PHYSICAL REVIEW B VOLUME 26, NUMBER 11 1 DECEMBER 1982

Phase transitions in systems with multispin interactions

K. A. Penson
Freie Universität Berlin, Institute of Theoretical Physics, Arnimallee 3, 1000 Berlin 33, West Germany

R. Jullien and P. Pfeuty
Laboratoire de Physique des Solides (associé au Centre National de la Recherche Scientifique) Bâtiment 510, Université Paris-Sud, 91405 Orsay, France
(Received 22 June 1982)

An Ising-type model including n-spin nearest-neighbor interactions is introduced. The ground-state properties of its Hamiltonian version are studied in one and two dimensions. The model is self-dual in one dimension. The mean-field theory indicates that for $n > n_c$ the transition may become first order. Finite-size scaling suggests that $n_c=4$ in one dimension. The critical exponents as functions of n are estimated.

The bulk of theoretical knowledge about the cooperative properties of interacting systems has been accumulated using models with pairwise interactions. The same can be said about the study of critical singularities near the phase transitions. From the very outset it was clear that the two-body interaction is only an approximation and n-body interactions ($n>2$) are more adequate descriptions of reality. There is evidence for important effects of many-body forces in different fields ranging from the theories of alloys[1] and surface problems[2,3] to the helix-coil transition,[4] the structure of solid ^{3}He (Ref. 5) and others.[6] Following Griffiths and Wood,[7(a)] the study of the critical behavior of systems with n-spin interactions ($n>2$) has been initiated by Baxter and Wu (BW).[7(b)] Their exact solution of the $n=3$ Ising model on a triangular lattice (the BW model) had shown that the $n=3$ transition has critical exponents which fundamentally differ from those of the $n=2$ (Onsager) case. Another system with four-spin interactions[8] can exhibit a line of varying critical exponents. The treatment of other many-body interactions seems to be prohibitively difficult. There is clearly a need for a model whose properties can be studied as a function of n.

In this Communication we respond to this need by introducing what is perhaps the simplest nontrivial model allowing for such a systematic approach. Consider a one-dimensional (1D) quantum spin system with the Hamiltonian

$$H_n=-J\sum_i\prod_{j=1}^{n}S_{i+j-1}^x-h\sum_i S_i^z\ , \tag{1}$$

with $(h/J)>0$, $n\geqslant 2$, and S_i^α ($\alpha=x,y,z$) being the Pauli matrices at the site i. For $D>1$, (1) generalizes to

$$H_n=-J\sum_{R(n)}\prod_{\text{all } i\in R(n)}S_i^x-h\sum_i S_i^z\quad (D>1)\ , \tag{2}$$

where $R(n)$ is a domain containing n neighboring spins on a D-dimensional lattice. $R(n)$ can be, for instance, a triangle with edge length $L-1$ with $n=L(L+1)/2$ spins (triangular lattice), etc.

For $n=2$, (1) and (2) reduce to the Ising model with a transverse field (ITF). For $h/J=0$ and $n=3$ on a triangular lattice, (2) is the classical BW model[7(b)] whose ground state is a quadruplet. It can be shown[6] that the general $h/J=0$ ground state of (1) or (2) is 2^{n-1}-fold degenerate (in 1D and for $n=3$ the four ground states consist of repeating patterns of $+++\cdots$, $+--\cdots$, $-+-\cdots$, $--+\cdots$, respectively, the generalization for $n>3$ being evident). For $h/J\to\infty$, the ground state is a singlet. In analogy to the ITF model it is believed that there must exist a critical field $(h/J)_c(n,D)$ where a phase transition in the ground state takes place with the opening of a gap Δ at $(h/J)_c$, with $\Delta\sim[(h/J)-(h/J)_c]^s$ between the singlet and the excited states. Using standard arguments[9] one concludes that the ground state of (1) or (2) in D dimensions is equivalent to a $(D+1)$, $h=0$ classical system for $T>0$ with n-spin couplings in D-dimensional (hyper)planes which are coupled by ferromagnetic two-body Ising interactions. For $D\geqslant 1$, $n>2$, there are no exact results available concerning the character of this transition.

