scattering experiments on $UO_2$. Our results demonstrate that the Monte Carlo technique is a useful tool to study the behavior of complicated spin systems.

It would be desirable to extend the Monte Carlo calculations to the study of complete phase diagrams for the type of spin systems considered here. In particular, by lowering the dimensionality of the order parameter by applying an external uniaxial stress or a magnetic field, we expect a crossover of the phase transition from first order to second order. This has been shown

experimentally[10] and theoretically[11] for MnO, and a similar behavior is expected for $UO_2$.[12] Such fluctuation-induced tricritical behavior can be studied by the numerical simulation methods described here, provided that an anisotropy term is added to the Hamiltonian.

[1]P. Bak, D. Mukamel, and S. Krinsky, Phys. Rev. Lett. 36, 52 (1976); D. Mukamel and S. Krinsky, Phys. Rev. B 13, 5065, 5078 (1976); P. Bak and D. Mukamel, Phys. Rev. B 13, 5086 (1976).

[2]S. A. Brazovsky and I. E. Dzyaloshinsky, Pis'ma Zh. Eksp. Teor. Fiz. 21, 360 (1975) [JETP Lett. 21, 164 (1975)]; S. A. Brazovsky, I. E. Dzyaloshinsky, and B. G. Kukharenko, Zh. Eksp. Teor. Fiz. 70, 2257 (1976) [Sov. Phys. JETP 43, 1178 (1976)].

[3]See K. G. Wilson and J. Kogut, Phys. Rep. 12C, 75 (1974).

[4]B. C. Frazer, G. Shirane, D. E. Cox, and C. E. Olsen, Phys. Rev. 140, A1448 (1965).

[5]P. Lethuiller, J. Pierre, G. Fillion, and B. Barbara, Phys. Status Solidi 15, 613 (1973).

[6]S. J. Allen, Phys. Rev. 167, 492 (1968).

[7]K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Adademic, New York, 1976), Vol. 5B, p. 1.

[8]O. G. Mouritsen and S. J. Knak Jensen, to be published.

[9]An alternative structure of $UO_2$, where the order parameter is a linear combination of those considered here, has been suggested by J. Faber and G. H. Lander, Phys. Rev. B 14, 1151 (1976). The Ginzburg-Landau-Wilson Hamiltonian, however, remains the same and the theory in Ref. 1 applies to this structure as well.

[10]D. Bloch, D. Hermann-Ronzaud, C. Vettier, W. B. Yelon, and R. Allen, Phys. Rev. Lett. 35, 963 (1975).

[11]P. Bak, S. Krinsky, and D. Mukamel, Phys. Rev. Lett. 36, 829 (1976).

[12]J. Sólyom and G. S. Grest, unpublished.

# Theory of the Residual Resistivity Anomaly in Potassium

Marilyn F. Bishop and A. W. Overhauser
*Department of Physics, Purdue University, West Lafayette, Indiana 47907*
(Received 12 May 1977)

The induced-torque experiments of Holroyd and Datars show evidence for an anomalous anisotropy in the residual resistance of potassium of about five to one. We show that this is consistent with the hypothesis that the conduction electrons are in a static charge-density–wave state. The importance of torque and de Haas–van Alphen experiments on the same specimen is emphasized.

The experiments of Holroyd and Datars[1] have verified the existence of the giant torque anomaly in potassium that was originally observed by Schaefer and Marcus.[2] The results show a variation of the induced torque with magnetic-field direction in spherical samples of potassium, an effect that is sizable even in the limit of zero magnetic field and becomes enormous for high fields. The low-field results imply that the residual resistivity of potassium is highly anisotropic, in contradiction to the simple theory of metals. The purpose of this Letter is to show that this anisotropy can be explained if the conduction electrons in potassium are in a static charge-density–wave state.

In an induced-torque experiment, a magnetic field is rotated with respect to a suspended sample, usually spherical in shape. The time variation of the field induces currents, which, by interacting with the field, exert a torque on the sample. The magnitude of this torque is measured as a function of both the direction and magnitude of the magnetic field. For a simple metal, i.e., a metal with a spherical Fermi surface, the induced torque, for a spherical sample, should be independent of the direction of the magnetic field. De Haas–van Alphen measurements on potassium seem to indicate that its Fermi surface is spherical to within 0.1%.[3] In contradiction, the gigantic anisotropies in the induced-torque experiments suggest that potassium is not so simple and that further study is needed.

In order to facilitate the examination of this problem, we present in Fig. 1 the data for sample $K$-10 of Holroyd and Datars.[1] The induced torque is plotted versus direction of magnetic field for axes of rotation along the growth axis [Fig. 1(a)] and perpendicular to the growth axis [Fig. 1(b)], for field values from 1 to 23 kG. The field was rotated at a speed of 22°/min, and the sample was kept at a temperature of 1.5 K. In order that the sample acquire a precise shape, the potassium was grown in a Kel-$F$ mold with a spherical cavity of diameter 1.11 cm, machined to within $10^{-3}$ in.[4] When the magnetic field was rotated in a plane perpendicular to the growth axis, as in Fig.