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CRITICAL PROPERTIES OF 2-DIMENSIONAL FERROMAGNET MODELS

In the paper it is shown by an example of heat capacity and, correspondingly, the thermic coefficient of stability for a magnetic system, that the lowest order of non-zero at the critical point derivative of a thermodynamic force with respect to the thermodynamic coordinate, according to the stability requirements, is odd. Thermodynamic properties of the 2-dimensional Potts model and the 3-spin model, valid for describing of the critical behavior of ferromagnetic systems with strong horizontal and weak vertical bonds, are studied. The whole set of thermodynamic characteristics of stability is calculated for these models, and varying of the critical behavior type with values of critical exponents of the thermodynamic quantities is studied. It is shown that in these 2-dimensional exactly solvable models both analytic and non-analytic behavior of heat capacity in the vicinity of the critical point is possible. It is shown, that the critical exponents of heat capacity for the 3-spin model and the Potts model for $q = 4$ are wholly corresponded to the conditions of thermodynamic stability and the first non-zero derivative at the critical point is the third order entropy derivative of temperature.

Keywords: thermodynamic stability, critical state, heat capacity, coefficients of stability, critical exponents.

У даній роботі на прикладі теплоємності й, відповідно, термічного коефіцієнта стійкості для магнітної системи показано, що похідною найнижчого порядку від термодинамічної сили за термодинамічною координатою, відмінною від нуля в критичній точці, згідно з вимогами стійкості, буде похідна непарного порядку. Досліджуються термодинамічні властивості двовимірної моделі Поттса та триспінової моделі, застосовних для опису критичної поведінки феромагнітних систем з сильними горизонтальними й слабкими вертикальними зв'язками. Для них розраховано повний комплекс термодинамічних характеристик стійкості й досліджено залежність типу критичної поведінки від значень критичних показників термодинамічних величин. Показано, що для цих двовимірних точно розв'язуваних моделей можлива реалізація як аналітичної, так і неаналітичної поведінки теплоємності в околі критичної точки. Обґрунтовано, що критичні показники теплоємності для триспінової моделі й моделі Поттса для $q = 4$ повністю відповідають вимогам термодинамічної стійкості й першою відмінною від нуля в критичній точці похідною буде похідна третього порядку від температури за ентропією.

Ключові слова: термодинамічна стійкість, критичний стан, теплоємність, коефіцієнти стійкості, критичні показники.

В данной работе на примере теплоемкости и, соответственно, термического коэффициента устойчивости для магнитной системы показано, что производной наинижшего порядка от термодинамической силы по термодинамической координате, отличной от нуля в критической точке, согласно требованиям устойчивости, будет производная нечетного порядка. Исследуются термодинамические свойства двумерной модели Поттса и трехспиновой модели, применимых для описания критического поведения ферромагнитных систем с сильными горизонтальными и слабыми вертикальными связями. Для них рассчитан полный комплекс термодинамических характеристик устойчивости и исследована зависимость типа критического поведения от значений критических показателей термодинамических величин. Обосновано, что для этих двумерных точно решаемых моделей возможна реализация и аналитического, и неаналитического поведения теплоемкости в окрестности критической точки. Показано, что критические показатели теплоемкости для трехспиновой модели и модели Поттса для $q = 4$ полностью соответствуют условиям термодинамической устойчивости и первой отличной от нуля в критической точке будет производная третьего порядка от температуры по энтропии.

Ключевые слова: термодинамическая устойчивость, критическое состояние, теплоемкость, коэффициенты устойчивости, критические показатели.

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1. Introduction

In a critical state the system is under extreme conditions – at the boundary of thermodynamic stability. The maximum growth of fluctuations takes place, which causes anomalies in behavior of thermodynamic quantities. One of the key tasks of critical state thermodynamics is identification of these anomalies, i.e. determination of behavior of thermodynamic parameters in the vicinity of critical points. There are several lines of attack on this problem, namely statistical (model), asymptotic and thermodynamic one.

The thermodynamic approach to the problem of a critical state provides for solution of the set task by thermodynamic method [1, 2], which considers the critical point as a point combining both subcritical (heterogeneous) and supercritical (homogeneous) state properties. In [1, 2] the problem of asymptotic behavior of thermodynamic parameters near the critical points was solved in general terms. The existence of four alternative types of behavior for thermodynamic quantities was ascertained. These types are classified by the value of one of the adiabatic stability coefficients (the ASC's) and by the value of the critical slope K_c of the phase equilibrium curve.