We report here on calculations with (1) and (2) which give first indications about the nature of these quantum phase transitions. First, in 1D an exact duality relation has been found which shows that the critical field for the second-order phase transition has the self-dual value $(h/J)_c=1$ independently of n. Next, H_n was treated with the molecular-field theory (MFT) which indicates that, for any n such that $3<n<\infty$, there is a first-order phase transition with $1<(h/J)_c(n)<2$, and $(h/J)_c(\infty)=1$. Finally, (1) and (2) were analyzed by the finite-size scaling (FSS) method in 1D for $2\leqslant n\leqslant 8$ and in 2D for $n=3$, 6 on a triangular lattice giving the estimates of values of $n_c(D)=4$ (1D), 3^-(2D) above which the transition may become first order as well as giving values of critical exponents α, β, and ν. The duality properties of (1) for given n are obtained from the transformation in 1D:

$$T_i^x=\prod_{j=0,1,2,\ldots}^{\infty} S_{i-nj}^z S_{i-nj-1}^z \; ; \quad T_i^z=\prod_{j=1}^{n} S_{i+j-1}^x ; \quad T_i^y=-S_i^y S_i^x \left(\prod_{j=1}^{n} S_{i+j-1}^x \right) S_i^z \left(\prod_{j=0,1,2,\ldots}^{\infty} S_{i-nj}^z S_{i-nj-1}^z \right) . \tag{3}$$

It can be shown that the operators T satisfy the usual $S=\frac{1}{2}$ spin commutation rules. Furthermore, if $h/J=g$, then (1) can be rewritten with the T's and $H_s(g)=gH_T(1/g)$ holds for the whole spectrum of H. In particular, if the model possesses a unique point at which the gap vanishes then it must occur at the point $g_c=1$ (duality). This extends then the exact result for $n=2$.

The MFT consists in approximating the coupling term in (1) by $J(\sigma^n-n\sigma^{n-1}S^x)$, with $\sigma=\langle S^x\rangle$, and by solving self-consistently for $\sigma=\sigma(h/J)$. For $n=2$ one obtains the second-order phase transition at $(h/J)_c=2$. For $n>2$ the multiplicity of solutions leads to a first-order phase transition at

$$(h/J)_c(n)=[n/(n-1)][n(n-2)/(n-2)^2]^{n/2-1} ,$$

$[1<(h/J)_c(n)<2]$, where σ undergoes a jump from $\sigma_c=[n(n-2)]^{1/2}/(n-1)$ to 0. Below $(h/J)_c(n)$, $\sigma(h/J)$ is the largest solution of $h/J=n\sigma^{n-2}(1-\sigma^2)^{1/2}$ and is equal to zero otherwise. $(h/J)_c \underset{n\to\infty}{\longrightarrow} 1$ and $\sigma(n=\infty)$ becomes the step function. We believe this last result to be exact since it corresponds to infinite-range multispin couplings. In higher dimension the results will be slightly modified but for $n\to\infty$ the transition is also expected to be of first order. This situation is reminiscent of q-state Potts model for which the MFT predicts a first-order transition for $q>3$ (all D) and where the transition *is* of first order for $q\to\infty$.[10] The MFT results cannot be trusted, however. The calculational method which should improve upon the MFT should preserve the intrinsic symmetry of H_n, for instance, the 2^{n-1}-fold degeneracy of its ground state. The block renormalization-group (RG) methods for quantum systems[11] cannot be used here since the RG generates interactions other that H_n, thus rendering the problem intractable.

We have applied the FSS method first formulated in Ref. 12 and later extended and refined.[13-15]

The FSS asserts that the correlation lengths for two finite systems with linear "sizes" L, L' and coupling constants g, g' are related by $\xi_L(g)=(L/L')\xi_{L'}(g')$. Since for our system H_n, the gap Δ corresponds to the reciprocal of the correlation length ξ (i.e., the dynamical critical exponent $z=1$) whence the FSS can be reformulated with Δ's. For both L, $L'\to\infty$ with a fixed ratio $L/L'=b$, the FSS represents a renormalization of the gap $\Delta(g)$ under a RG transformation $g'=R_b(g)$. For finite L and L', the FSS is only an approximation ("phenomenological scaling"[13]). The fixed point g^* of the R_b transformation is the solution of

$$\Delta_{L'}(g^*)=b\Delta_L(g^*) . \tag{4}$$

$g^*=g^*(L,L')$ should tend to exact value g_c if L, $L'\to\infty$ with $L/L'=b$. The exponent $\nu=s$ can be obtained by linearizing (4) near $g=g^*$. Other exponents (α, β, etc.) are obtained from similar considerations.[14,15]

