

## Self-consistent approximation of a phase transition as a theory of a constrained system

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We show that the various self-consistent theories of a phase transition (the Hartree approximation, the self-consistent phonon approximation, the generalized spherical model of Brout) exhibit the same properties: The transition is of first order, and in the disordered phase the critical indices are  $\gamma = 2$ ,  $\alpha = -1$ . Applying the Fisher renormalization theory, we find that these properties come from the constraint given by the self-consistent condition. The constraint induces a first-order transition in the ordered phase and a renormalization of the critical exponents in the disordered phase.

### I. INTRODUCTION

In the theory of phase transition, there has recently been interest in approximate solutions which go a step beyond the mean-field theory (MFT): the self-consistent approximations. Depending on the adopted formalism, different names have been given. In the frame of the Landau theory, it is called the Hartree approximation<sup>1</sup> (HA). It is known as the self-consistent phonon (SCP) approximation in the study of structural phase transitions.<sup>2</sup> In his treatment of the Ising model, Brout<sup>3</sup> developed the "generalized spherical model," which is also a self-consistent approximation. Recently, Lines<sup>4</sup> presented his correlated-effective-field theory (CEF), which is general enough to include the SCP approximation and the Brout model as particular cases.

In Ref. 1 Amit and Zannetti gave detailed calculations of the HA (in the case of a scalar order parameter), and we briefly recall their results. In the disordered phase, the critical indices are  $\gamma = 2$ ,  $\nu = 1$ , and  $\alpha = -1$ , but these indices are defined for a temperature  $T_0$ , which is not the true transition temperature. In the ordered side, the transition is of first order and the transition temperature  $T_v$  is greater than  $T_0$ .  $T_0$  is merely the stability limit of the disordered phase. It is the purpose of this paper to show that the SCP approximation and the Brout model have the same properties. In the case of the SCP theory it is already known that the transition is of first order<sup>5</sup> (at least in three dimensions), and we shall show that in the disordered phase we have also  $\gamma = 2$ ,  $\alpha = -1$ .

Apparently, the Brout model gives a second-order transition and does not seem to belong to the same class of approximations. But Brout noted<sup>6</sup> that his model has a "deep flaw": the curve  $R(H)$  ( $R$ , magnetization;  $H$ , magnetic field) has the shape indicated in Fig. 1 for  $T \geq T_c$  (transition temperature), which is unacceptable at a second-order transition. This type of curve is very well known in ferroelectricity as a "double hysteresis loop." Among the experimentalists, it is considered as

the best experimental proof of a first-order transition.<sup>7</sup> This suggests that a re-examination of the results of the Brout model would be worthwhile. Effectively, we found that this model exhibits a first-order transition.

The second purpose of this paper is to find the reason for the appearance of a first-order transition in these theories. The clue is to see these approximations as expressing a constraint for the MFT, in the sense of Fisher.<sup>8</sup> Recently, Imry *et al.*<sup>9</sup> showed that a constrained system may exhibit a perfect second-order transition or a renormalized one, or a first-order transition. We shall show below that effectively the constraint in a self-consistent approximation is such that the transition becomes a first-order transition.

### II. SCP APPROXIMATION

We follow the exposition of Lines and consider a local potential for  $N$  coupled oscillators

$$V(x_i) = a_1 x_i^2 + a_2 x_i^4 - \frac{1}{2} \sum_j v_{ij} x_i x_j, \quad (1)$$

where  $x_i$  is the displacement of the  $i$ th oscillator. We write

$$\begin{aligned} x_i &= \langle x \rangle + u_i, \\ u_i &= \frac{1}{\sqrt{N}} \sum_q u(q) e^{-i\vec{q} \cdot \vec{i}}, \\ v(q) &= \sum_q v_{ij} e^{-i\vec{q} \cdot (\vec{i}-\vec{j})}, \end{aligned}$$

where  $\langle x \rangle$  is the thermodynamic mean value of  $x_i$ . From (1) we obtain the three basic equations of the SCP approximation (see Ref. 4 for details)

$$h = [2a_1 - v(0) + 12a_2 \langle u_i^2 \rangle] \langle x \rangle + 4a_2 \langle x \rangle^3, \quad (2a)$$

$$\ddot{u}(q) = -\Omega^2(q) u(q),$$

$$\Omega^2(q) = 2a_1 + 12a_2 \langle x \rangle^2 + 12a_2 \langle u_i^2 \rangle + v(q), \quad (2b)$$

$$\langle u_i^2 \rangle = \frac{1}{N} \sum_q \frac{\hbar}{2\Omega(q)} \left[ \coth \frac{\hbar\Omega(q)}{2kT} \right]. \quad (2c)$$