The most informative of the ASC's is thermic coefficient of stability, related to heat capacity of system, $(\partial T/\partial S)_M = T/C_M$. It can be explained, first of all, by the fact that according to the first Gibbs lemma the heat capacity C_M is proportional to fluctuations of energy, i.e. C_M determines the fluctuation level growth in the critical point. At the first and the second type of critical behavior $(\partial T/\partial S)_M = \text{const}$ and the level of fluctuations is low. At the third and the fourth type $(\partial T/\partial S)_M \to 0$ and fluctuations reach the large values. The most "fluctuating" is the fourth type, where all the stability characteristics tend to zero.

The analysis reveals that the first type corresponds to experimental data and to models in the self-consistent field approximation. The second and the forth type of critical behavior are intrinsic for ferromagnets and ferroelectrics [3, 4].

The exact solvable models of statistical physics and their applicability to describing of real critical phenomena are always in supreme concern of scientists who deal with the problem of phase transitions and critical state. This paper considers the study of the critical properties for certain statistical models by applying the thermodynamic method of investigation of critical states for one-component equilibrium systems [1, 2], based on the introduction of the constructive definition of a critical state through the system of homogeneous linear equations and concurrent examination of critical state stability conditions.

2. The 3-spin model

Solving the 8-vertex model [5-7] has generated interest in models with multispin interactions, especially in the model with interaction of three spins on a triangular lattice. In such model every site i of the triangular lattice is occupied by spin σ_i taking the value $+1$ or -1. The energy of a certain spin configuration is

$$\mathcal{E} = -J\sum \sigma_i \sigma_j \sigma_k \qquad (1)$$

where the summation is carried on over all the triangular sides of the lattice.

When calculating the free energy for the 3-spin model, it was noticed [6, 7] that obtained results coincide exactly with those for a special case of the 8-vertex model, and the 8-vertex model has four-fold symmetry of spin configurations. Taking advantages of the properties obtained, R. Baxter found the transformation of the 3-spin model on the triangular lattice into the 8-vertex model on the square lattice. As the free energy and the spontaneous magnetization for the 3-spin model coincide with the relevant functions for the 8-vertex model when the interaction parameter is $\mu = 3\pi/4$, the critical exponents of the model under consideration takes the values:

$$\alpha = \alpha' = 2/3, \quad \beta = 1/12, \quad \gamma = 7/6, \quad \delta = 15. \tag{2}$$

From these data, the asymptotic behavior of basic stability characteristics was analyzed. When approaching the critical point, all the thermodynamic parameters tend to zero, moreover, the quantities $(\partial H/\partial M)_S$ and $(\partial H/\partial M)_T$ (the reciprocal adiabatic and isothermic susceptibilities) vanish faster than the others. As $\gamma > \alpha$, the value of the critical slope is $K_c = 0$. This corresponds to the fourth type of critical behavior, which is peculiar for ferromagnets and ferroelectrics. Also, this is particular case of the results obtained in [4] for the range $\frac{\pi}{2} < \mu < \frac{15\pi}{16}$. But the special attention attracts the fact, that the 3-spin model satisfies the conditions of the critical state absolutely.

The analytic structure of the thermodynamic method [1, 2] is defined by the expansion of the internal energy (its magnetic part) $U(S,M)$ in series in entropy S and magnetization M in the vicinity of the critical point. It was shown [1, 2], that according to stability conditions of the critical state $\delta^2 U \geq 0$ under $\sum_{n=2}^{\infty} \frac{1}{n!} \delta^n U(\delta' S, \delta' M) > 0$, the lowest non-zero (and non-equal to infinity) derivative of a thermodynamic force with respect to the generalized thermodynamic coordinate (an external parameter of the system) is an odd order derivative. For example, for S-derivative of T (in the case of constant magnetization M) such derivatives may be $(\partial T/\partial S)_M$, $(\partial^3 T/\partial S^3)_M$, or $(\partial^5 T/\partial S^5)_M$, …. Let us denote the order of that derivative n. Consider an asymptotic behavior of these quantities. Assume $(\partial^n T/\partial S^n)_M = a \neq \{0, \infty\}$ and $(\partial^k T/\partial S^k)_M = 0$ for $k < n$. This implies $|T - T_c| \approx a|S - S_c|^n$ in the vicinity of the critical point when $M = M_c = 0$. Therefore, $(\partial S/\partial T)_M \approx \tau^{1/n-1}/an$, $\tau = |T - T_c|$. Hence, the sequence of such derivatives corresponds to the sequence of the critical exponents:

$$n = 1, 3, 5, \ldots \to \infty \quad \Leftrightarrow \quad \alpha = 0, \ \frac{2}{3}, \ \frac{4}{5}, \ldots, \ \frac{n-1}{n}, \ldots \to 1. \tag{3}$$