We have found $\Delta(g)$ for H_n for $2\leq n\leq 8$ in 1D and for $n=3$, 6 in 2D. The block sizes L were chosen to be multiples of n: for $n=2$ we used $L=(2, 4, \ldots, L_{\max}^{(e)})$, $n=3$ with $L=(3, 6, \ldots, L_{\max}^{(0)})$, etc., with $L_{\max}^{(e)}=16$ and $L_{\max}^{(0)}=15$ spins. The Lanczös scheme was used.[14] We have calculated the fixed points $g^*=(h/J)_c$, the ground-state energy $E_0(g)/L$ with its derivatives and the exponents α, β, and ν. The results for ν in 1D are represented on Fig. 1. The $1/L$ plots for given n are aligned on almost straight lines and the extrapolated values $\nu_\infty(n)$ are in the insert. We obtained $\nu_\infty(3)\cong 0.72$ and $\nu_\infty(4)\approx 0.5$. For $n>4$ no extrapolation for the exponents can be made because the number of points obtained is too small. It is characteristic that the "initial" points of $\nu_L(n)$ (for $L=2n$) decrease below 0.5 (see Fig. 1). In studying first-order transitions using the FSS, care should be exerted since the assumption of FSS that $\xi_\infty(g_c)=\infty$ may not be satisfied. If the transition is "weakly" first order, ξ_∞ is very large but finite at g_c. Thus, strictly speaking, ν cannot be defined. But an "apparent" ν'_∞ can still be calculated as one would be studying a second-order case. If, with increasing n, the first-order character increases [and $\xi_\infty(g_c)$ decreases] the apparent ν'_∞ would tend to zero.

The determination of n_c for H_n may be only a subject of estimation. Let us assume that for $n=n_c$, $(1/L)E_0(g)$ near g_c is linear in $|g-g_c|$ with a discontinuous first derivative at g_c. Since $E_0\sim|g-g_c|^{2-\alpha(\alpha')}$ then $\alpha=\alpha'=1$. With the hyperscaling $(D+z)\nu=2-\alpha$ with $z=1$, $\nu_c=\nu(n_c)=(D+1)^{-1}$ results. For $n<n_c$, $\nu>\nu_c$, and for $n>n_c$, ξ may remain finite. Another evidence is provided by the behavior of $-(1/L)\partial E_0(g,n)/\partial g$ corresponding to $\langle 0|S^z|0\rangle = \langle S^z\rangle$, which is the entropy of the $(D+1)$ classical system. The discontinuity of $\langle S^z\rangle$ is the latent heat. We present the curves of $-\langle S^z\rangle$ for $n=3$, 5 in 1D in Figs. 2(a) and 2(b). The slopes of $-\langle S^z\rangle$ at $g_c=1$ are increasing and away from $g_c=1$ are decreasing with n. This is strongly suggestive of a discontinuity at $g_c=1$ building up with n. The values of $\alpha(n)$ and $\beta(n)$ are

