Critical point of infinite type

L. Benguigui
Physics Department and Solid State Institute, Technion–Israel Institute of Technology, Haifa, Israel
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We show that a critical point of infinite type is in fact a special case of first-order transition between two states: one perfectly ordered, and a disordered one. The analogy with exact models is pointed out.

I. INTRODUCTION

The concept of critical points of different type or order was introduced at almost the same time by Schulman[1] and by Chang *et al.*[2] In this paper, we investigate the properties of a critical point of infinite type, i.e., what happens if one considers the limit of critical points of finite type t as $t \to \infty$. This question is not only of academic interest since our main result is that some exact models have critical points of infinite type, the best known among them being the Slater potassium-dihydrogen-phosphate (KDP) model.[3] The ferroelectric models with the ice rule seem to be impossible to classify among the other models like the Ising or Heisenberg models. Although Sutherland[4] has mentioned that in two dimensions the KDP model is characterized by $\beta=0$, the F model by $\beta=\infty$ and the Ising model by $\beta=\frac{1}{4}$, taking an intermediate position, no systematic classification has been proposed. Thus, we shall study the properties of critical point with $t=\infty$ and discuss the possibility of classifying the ice rule models under a general classification.

II. DEFINITION

We recall briefly the definition of the type of a critical point, as given by Schulman who used the catastrophe theory.[5] A critical point can be seen as a catastrophe and consequently for phase transitions involving one order parameter the state of the system is described by a polynomial of one variable. The type t is defined by half the degree of polynomial. Here we consider only polynomials with even powers (symmetric critical points),

$$F(\mu)=\mu^{2t}+\sum_{j=1}^{t-1} U_{2j}\mu^{2j}\,. \tag{1}$$

The variable μ is related to the order parameter and the U_{2j} are functions of the temperature T and of $t-2$ fieldlike parameters. At the transition point, all the U_{2j} coefficients vanish

$$U_{2j}(T;Y_1,\ldots,Y_{t-2})=0,\quad j=1,\ldots,t-1\,. \tag{2}$$

These determine $t-1$ hypersurfaces in the thermodynamic space whose intersection is the critical point of type t. Benguigui and Schulman[6] have shown that a symmetric critical point of type t is located on a line of critical points of type $t-1$, at the point where the second-order transition becomes of first order.[7]

A critical point of infinite type may occur in one of the two following cases:

Case I. The number of the Y_j variables goes to infinity and, following Eq. (2), at the critical point all the coefficients of the polynomial (which is now an infinite series) become null simultaneously.

Case II. All the coefficients of the polynomial, as long as we can take it, become null accidentally for a set of particular values of T and Y_j. The number of the Y_j variables is finite in this case. This situation bears some similarity to an essential singularity.

One notes the advantage of Schulman's definition which gives a critical point of infinite type even if the number of the Y_j variables is finite. This is not possible in Chang's definition since a critical point of type t is the point where t phases become critical.

III. TRANSITION WITHOUT EXTERNAL FIELD

We start with the Landau-Wilson Hamiltonian for a critical point of type t:

$$\mathcal{H}=\int \left[a\,P^2(\vec{x})+b P^{2t}(\vec{x})+U(\nabla P)^2\right] d_d V\,, \tag{3}$$

with $a=A(T-T_c)$. In order to calculate the properties for $t\to\infty$, we shall determine them first for t finite and only afterwards let $t\to\infty$. Formally letting $t\to\infty$ in the Hamiltonian is not readily subject to interpretation. The calculation of the critical exponents for a critical point of type t is a complicated problem.[2,8] One can do an ϵ expansion[9] where $\epsilon=2t/(t-1)-d$. The borderline dimension $d_B=2t/(t-1)$ is such that for $d>d_B$ the classical theory may be used. It is already known that for $d=3$, it suffices that $t>3$ to get classical results. The important point is that $d=2$ becomes the borderline dimension for

$t=\infty$. Thus we have the important result that the classical theory gives the correct results for $t=\infty$, even for $d=2$. For $d=d_B$, it is in general necessary to include logarithmic correction. However for $t=\infty$, this correction is meaningless below T_c and does not seem to exist for $T>T_c$, as can be seen from comparison with exact models.

For $T<T_c$, the classical result is obtained by taking the following approximation. The exact partition function $Z \propto \int e^{-\mathcal{H}/kT} DP(\kappa)$ is replaced by $Z_{cl} \propto e^{-\mathcal{H}(P_0)/kT}$ where P_0 is the value of P which minimizes (3). Following the usual procedure, we get

$$P_0 = (-a/bt)^{1/2(t-1)} \quad \text{or} \quad P_0 \propto (T-T_c)^{1/2(t-1)} \tag{4a}$$

for the order parameter;

$$\chi^{-1} = -4a(t-1) \tag{4b}$$

for the susceptibility;

$$C = [1/(t-1)]A^2(-a)^{(2-t)/(t-1)}(1/bt)^{1/(t-1)},$$

$$\alpha' = t - 2/(t-1) \tag{4c}$$

for the specific heat.