For the derivatives $(\partial T/\partial S)_M, (\partial^3 T/\partial S^3)_M, \ldots (\partial^n T/\partial S^n)_M, \ldots$ the corresponding exponent is a known critical index of heat capacity α. When $n = 3, 5, 7, \ldots$ the divergent heat capacity C_M with the fractional values of exponent α takes place. For the 3-spin model $\alpha = 2/3$, and this implies, that the lowest non-zero derivative is the third order derivative $(\partial^3 T/\partial S^3)_M$. The analogous analysis can be carried out for the other adiabatic parameters also.

It is known that in the renormalization group theory the true values of the critical exponents are obtained by the perturbative approach method in small parameter $\varepsilon = 4 - d$ [8], accounting for the first terms of the ε-expansion. In this case an efficient assumption concerning the fractal spatial dimension d takes place. In case under study the perturbation theory leads to the idea of the fractal orders of the derivatives n (Fig. 1) and the small parameters $\sigma = n - n_0$ where n_0 is the nearest to n integer odd number. At this the critical indices are given by expression $(n-1)/n$. E.g., for $(\partial T/\partial S)_M$ near $n_0 = 1$, when $\sigma = 1/7$, one obtains $\alpha = 1/8$, which corresponds to the 3-dimensional Ising model [9].

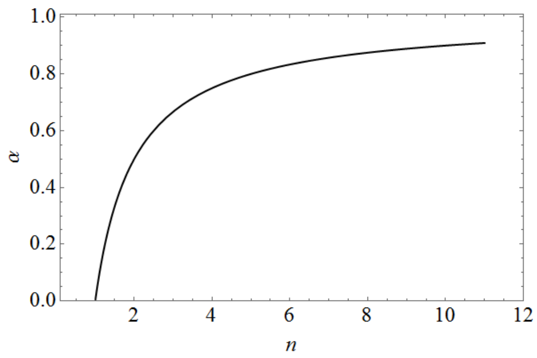


Fig. 1. The order of the ASC's derivative plot of the critical exponent for heat capacity.

3. The 2-dimensional Potts model

Another model, that is of certain interest from viewpoint of the thermodynamic stability requirements, is the Potts model [6, 10, 11]. It is a generalization of the 2-dimensional Ising model [6, 9]. The model is not solved exactly, but it can be presented as a vertex model with the antiparallel order and its critical behavior was investigated well enough.

The Potts model can be formulated for any graph, i.e. for an arbitrary set of vertices (sites) and edges (lines), which join pairs of vertices. Every vertex is associated with a certain parameter σ_i which can take on q values (suppose, $1, 2, \ldots, q$). The peculiarity of this model is that q effects on the type of the phase transition. When $q > 4$ the phase transition is of the first kind (with latent heat of transition), and it is continuous if $q \le 4$. The latter is just the matter of our consideration.

When $q = 1$, the values of the critical exponents are equal to

$$\alpha = -\tfrac{2}{3},\ \beta = \tfrac{5}{36},\ \gamma = \tfrac{19}{18},\ \delta = 15. \tag{4}$$

At $q = 2$ the Potts model becomes the Ising one and the critical exponents are

$$\alpha = 0,\ \beta = \tfrac{1}{8},\ \gamma = \tfrac{7}{4},\ \delta = 15. \tag{5}$$

When $q = 3$,

$$\alpha = \tfrac{1}{3},\ \beta = \tfrac{1}{9},\ \gamma = \tfrac{13}{9},\ \delta = 14, \tag{6}$$

and critical indices coincide with those of the hard hexagon model [6].

At $q = 4$

$$\alpha = \tfrac{2}{3},\ \beta = \tfrac{1}{12},\ \gamma = \tfrac{4}{3},\ \delta = 15, \tag{7}$$

that overlaps with the results for the 3-spin model discussed above (indices α and β).

R. Baxter showed simple dependence of critical exponents of the Potts model on the interaction parameter (like the 8-vertex model) [6], to be more precise, on $y = 2\mu/\pi$:

$$\alpha = \frac{2-4y}{3-3y},\ \beta = \frac{1+y}{12},\ \gamma = \frac{15-16y+y^2}{12(1-y)},\ \delta = \frac{15-8y+y^2}{1-y^2}. \qquad (8)$$

At $q = 1, 2, 3, 4$ the parameter y consequently takes the values $\frac{2}{3}, \frac{1}{2}, \frac{1}{3}, 0$. So, as in the Baxter model, in the Potts one the violation of the universality hypothesis takes place [4].