In (2a)  $h$  is the field conjugate of  $\langle x \rangle$ . In the follow-

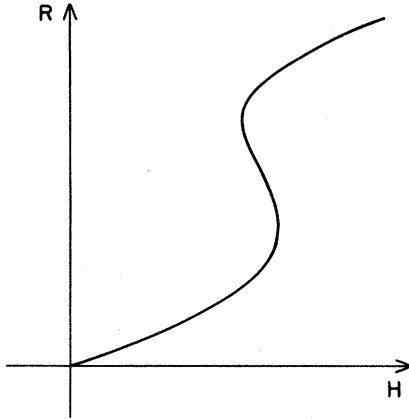


FIG. 1. Curve  $R(H)$ , magnetization vs magnetic field, in the Brout treatment of the Ising model, for  $T \geq T_c$ .

ing we shall assume that  $\hbar\Omega(q) \ll kT$  and  $v(q) = v(0) - \gamma^2 q^2$ . From (2a), we have for the susceptibility  $\kappa$

$$\kappa^{-1} = \chi = \left( \frac{\partial \hbar}{\partial \langle x \rangle} \right)_{\langle x \rangle=0} = 2a_1 - v(0) + 12a_2 \langle u_i^2 \rangle, \quad (3)$$

and  $\langle u_i^2 \rangle$  is determined consistently by (2b) and (2c),

$$N \langle u_i^2 \rangle = \sum_q \frac{kT}{\Omega^2(q)} = \sum_q kT [2a_1 + 12a_2 \langle u_i^2 \rangle - v(q)]^{-1}$$

or

$$N \langle u_i^2 \rangle = kT \sum_q (\chi + \gamma^2 q^2)^{-1}.$$

Using a Debye approximation, we get

$$\langle u_i^2 \rangle = \frac{VkT}{2\pi^2 N} \int_0^{q_m} \frac{q^2 dq}{\chi + \gamma^2 q^2}, \quad (4)$$

$$\langle u_i^2 \rangle = \frac{VkT}{2\pi^2 N} \left( \frac{q_m}{\gamma^2} - \frac{\chi^{1/2}}{\gamma^3} \arctan \frac{\gamma q_m}{\chi^{1/2}} \right).$$

$q_m$  is the cutoff in the Debye approximation and is related to  $N$  by the relation  $N = Vq_m^3/6\pi^2$  ( $V$  is the volume of the system). The implicit equation giving  $\chi$  is deduced from (3) and (4),

$$\chi = 2a_1 - v(0) + \frac{6a_2 kTV}{\pi^2 N \gamma^2} \left( q_m - \frac{\chi^{1/2}}{\gamma} \arctan \frac{\gamma q_m}{\chi^{1/2}} \right). \quad (5)$$

The inverse of the susceptibility is null for the temperature

$$T_0 = [v(0) - 2a_1] \pi^2 N \gamma^2 / 6a_2 V k q_m.$$

For  $T - T_0 \ll T_0$ , Eq. (5) reduced to

$$\chi^{1/2} = (2q_m \gamma / \pi T) (T - T_0), \quad (6)$$

which shows that the index  $\gamma$  is equal to 2.

To find the specific heat we calculate the internal energy  $E = N \langle V_i \rangle$ , and we have

$$\frac{E}{N} = a_1 \langle x_i^2 \rangle + a_2 \langle x_i^4 \rangle - \frac{1}{2} \sum_j u_{ij} \langle x_i x_j \rangle,$$

or

$$\frac{E}{N} = [a_1 - \frac{1}{2} v(0)] \langle x \rangle^2 + a_1 \langle u_i^2 \rangle + a_2 (\langle x \rangle^4 + 6 \langle x \rangle^2 \langle u_i^2 \rangle + \langle u_i^4 \rangle) - \frac{1}{2} \sum_j v_{ij} \langle u_i u_j \rangle.$$

Writing that

$$\sum_j v_{ij} \langle u_i u_j \rangle = \frac{1}{N} \sum_q v(q) \langle u(q) u(-q) \rangle,$$

and  $\langle u_i^4 \rangle \approx 3 \langle u_i^2 \rangle^2$ ,

we find for the specific heat per oscillator

$$\frac{C}{N} = \frac{\partial}{\partial T} \left( \frac{E}{N} \right) = \frac{k}{2} - \frac{1}{2} \langle u_i^2 \rangle \frac{\partial \chi}{\partial T}. \quad (7)$$

From (4) and (5), we find that when  $(T - T_0) \ll T_0$ ,

$$\frac{C}{N} = \frac{k}{2} - \frac{12kN}{\pi^2} \left( \frac{T - T_0}{T} \right), \quad (8)$$

which shows that  $\alpha = -1$ .