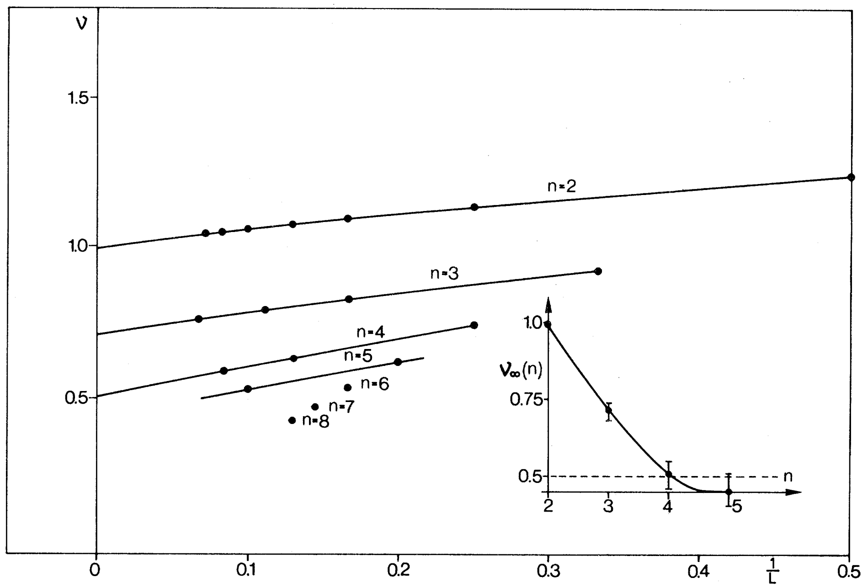

FIG. 1. The exponent ν calculated for $n=2, 3, \ldots, 8$, $L \leq 16$. The extrapolated ($L=\infty$) values of ν are in the insert together with their error bars (1D).

consistent with this picture.[6] (Note that one may also have a latent heat with a continuous order parameter and with ξ diverging[15]). However, the accuracy of the present and previous FSS studies[16,17] is not sufficient to determine the nature of such a discontinuity: it is impossible to distinguish a curvature *near* g_c (case $\alpha<1$) from a jump at g_c. In contrast, the accuracy of determination of g_c is very good.[6] Thus the FSS reproduces well the self-dual value $g_c=1$, which, strictly speaking, yields only a second-order transition point.

We have also performed the calculations in 2D for $n=3$ and $n=6$ interactions on a triangular lattice using triangular blocks of edge length $L-1=1, 2, 3, 4$

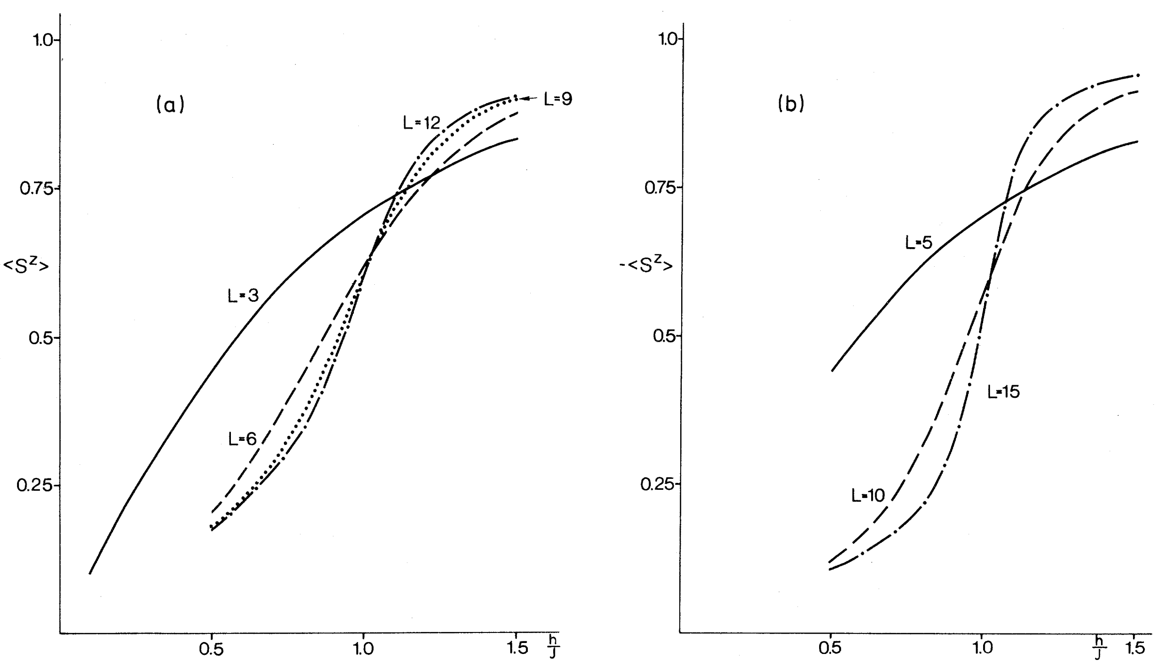

FIG. 2. (a): $-(1/L)\ \partial E_0(n,g)/\partial g$ as a function of g for $n=3$ ($L=3, 6, 9, 12, 15$) in 1D. (b): $-(1/L)\ \partial E_0(n,g)/\partial g$ as a function of g for $n=5$ ($L=5, 10, 15$) in 1D.