Now if $t \to \infty$, we get

$$P=1, \quad \text{i.e.,} \quad \beta_\infty = 0, \quad \delta_\infty = \infty, \quad \beta\delta = 1,$$

$$\chi = 0, \quad C = 0.$$

Since $P=1$, this means that the system is completely ordered and there are no spatial fluctuations. Consequently we get $\chi=0$ and $C=0$. It is interesting to note that $\chi \to 0$ and $C \to 0$ for $t \to \infty$ because the amplitudes go to zero. By continuity, one can say that the exponent γ' and α' are both equal to 1, although $\chi=0$ and $C=0$ can be interpreted as $\gamma'=0$ and $\alpha'=0$.

Above T_c, $P=0$ and from the above results, we see that the transition becomes of first order, but without thermal hysteresis. The latent heat is equal to AT_c. The classical approximation above T_c consists of taking only the first and third terms in (3) and we get the Gaussian model, i.e., $\gamma=1$ and $\alpha=\frac{1}{2}$. There is an asymmetry in the behavior of the system above and below T_c. In particular for t finite one expects that $\alpha'(t)=\alpha(t)$. The fact that $\alpha \to \frac{1}{2}$ for $t \to \infty$ does not mean that α exhibits a discontinuity. One rather expects a crossover from a region where C behaves like $(T_c-T)^{-1/2}$ to region with $C \propto (T_c-T)^{-\alpha(t)}$. For $t \to \infty$, this region disappears.

IV. TRANSITION WITH AN EXTERNAL FIELD

For t finite, the curve $P(T)$ with $E \neq 0$ has an inflection point. [Now, the Hamiltonian (3) contains a term EP.] Let be P_i and T_i the values of the order parameter and of the temperature of the inflection point ($T_i > T_c$). Clearly P_i and T_i are functions of E. First we calculate dP/dT. We get

$$\frac{dP}{dT} = -\frac{AP}{A(T-T_c)+bt(2t-1)P^{2t-2}}. \tag{5}$$

d^2P/dT^2 is null if

$$2A(T-T_c)+bt(2t-1)(4-2t)P^{2t-1}=0,$$

i.e., P_i is given by

$$P_i = [4A(T_i-T_c)/bt(2t-1)(2t-4)]^{1/(2t-1)}. \tag{6}$$

Now, if $t \to \infty$, $P_i \to 1$. In order to calculate T_i, we use the relation

$$E = \frac{\partial G}{\partial P} = 2A(T_i - T_c)P_i + 2btP_i^{2t-1} \tag{7}$$

(G is the free energy).

Using (6), (7) becomes, if $t \to \infty$,

$$E = 2A(T_i - T_c). \tag{8}$$

Now from (5), it is easy to see that if $T \to T_{i-}$, $dP/dT \to 0$, and if $T \to T_{i+}$,

$$\frac{dP}{dT} \to -\frac{1}{T_i - T_c} = -\frac{2A}{E}.$$

The schematic variations of P as function of T are given on Fig. 1, for some values of E. Thus, with an external field, the transition is no longer a first order transition but a second order one: P is now continuous, but has a discontinuity in its derivative at T_i. This temperature is the new transition temperature.

V. COMPARISON WITH EXACT MODELS

(i) Bowers and McKerrell model.[10] In this model, the Hamiltonian which describes an assembly of N spins contains two-point, four-point, . . . , $2n$-point interactions:

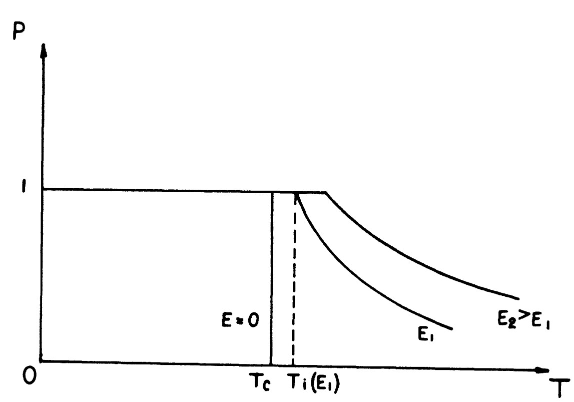

FIG. 1. Schematic variation of P and T, for different values of the external field if $t=\infty$.

$$H=-\sum_{r=1}^{n} J_{2r} S^{-2r} N^{-(2r-1)} \sum_{i_1,\ldots,i_{2r}} S^2_{i_1},\ldots,S^2_{i_{2r}}.$$

The interaction strengths J_{2r} are independent of the distance between the spins. For interactions up to n one can get, using a special choice of the J_{2r}, a critical point of type $t=n+1$, with the same critical exponents as those found above. For a spin $s=\frac{1}{2}$, the interactions J_{2r} must be equal to $J_2/2r(r-1)$. One gets a critical point of type $t=\infty$, if $n\rightarrow\infty$, and J_{2r} decreases with the number of spins involved. At the limit, the interaction which includes all the spins ($n=\infty$) has null strength. This model is an example of case I.