### III. BROUT MODEL

We start with the Hamiltonian of the Ising model

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} v_{ij} x_i x_j,$$

and we shall use the Fourier transforms  $x_q$  of  $x_i$ ,

$$x_q = \frac{1}{\sqrt{N}} \sum_i x_i e^{i\mathbf{q} \cdot \mathbf{i}},$$

and of the Fourier transform  $v(q)$  of  $v_{ij}$ . Brout writes

$$\mathcal{H} = -\frac{1}{2} \sum_q v(q) |x_q|^2,$$

and proposes for  $\langle |x_q|^2 \rangle$  the following expressions. In the disordered phase,

$$\langle |x_q|^2 \rangle = [1 - \beta[v(q) - \mu]]^{-1} \quad (\beta = 1/kT), \quad (9a)$$

and, in the ordered phase,

$$\langle |x_q|^2 \rangle = [1 - \beta(1 - R^2)[v(q) - \mu]]^{-1}. \quad (9b)$$

$\mu$  is a temperature-dependent parameter which must be determined through the sum rule  $\sum_q \langle |x_q|^2 \rangle = N$ . First we shall show that the transition is of first order. In the ordered phase,  $R$  is given<sup>3,4</sup> by the two following equations:

$$R = \tanh \frac{R[v(0) - \mu]}{kT} \quad (10)$$

and

$$N = \sum_q \langle |x_q|^2 \rangle$$

$$= \sum_q \{1 - (1 - R^2)\beta[v(0) - \mu - \gamma^2 q^2]\}^{-1}. \quad (11)$$

We want to calculate  $dR/dT$  for  $R=0$ . If its value is infinite negative the transition is of second order, and if not, it is of first order. From (11), we get

$$N(1 - R^2) = \frac{V}{2\pi^2} \left\{ \frac{q_m k T}{\gamma^2} - \frac{(kT)^{1/2}}{\gamma^3} \left( \frac{1}{1 - R^2} - \frac{v(0) - \mu}{kT} \right) \right. \\ \left. \times \arctan \left[ \gamma q_m / (kT)^{1/2} \left( \frac{1}{1 - R^2} - \frac{v(0) - \mu}{kT} \right)^{1/2} \right] \right\}. \quad (12)$$

$R$  is equal to zero for  $T_0$  defined by  $T_0 = 2\pi^2 \gamma^2 N / v q_m k$ . (Here also  $q_m$  is the cutoff of the Debye approximation.) Near  $T_0$ , taking into account that  $R \ll 1$ , we have from (12),

$$R^2 = [v(0) - \mu] / kT - 1 + K[(T - T_0) / T_0]^2, \quad (13)$$

with  $K = 12/\pi^2$ . Now, we develop (10) near  $R \approx 0$ ,

$$R = \{[v(0) - \mu] / kT\} R - \frac{1}{3} \{[v(0) - \mu] / kT\}^3 R^3$$

or

$$R^2 = 3 \{[v(0) - \mu - kT] / [v(0) - \mu]^3\} k^2 T^2. \quad (14)$$

Combining (13) and (14), and since near  $T_0$   $v(0) - \mu \approx kT_0$ , we find

$$R^2 = (6/\pi^2) [(T - T_0) / T_0]^2. \quad (15)$$

Thus  $dR/dt$  is finite. We adopt the positive value, since we exclude that  $R$  goes to zero with finite negative slope.

In the disordered phase the susceptibility  $\kappa$  is equal to

$$\beta \langle |x_q|^2 \rangle = \beta \{1 - \beta[v(0) - \mu]\}^{-1}.$$

Writing  $v(0) - \mu = kT_c(T)$ , we shall see below that the condition  $N = \sum_q \langle |x_q|^2 \rangle$  can be written in the disordered phase, when  $T - T_0 \ll T_0$ ,

$$(T - T_c)^{1/2} = (2q_m \gamma / \pi k^{1/2}) (T - T_0) / T. \quad (16)$$

This permits the calculation of  $\kappa$  as a function of  $T - T_0$ , and we get

$$\kappa^{-1/2} = (2q_m \gamma / \pi T) (T - T_0),$$

which is identical with (6). The specific heat in the disordered phase is calculated as above, from the mean value of  $\mathcal{H}$ , i.e.,  $E = \langle \mathcal{H} \rangle = -\frac{1}{2} \sum_q v(q) \times \langle |x_q|^2 \rangle$ , with  $\langle |x_q|^2 \rangle$  given by (9a).

