PHASE TRANSITIONS OF CONTINUOUS ORDER

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I. Conjecture of a New Type of Phase Transition

In discussions of phase transitions it is most useful to describe the state of a large system by its intensive thermodynamic variables, also called "fields". These field variables, like temperature, pressure, magnetic field, or chemical potentials, are always identical in two coexisting phases in contrast to the "density" variables like entropy, particle density, or magnetization. The appropriate thermodynamic potential which is a function of the field variables is called the free energy. In the Ehrenfest scheme there is said to be a phase transition of the n-th order at some point P in the space of field variables, if at this point all derivatives of the free energy with respect to the variables exist continuously up to order n-1, but in the n-th order discontinuities or divergencies show up. More generally a phase transition of a thermodynamic system is associated with the singularities of the free energy.

Usually the set of singular points forms one or several smooth hypersurfaces in the space of field variables. Singular behavior shows up if one crosses the hypersurface at some point P by varying some locally defined variable x assumed to be orthogonal on the surface. In realistic systems, for instance magnets or fluids, one observes a rather restricted class of phase transitions: When crossing the hypersurface, discontinuities in the first derivatives show up indicating a first order transition; only on the edges of the singular hypersurfaces the phase transitions may change to second order and thus give rise to critical behavior.

As an example we consider a simple ferromagnetic system. There are two field variables: the magnetic field, $-\infty<B<\infty$, and the temperature, $0\leq T<\infty$. The singular hypersurface in this case is the line: $B=0$, $0\leq T\leq T_C$. When crossing the interior part of this line, $T<T_C$, we have the singular behavior:

$$F(B,T)-F(0,T) = -|B|\cdot M_0(T), \quad B\to 0 \tag{1}$$

where M_o is the spontaneous magnetization ; at $T=T_c$, the edge of the singular line, one observes the well-known critical behavior.

In contrast to the usual behavior described above, I would like to conjecture a new type of phase transition corresponding to another simple type of singularity. This conjecture will be supported by the model calculation of the next section. Again we consider a smooth hypersurface of singular points P with the locally defined orthogonal field variable x, x=0 on the surface. Then the leading singular part of the free energy should have the form:

$$F_{sing} \sim |x|^{\kappa(P)} \quad , \; x \to 0 \; , \qquad (2)$$

where the exponent $\kappa(P)$ characterizing the power law singularity is assumed to be a continuous function on the hypersurface. For obvious reasons this new type will be called a phase transition of continuous order. If at some fixed point P: $n-1<\kappa\leq n$, n integer, we have an n-th order phase transition at P according to the Ehrenfest classification scheme. To supplement the above definition it also seems natural to assume that the exponent κ approaches infinity, if the singular point P tends to the edge of the surface. This would correspond to a smooth "fading away" of the singularity in the free energy. A border-line case of a continuous phase transition would be the situation where the exponent κ remains "infinite" on the whole singular hypersurface. This means that the singularity of the free energy is weaker than any power.

In the example of the simple magnetic system discussed above, we would expect a singular line in the B,T-plane, B=0, $0\leq T\leq T_\infty$, and the following behavior of the free energy:

$$F = F_{\mathbf{reg.}}(B^2) + A(T)|B|^{\kappa} \; , \; B\to 0. \qquad (3)$$

Because of symmetry the regular part of the free energy is a function of B^2. The exponent $\kappa(T)$ is expected to increase monotonously from unity at T=0 to infinity at some finite temperature T_∞. As long as $\kappa=1$, we have a first order phase transition with nonvanishing magnetization in zero field, thus the system is ordered in the usual sense. If $\kappa>1$, the zero field magnetization vanishes and there is no longer usual long range order; however, there is still a phase transition up to T_∞, beyond which the free energy will be an analytic function.

II. The Ferromagnetic Ising Model on a Cayley Tree

To support the above conjecture we shall now show that the ferromagnetic Ising model with nearest neighbour interaction on a Cayley tree lattice exhibits such a phase transition of continuous order[1]. A Cayley tree of connectivity K (also called branching ratio) is a continuously branching lattice without cycles. It may be constructed by connecting K+1 n-generation branches to a central site. An n-generation branch itself is defined as an initial site connected to K (n-1)-generation branches; a 1-generation branch is a single site. The thermodynamic limit corresponds to letting n go to infinity. As the linear chain (K=1) is well-known, we here consider $K \geq 2$.

The partition function of the model is given by

$$Z(t,b) = \sum_{\sigma_i = \pm 1} \exp\left\{ b \sum_i \sigma_i + t^{-1} \sum_{\langle ij \rangle} \sigma_i \sigma_j \right\} \tag{4}$$

with a reduced temperature, $t = (\beta J)^{-1}$, where J is the nearest neighbour coupling, and a reduced field $\beta B = b$. This model is almost soluble in closed form. As there are no cycles on a Cayley tree, a path connecting two sites is unique. In performing the trace in (4) one can start with the surface sites and one may proceed step by step towards the interior of the tree. This procedure which, of course, resembles the transfer matrix method results in a recurrence relation for the partition function of an n-generation branch(2):

$$Z^{\pm}_{n+1} = e^{\pm b} \left[Z^{+}_{n} \cdot e^{\pm t^{-1}} + Z^{-}_{n} \cdot e^{\mp t^{-1}} \right]^{K}, \quad Z^{\pm}_{1} = e^{\pm b} \tag{5}$$

where the $\pm$ sign indicates that the initial site spin is kept fixed to $\sigma = \pm 1$, respectively. Using the probability ratio $e^{2x_n} = Z^{+}_{n}/Z^{-}_{n}$, expression (5) is rewritten as