($n=3$) and $L-1=2$, 3, 4 ($n=6$). The extrapolated ($L=\infty$) values of ν and g_c are $\nu_\infty(3)=0.38$, $\nu_\infty(6)=0.15$, $g_c(3)=2.45$, and $g_c(6)=0.68$. These reductions of both ν_∞ and g_c (the duality does not hold) indicate that the transition may become first order for $3<n<6$. We tend to believe that these evidences for possible crossover from second- to first-order phase transitions should encourage further study of H_n in $D\geqslant1$. Several extensions are possible: first, the increase of block sizes L would give more reliable values for the exponents; second, the inclusion of interactions with different n's, $H_n+H_{n'}+\cdots$ would give an indication for mutual relevance of n, n' terms and would lead to more complicated phase diagrams, quantum multicritical points, etc.[18] The question of possible duality of multispin interactions in higher D is also of current interest.[19] We are studying these questions at present. Finally, the state of knowledge about H_n is reminiscent of the very early stage of study of Potts-type models. It would be intriguing to guess when rigorous analytic results about H_n will be obtainable.

ACKNOWLEDGMENTS

K.A.P. thanks Professor K. H. Bennemann for discussions and support. This work was supported by the Deutsche Forschungsgemeinschaft, Bonn. The support of NATO through Grant No. R.G.106.81 is acknowledged.

---

[1]G. B. Taggart and R. A. Tahir-Kheli, Prog. Theor. Phys. 47, 370 (1972); C. G. Shirley and S. Wilkins, Phys. Rev. B 6, 1251 (1972).
[2]R. C. Kittler and K. H. Bennemann, Solid State Commun. 32, 403 (1979).
[3]K. Binder and D. P. Landau, Phys. Rev. B 21, 1941 (1980).
[4]B. H. Zimm and J. K. Bragg, J. Chem. Phys. 31, 526 (1959).
[5]M. Roger, J. M. Delrieu, J. H. Hetherington, Phys. Rev. Lett. 45, 137 (1980).
[6]K. A. Penson, R. Jullien, and P. Pfeuty (unpublished).
[7](a) H. P. Griffiths and D. W. Wood, J. Phys. C 5, L253 (1972); (b) R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. 21, 1294 (1973).
[8]R. J. Baxter, Ann. Phys. (N.Y.) 70, 193 (1972).
[9]E. Fradkin and L. Susskind, Phys. Rev. D 17, 2637 (1978).
[10]R. Kotecký and S. B. Shlosman, Comm. Math. Phys. 83, 493 (1982).
[11]P. Pfeuty, R. Jullien, and K. A. Penson, in *Real Space Renormalization,* Topics in Current Physics, edited by Th. W. Burkhard and J. M. J. van Leeuven (Springer, Heidelberg, 1982), Vol. 30.
[12]M. E. Fisher and M. E. Barber, Phys. Rev. Lett. 28, 1516 (1972).
[13]M. P. Nightingale, Physica (Utrecht) 83A, 561 (1976).
[14]H. H. Roomany, H. W. Wyld, and L. H. Holloway, Phys. Rev. D 21, 1557 (1980).
[15]M. E. Fisher and A. N. Berker, Phys. Rev. B 26, 2507 (1982).
[16]C. J. Hamer, J. Phys. A 14, 2981 (1981).
[17]W. Kinzel, E. Domany, and A. Aharony, J. Phys. A 14, L417 (1981).
[18]For $n=2$, $n'=4$ the model is similar to the Ashkin-Teller model [see R. V. Ditzian, J. R. Banavar, G. S. Grest, and L. P. Kadanoff, Phys. Rev. B 22, 2542 (1980)], and to the generalizations thereof [see G. S. Grest and M. Widom, Phys. Rev. B 24, 6508 (1981)].
[19]P. A. Pearce and R. J. Baxter, Phys. Rev. B 24, 5295 (1981).