$$E = -\frac{1}{2} \sum_q \frac{v(q)}{1 - \beta[v(q) - \mu]},$$

$$E = -\frac{1}{2} \sum_q \left[ \frac{1}{\beta} \left( -1 + \frac{1}{1 - \beta[v(q) - \mu]} \right) + \frac{\mu}{1 - \beta[v(q) - \mu]} \right],$$

$$E = -\frac{1}{2} N \mu,$$

taking into account the constraint  $N = \sum_q \{1 - \beta[v(q) - \mu]\}^{-1}$ . We have

$$\frac{C}{N} = -\frac{1}{2} \frac{d\mu}{dT}.$$

Using as above the notation  $v(0) - \mu = kT_c(T)$ , we can write

$$\frac{C}{N} = \frac{k}{2} \frac{dT_c}{dT}.$$

The derivative  $dT_c/dT$  is deduced from (16), and we get

$$\frac{C}{N} = \frac{k}{2} - \frac{12k}{\pi^2} N \frac{T - T_0}{T}, \quad (17)$$

which is identical with (8), the expression of the specific heat in the SCP approximation.

#### IV. CONSTRAINT

In Fisher's theory<sup>8,9</sup> it is supposed that the free energy of a system exhibiting a second-order transition depends on  $T$  and on another parameter  $\xi$  in the following form:

$$G = g_0(\xi, T) + g_1(\xi, T) |T - T_c(\xi)|^{2-\alpha}.$$

$\alpha$  is the critical index of the specific heat. A constraint is defined by a relation between  $T$ ,  $\xi$ , and its conjugate  $x(\xi, T) = \partial G / \partial \xi$ ,  $F(T, \xi, x) = \theta$ . In the  $T - \xi$  plane, the line defined by  $F(T, \xi, x(\xi, T)) = \theta$ , or  $\xi = \xi^R(T)$ , and the line  $T = T_c(\xi)$  cross at the temperature  $T_0$ . In order to calculate the properties of the constrained system, it is necessary to compute the relation between  $|T - T_c(\xi)|$  and  $|T - T_0|$ . If this function is single valued, the transition is of second order (with or without renormalization), and if it is a triple valued, the transition is of first order.

We shall work in the frame of the Brout model, since we can identify the parameter  $\mu$  and the parameter  $\xi$  of the renormalization theory. The constraint is the sum rule  $N = \sum_q \langle |x_q|^2 \rangle$ . As this constraint does not take the same form in the disordered and ordered phases [see expressions (9a) and (9b)], we must perform the calculations in both.

##### A. Disordered phase

We calculate explicitly the constraint

$$N = \sum_q \langle |x_q|^2 \rangle = \sum_q \frac{1}{1 - \beta[v(q) - \mu]}, \quad (18)$$

$$N = \frac{V}{2\pi^2} \left( \frac{kT q_m}{\gamma^2} - \frac{kT}{\gamma^3} [kT - v(0) + \mu]^{1/2} \right. \\ \left. \times \arctan \frac{\gamma q_m}{[kT - v(0) + \mu]^{1/2}} \right). \quad (19)$$

This is the explicit form of the function  $\xi^R(T)$  and the intersection with the curve  $T_c(\mu) = [v(0) - \mu] / k$  is equal to  $T_0 = 2\pi^2 \gamma^2 N / V q_m k$ . Thus (19) becomes

$$\frac{q_m k}{2\pi^2 \gamma^2} (T - T_0) = \frac{k^{3/2} (T - T_c)^{1/2}}{\gamma^3} \arctan \frac{\gamma q_m}{k^{1/2} (T - T_c)^{1/2}}, \quad (20)$$

which is the required expression. As this is a single-valued function, there is only renormalization of the critical exponents. When  $T - T \ll T_0$ , Eq. (20) can be written

$$q_m (T - T_0) = (\pi k^{1/2} / 2\gamma) (T - T_c)^{1/2},$$

which is the expression (16) above. Thus the critical exponents of the unconstrained system<sup>6</sup>  $\gamma = 1$  and  $\alpha = \frac{1}{2}$  become  $\gamma = 2$  and  $\alpha = -1$ , in agreement with the Fisher predictions.