(ii) Crossed Ising chains. Jüngling and Obermair model.[11] This model describes horizontal and vertical crossed Ising chains with different interaction strength between spins of the horizontal and vertical chains. If the distance between the vertical chains increases infinitely but the interaction strength of the spins of the horizontal chain also increases infinitely, a first-order transition appears between two states, a perfectly ordered one and a disordered one. However, above T_c, the properties of the system are not exactly the same as the Gaussian model. This is an example of case II.

(iii) Slater KDP model.[3] It is most interesting that the Slater KDP model has *exactly* the same properties found above for $t=\infty$, without and with external field. For the complete equivalence, it is only necessary to choose $A=\frac{1}{2}(k\ln 2)$. Thus the latent heat is $AT_c=\frac{1}{2}(k\ln 2)$ and $dT_i/dE=1/2A=1/k\ln 2$. This example of a critical point of infinite type belongs to the case II.

VI. REMARKS

One can also define a first order transition of type t, using the above remark that a critical point of type $t+1$ is located, in the thermodynamical space, on the line of critical points of type t, where the transition goes from a second to a first-order transition. The first-order transition is also of type t. For first-order transition, the classical theory can be used, in the absence of an external field.[12] Thus the free energy per unit volume is

$$G=aP^2+cP^{2t-2}+bP^{2t}.$$

It is easy to show that the discontinuity in P at the transition temperature T_c' is equal to

$$P_0=[-2a(t-1)/c]^{1/2(t-2)},$$

which goes to 1 when $t\rightarrow\infty$. The transition temperature T_c' in lower than T_c, but goes to it when $t\rightarrow\infty$. Thus the difference between the first and second order transition disappears for $t\rightarrow\infty$. This explains why the second order transition becomes of first order at $t\rightarrow\infty$.

The results of the preceding sections show that the KDP model with the ice rule can be included in the classification of critical points of different type. The question is, can one also include the opposite model with the ice rule, namely the F model. This can be done but formally, by putting $t=1$ in the formulas (4). We get $\beta=\infty$, $\chi=\infty$, or $\gamma'=\infty$ and $\alpha'=-\infty$. The derivatives of P also have an infinite exponent. This is qualitative agreement with the exact results.[13]

$$P_0\propto(T_c-T)^{1/2}\{\exp[-g/(T_c-T)^{1/2}]\},$$

$$\chi\propto(T_c-T)^{-1}\{\exp[\pi^2/2(T_c-T)^{1/2}]\},$$

$$G\propto\exp[-\pi^2/(T_c-T)^{1/2}].$$

VII. CONCLUSION

In the case of a critical point of infinite type, it is possible to use the classical theory and to let $t\rightarrow\infty$ to get the correct results. Thus the properties of a critical point of infinite type are: (i) The transition is a very special first-order transition, without hysteresis and the order parameter jumps suddenly, at T_c, from 1 to 0; (ii) the latent heat is given by $u=AT_c$; (iii) below T_c, the susceptibility X and the specific heat C are null (as a result of the perfect ordering); (iv) above T_c, χ and C diverge: $\chi\propto(T_c-T)^{-1}$ and $C\propto(T_c-T)^{-1/2}$; (v) with an external field, the transition becomes also a special case of second-order transition and the value of the new transition temperature is linear in the field.

The KDP model is an example of a critical point of infinite type. We conclude also that the properties of the KDP model are dimension independent as are those of the classical theory. Considering the limits $t\rightarrow 1$ and $t\rightarrow\infty$, one can include the ferroelectric models with the ice rule in a general classification of critical points.

The main and most important property of the critical point of infinite type is the sudden transition from a perfectly ordered state ($P=1$) to a disordered one ($P=0$). The interesting question is: what are the ingredients that must be incorporated in a particular model to get such a behavior? From the three examples we quoted, it is clear that it is necessary to include infinite interactions (in number or in strength). This insures that, in the ordered state, the system is perfectly ordered. However, these interactions must have some kind of opposition in order that a phase transition occurs. Thus, in the Bowers-McKerrell model, $n\rightarrow\infty$ but $J_{2n}\rightarrow 0$. In the Ising analog of the KDP model the two-spin interactions go to infinity but the four-spin interaction also goes to infinity.

As it is known[14] the two-spin interactions favor ordering but the four-spin interaction plays an opposite role. In the Jüngling and Obermair model the interaction strength in the horizontal chains goes to infinity, but the distance between the vertical chains also goes to infinity.

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