

Critical singularities: A fractal model

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(Submitted 20 March 1991)

Zh. Eksp. Teor. Fiz. **102**, 508–510 (August 1992)

A model is discussed in which a thermodynamical potential singularity results from a continuous change in the fractal dimensionality of the fluctuation phase in the vicinity of the transition temperature. The corresponding specific-heat singularity is found to be logarithmic.

The use of the fractal dimensionality concept for describing critical phenomena was first suggested in Ref. 1. The concept has received support from direct (numerical) Ising model calculations² and is also corroborated by the scale-invariant theory of critical phenomena.^{3–7} In particular, calculations of the magnetization M show evidence² for fractal behavior of the form

$$\langle |M| \rangle \propto L^{\mathcal{D}}, \quad \mathcal{D} < d \quad (T = T_c), \quad (1)$$

where L is the linear size of the system and d denotes the dimensionality of space. Since, on the other hand, the quantity $\langle M \rangle$ should vanish at $T = T_c$, it is immediately clear that the regions $M < 0$ and $M > 0$ must differ in their volume for any actual distribution resulting in M ; by relating this difference to a certain type of clusters (known as “resultant dominant clusters”), a theory capable of explaining relation (1) and consistent with the scaling concept⁷ may be developed.

It is clear, however, that the thermodynamic potential is by no means determined by the “dominant” clusters alone but, rather, by all physical units comprising the volume of the system.

The present fluctuation region model assumes that at $T > T_c$ a D -dimensional fractal structure occurs for the low-symmetry phase which is stable for $T < T_c$. A similar model has in fact been used by Andreev⁸ in his search for the thermodynamic potential singularity involved in first-order transitions; also by Bruce and Wallace,⁹ in connection with second-order transitions. In both studies, fluctuation-induced droplets were introduced to play the role of the unstable phase, and in the latter paper the idea of treating the droplets as fractals was (tentatively) put forward.

Let V be the (constant) volume of the system and φ_1 and φ_2 the potential densities of its pure phases; clearly, $\varphi_1(T_c) = \varphi_2(T_c)$. In the region $T > T_c$ (say) the potential of the system may be defined as

$$F = \varphi_1 v + \varphi_2 (V - v). \quad (2)$$

Here v is the volume of the (unstable) fluctuation phase, and one readily sees that the fractal character of this phase corresponds, in a sense, to the lack of smoothness in the phase boundary; otherwise, a first-order transition would result. We denote by D the dimensionality of the set formed by the fluctuation phase, and we consider D to be a continuous function of temperature [$D \equiv D(T)$], so that $D(T_c) = d$. This implies that D is not identical with the quantity \mathcal{D} in (1) and reflects the fact that not only clusters with a specific sign of M , but also the totality of all $M^2 \neq 0$ and $M = 0$ clus-

ters determine the magnitude of the thermodynamic potential—as one might expect when the entire volume of the system is taken into account.

Consider a fluctuation phase occupying a region with linear dimensions on the order of the correlation length r_c . The exact dimensionality of a fractal set is known to be given by the limit

$$D = \lim_{\rho \rightarrow 0} \frac{\ln K(\rho)}{\ln(r_c/\rho)}, \quad (3)$$

where $K(\rho)$ is the number of d -cubes covering the set. Clearly, however, this definition is of limited practical value because there is actually no quantity available to use as ρ . To remedy this, we may replace (3) by a formally equivalent definition

$$D = \lim_{r_c \rightarrow \infty} \frac{\ln K(r_c)}{\ln(r_c/\rho)}, \quad (4)$$

and, because $r_c \rightarrow \infty$ in the limit as $T \rightarrow T_c$, it is precisely in the fluctuation region that (4) may be understood literally: the quantity ρ may simply be interpreted as representing the average interparticle separation. It thus follows that the present formulation is only adequate for sufficiently large ratios r_c/ρ , that is, exactly in the immediate vicinity of T_c .

For a region whose d -volume is r_c^d , the d -volume of the fluctuation phase is then given by

$$v = \rho^d K(r_c) = r_c^d (\rho/r_c)^{d-D}; \quad (5)$$

note that the volume of the fractal set is identical to its d -dimensional measure¹⁰ with this definition. Assuming $d - D(t)$ to be an analytic function of $T = T_c$ [so that $d - D(T) = b(T - T_c) + \dots$, and remembering that $r_c \propto |T - T_c|^{-\nu}$, we rewrite (2) in the form

$$F = \varphi_2 V + (\varphi_1 - \varphi_2) v,$$

and set $t = T - T_c$ to obtain

$$F = V \varphi_2 + r_c^d (at)^{\nu b t} (\varphi_1 - \varphi_2), \quad a = \text{const.} \quad (6)$$

The singular part of the potential then follows, assuming $\varphi_1 - \varphi_2 \propto t$ in the small t limit, as

$$F_{\text{sing}} \propto r_c^d t^2 \ln t. \quad (7)$$

As is customary, we should not identify r_c^d with the volume of the system [more precisely, though, it is the ratio of the potential (7) to r_c^d which (automatically) yields the F den-

sity]. We find then that close to T_c the specific heat of the system behaves like

$$c \propto \ln t, \quad (8)$$

and it is readily seen that the correct sign of c is ensured by the thermodynamic equilibrium condition $\varphi_1 - \varphi_2 > 0$ for $T > T_c$. An interesting point to note is that it is precisely the condition $D(T_c) = d$ (see above) that gives our formulation a direct "mechanical" meaning; it can be seen, namely, that the ratio of the d -volume of the primary (stable) phase to the entire volume of the system (on the corresponding side of T_c) remains finite—as indeed it should. This should be contrasted with the case $D(T_c) < d$, for which the ratio of the volume of the stable phase to that of the entire system goes to zero when the size of the system increases without bound.

According to the above model, then, the thermodynamic potential singularity at $T = T_c$ results from an assumption concerning the fractal nature of (in fact, the shape of the "droplets" in) the fluctuation phase of the system (cf. the "ramified cluster" approach due to Domb,¹¹ in which the surface-to-volume ratio remains finite in the limit as the volume tends to infinity).

It is easily seen, further, that the present result is by no means inconsistent either with (1) or, more generally, with the critical exponent concept;¹² in the latter context, our re-

sult is simply equivalent to specifying the value of one of the exponents ($\alpha = 0$) under conditions of constant volume.

We note, finally, that the same results may of course be obtained directly from the partition function of the system by integrating over only those particle configurations in which some of the particles assemble to form a phase filling a set of dimensionality D such that $D \rightarrow d$ as $T \rightarrow T_c$.

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Translated by E. Strelchenko