#### B. Ordered phase

In this case the constraint is given by the expressions (11) and (12). When  $T_c - T \ll T_c$ , we have  $R^2 = 3T^2(T_c - T)/T_c^3$ , and (12) can be written

$$\frac{k q_m}{2\pi^2 \gamma^2} (T_0 - T) = \frac{3NT^2}{T_0^3} (T_c - T) - \frac{\pi k^{3/2} T}{\sqrt{2} \gamma^3} (T_c - T)^{1/2}. \quad (21)$$

It is clear that the expression (21) giving  $T_0 - T$  as a function of  $T_c - T$  is a double-valued function ( $T < T_0, T_c$ ), and the transition is of first order.

We get an interesting and new result. The constrained system exhibits a first-order transition because the constraint forces it in the ordered side only. This means that the result of Imry *et al.*<sup>9</sup> must be completed: In order to get a first-order transition the function giving  $T_0 - T$  as a function of  $T_c - T$  must be only double valued. We see that the theory of the constrained system explains the properties of the self-consistent approximation: first-order transition and renormalization of the exponents in the disordered phase.

#### V. REMARKS

(i) Although we have not a complete proof, we think that the CEP theory of Lines also exhibits the same properties as found above. Our feeling is based on the results of the SCP approximation and of the Brout model, which are two particular cases of the CEP.

If this is correct, the results of Lines,<sup>10</sup> who used his theory for an anisotropic potential in order to describe uniaxial ferroelectrics, are immediately understood. He finds that in the disordered phase the susceptibility  $\kappa$  is proportional to

$$\frac{(T - T_0)}{\log_{10}(1/T - T_0)}$$

and the specific heat  $C$  is equal to

$$A - \frac{B}{\log_{10}(1/T - T_0)}$$

( $A$  and  $B$  are two constants). These are exactly the results of Fisher's renormalization theory,<sup>8</sup> when the specific heat of the unconstrained system

has a logarithmic divergence. And when the constraint of the CEP theory is relaxed, it is found<sup>11</sup> that in the case of an anisotropic potential the divergence of the specific heat is logarithmic.

(ii) If the equivalence of the different types of self-consistent approximation are complete in the disordered phase (see Secs. II and III), in the ordered phase the equivalence is only qualitative. However, the ordered phase has an interesting property. If we expand the free energy in function of the order parameter (say  $\langle x \rangle$ ) of the SCP approximation, we find [with the help of the expressions (2a)–(2c)] that (if  $T - T_0 \ll T_0$ )

$$G = A(T - T_0) \langle x \rangle^2 - B \langle x \rangle^3 T + a_2 \langle x \rangle^4, \quad (22)$$

where  $A$  and  $B$  are functions of the parameters of the model [ $a_1, a_2, q_m$  and  $v(0)$ ]. This is an example of a first-order transition predicted by Landau.<sup>12</sup> But in (22) it is clear that  $G$  must be invariant by changing  $\langle x \rangle$  in  $-\langle x \rangle$ . This means that in (22)  $\langle x \rangle$  stands for the absolute value of the order parameter. It seems that the appearance of the  $\langle x \rangle^3$  term has nothing to do with critical behavior, as speculated by Conte.<sup>5(b)</sup>

(iii) A common feature of this type of approximation is the factorization of the correlation functions. As a result, in the neighborhood of the transition the approximation is no longer valid. Various criterions have been given in order to estimate the "critical region" in which the approximation breaks down.<sup>1,5(a),13</sup> Outside the critical region, the system exhibits classical behavior of a second-order transition, with an apparent transition temperature equal to  $T_0$ ,  $\beta = \frac{1}{2}$ ,  $\gamma = \gamma' = 1$ , and a jump in the specific heat. Pietrass<sup>13</sup> proposed using the SCP (outside the critical region) to describe a second-order transition. However, the results of the preceding section show that the appearance of the first-order transition is an intrinsic property of the approximation, and we cannot call it a "spurious" one. This approximation may be more suitable for the structural transitions with a first-order character, such as the  $\alpha$ - $\beta$  transition of the quartz.<sup>14</sup>

#### VI. CONCLUSION

The main result is that the appearance of a first-order transition in the self-consistent approximation is a genuine property of the theory. This has been shown by using the Fisher theory of the renormalization extended by Imry *et al.*<sup>9</sup> The self-consistent condition, which assures the consistency of the theory, can be seen formally as a constraint. The interesting and new point is that although the physical meaning of the constraint is the same in the ordered and disordered phases, the consequence is not the same in the two phases. In the ordered phase, the constraint induces a phase change be-

fore the order parameter becomes zero, i. e., the transition becomes of first order. In the disordered

phase there is a renormalization of the critical indices.

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