The analysis of behavior of the ASC's for the Potts model (Fig. 2) enables to ascertain, that at $q = 1$ the stability coefficients asymptotically behave as:

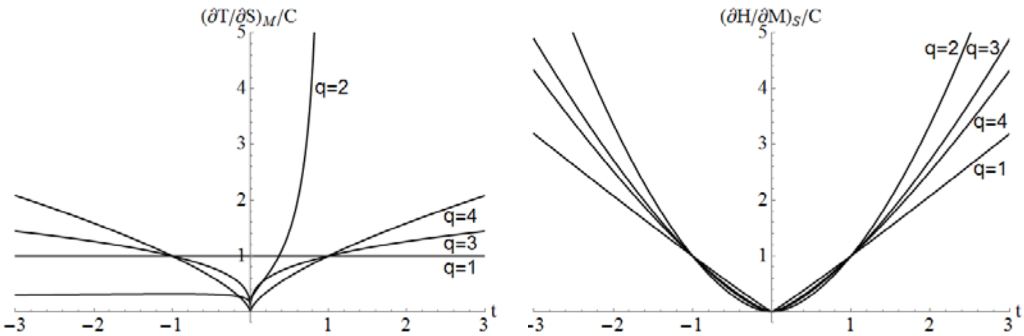
$$\left(\frac{\partial T}{\partial S}\right)_M \sim (-t)^{-2/3},\quad \left(\frac{\partial H}{\partial M}\right)_S \sim (-t)^{19/18}.$$

where $t = (T - T_c)/T_c$; i.e. the second type of critical behavior with the slope of the phase equilibrium curve at the critical point $K_c = 0$ is realized. The energy fluctuations in this case are tempered and fluctuations of the magnetic orientation are large.

If $q = 2$, then $\alpha = 0$ (logarithmic divergence) and $\gamma = 7/4$ leads to the fourth type of critical behavior with the critical slope $K_c = \infty$. The energy and magnetic orientation fluctuations are extremely large. At $q = 3$ the ASC's are given by

$$\left(\frac{\partial T}{\partial S}\right)_M \sim (-t)^{1/3},\quad \left(\frac{\partial H}{\partial M}\right)_S \sim (-t)^{13/9},$$

and the fourth type of critical behavior with $K_c = 0$ is realized.



(a) **(b)**

Fig. 2. Temperature-dependence plot of thermic (a) and magnetic (b) ASC's for the Potts model.

In this model the case $q = 4$ is of peculiar interest:

$$\left(\frac{\partial T}{\partial S}\right)_M \sim (-t)^{2/3},\quad \left(\frac{\partial H}{\partial M}\right)_S \sim (-t)^{4/3}.$$

Here the fourth type of critical behavior with $K_c = 0$ takes place as well, but this case satisfies the stability conditions completely and we have the same situation as in the 3-spin model: the lowest non-zero derivative is the third order derivative $\left(\partial^3 T/\partial S^3\right)_M$.

However, considered models are not the only models, obeying the condition (3). Thus, the value of critical exponent $\alpha = 0$ corresponds to the classical models, the Lieb model when $T < T_c$, the Potts model at $q = 2$, the Baxter and Ashkin – Teller models at $\mu = \pi/2$ [6]. The other possibilities are considered before, while studying the critical behavior of 2-dimensional models [3, 4]. For example, $\alpha = 2/3$ corresponds, together with the 3-spin model and the Potts one at $q = 4$, also to the Baxter model when $\mu = 3\pi/4$ and to the Ashkin – Teller one at $\mu = 0$. The value $\alpha = 4/5$ corresponds to the Baxter model at $\mu = 5\pi/6$. The limit value of critical exponent $\alpha = 1$ corresponds to the 6-vertex Lieb when $T > T_c$, which is the threshold case of the Baxter model at $\mu = \pi$.

4. Conclusions

The performed analysis enables us to conclude, that according to the conditions of thermodynamic stability of the critical state both analytic and non-analytic behavior of heat capacity is possible and both of these cases take place. In the models considered (the 3-spin model, the Potts model) the second and the fourth types of critical behavior are possible, which are peculiar for ferromagnets, as it was shown before [1-4], and which differ in the level of fluctuation growth of the energy and magnetization. This is in good agreement with experimental data.

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