$$x_{n+1} = b + h(x_n), \quad h(x) = \frac{K}{2} \ln \frac{1 + \frac{\gamma}{K} \tanh x}{1 - \frac{\gamma}{K} \tanh x} \tag{6}$$

with $x_1 = b$ and the temperature parameter

$$\gamma(t) = K \cdot \tanh \frac{1}{t} \quad . \tag{7}$$

Using (5) the free energy per site in the thermodynamic limit can be derived as the sum:

$$f(t,b) - f(t,0) = \frac{K-1}{2} \sum_{n=1}^{\infty} K^{-n} \ln \left[1 + \frac{\sinh^2 x_n}{\cosh^2 t^{-1}} \right], \tag{8}$$

where the zero field result, $f(t,0) = \ln(e^{t^{-1}} + e^{-t^{-1}})$, is analytic in t(or T)(2). We notice that the surface sites still contribute to the sum (the n=1 term) in the thermodynamic limit, as their ratio to the total number of sites tends to the finite value $\frac{K-1}{K}$, a consequence of the unusual topology of the pseudolattice.

Eqs. (6) and (8) cannot be solved in closed form. However, the singularities of the free energy can be discussed completely. First one notices that each x_n and the summand in (8) are analytic functions of b and t near their real axis, respectively; furthermore, both (6) and (8) are convergent. Therefore, singularities can arise only from nonuniform convergence. However, one can show[(1),(3)] that the convergence is uniform and thus the free energy is analytic, if the map $x_n \to x_{n+1}$ is contractive near the fix point (point of convergence), i.e.

$$|x_{n+1} - x_n| < \alpha |x_n - x_{n-1}| \ , \ \alpha < 1, \ n \geq N_o . \tag{9}$$

The quantity α may be replaced by $|h'(x_\infty)|$ where x_∞ is the fix point. Simple inspection of (6) then yields the result[(1)]: The free energy is analytic in t and b except for the singular line, b=0, $0 \leq T \leq T_\infty$, where $\gamma(T_\infty)=1$ defines the transition temperature.

The precise form of the singularities for $b \to 0$, $T \leq T_\infty$, can be studied by solving linear recurrence relations which are upper and lower bounds to (6) and which also give upper and lower bounds to (8), both displaying the same singular behavior. The final result is[(1)]:

$$f(t,b) = f_{reg.}(b^2) + A(T) \cdot |b|^\kappa \{1+O(|b|)\} \ , \ b \to 0 \tag{10}$$

where the exponent is

$$\kappa = \frac{\ln K}{\ln \gamma(t)} \tag{11}$$

which varies between unity at T=0 ($\gamma(0)=K$) and infinity at $T=T_\infty$ where the singularity fades away. Thus we have a continuous phase transition as explained in the first section. In particular, it turns out that for even integers, $\kappa=2l$, the singular behavior changes to $b^{2l}.\ln|b|$ due to a compensation of divergencies in A(T) and the corresponding coefficient in $f_{reg.}$.

As $\kappa>1$ for T>0, the spontaneous magnetization vanishes. Therefore order in the usual sense is achieved only at zero temperature. One notices, however, that the susceptibility $\chi = -\frac{\partial^2 f}{\partial b^2}\Big|_{b=0}$ diverges if $\kappa \leq 2$, i.e. for $T \leq T_2$ where T_2 is defined by

$$\gamma^2 = K, \ 0<T_2<T_\infty \ . \tag{12}$$

For comparison, in the usual type of phase transition order sets in abruptly or continuously at the critical point T_c. In our case the line of continuous phase transitions interpolates between the high-temperature disordered state and the zero temperature ordered state; the onset of order at T_c in the usual situation is thus stretched to the line $0 \leq T \leq T_\infty$.

III. Extensions and Outlook

The above analysis has been extended to the corresponding antiferromagnetic situation[3]. Including a staggered field H into the discussion the free energy F(T,B,H) is represented in a 3-dimensional space of field variables. The formalism is somewhat more involved, but similar as in Section II. Again the singularities can be worked out by studying recurrence relations. We obtain two pieces of singular surfaces. When crossing the first surface perpendicularly, we again find the singular behavior $|x|^{\kappa}$ where $\kappa(P)\geq 1$ varies continuously on the surface, going to infinity on the edge. On the second surface which in fact joins the first one, κ stays strictly infinite. This is therefore a border-line case as explained in the first section where the singularity is weaker than any power. So far we have not yet been able to determine the precise form of the weak singularity.

The continuous phase transition for the Ising model on the Cayley tree evidently is a consequence of the topology of the pseudolattice. However, its occurrence in more realistic physical situations is possible; we have at least two other situations in mind:

a) For random ferromagnets one considers a fraction p of magnetic atoms and a fraction 1-p of unmagnetic atoms distributed at random on a regular lattice. It is known that the critical temperature $T_c(p)$ is a decreasing function with decreasing p, vanishing for $p\leq p_o$, the percolation limit. However, Griffiths[4] has proven that the free energy is singular up to $T_c(1)$ for all p. The precise nature of the singularities is not yet known. Recently Domb[5] has argued that the ramified magnetic clusters are dominating the singular behavior. In view of the fact that Cayley tree graphs are special ramified clusters, it is conjectured that a random ferromagnet is another candidate for a continuous phase transition, possibly of the border-line case.

b) Two dimensional models with continuous symmetry are known not to have long range order. However, series expansions seem to indicate that the susceptibility is diverging below some temperature[7], although this fact is far from being proven. Again it is conjectured that in these systems a phase transition of continuous order may take place.

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