
THERMODYNAMICS OF MODELS WHERE THE UNIVERSALITY HYPOTHESIS IS VIOLATED

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Critical properties of some two-dimensional exactly solved models of statistical mechanics — such as the Baxter eight-vertex, three-spin, Potts, and Ashkin—Teller ones — have been considered. The behavior of the complete set of stability characteristics for these models has been examined in the vicinity of the critical point. The types of the critical behavior have been determined. The violation of the universality hypothesis in the Baxter and Ashkin—Teller models has been explained.

1. Introduction

The main task of the critical state theory is to determine the behavior of thermodynamic quantities in the critical region. There are several ways to solve this problem. One of them is connected with the exact calculation of the partition function, which is used afterwards to find the behavior of all thermodynamic characteristics of the stability. Nowadays, this way is feasible only for model considerations. In the framework of this approach, two-dimensional models, which allow the exact solutions to be obtained, are of high importance. These models form the “capital” of statistical mechanics and help us to understand certain thermodynamic properties of specific systems and the run of critical phenomena in them at a qualitative level. The second approach is related to the analysis of the asymptotic behavior of thermodynamic quantities in the vicinity of the critical point. The significant progress has been achieved in this direction. The scaling law and universality hypotheses, as well as the renormalization group method in all its variants, are very important here. It turned out that there is a

large class of real systems and models, for which the scaling law and universality hypotheses are satisfied. However, along with them, there is a number of real systems and consistent models, for which the hypotheses mentioned are violated. These include, e.g., the Lieb six-vertex ferroelectric model and the model of hard squares, in which the scaling law hypothesis becomes violated, or the Baxter eight-vertex and Ashkin—Teller models, where the universality hypothesis is violated [1]. A third approach consists in solving the given task in the general form, making use of the thermodynamic method [2,3], in which the critical point is considered as a point combining the properties of sub- and supercritical (heterogeneous and homogeneous) states.

The task of this work was to study the critical behavior of the thermodynamic parameters of the mentioned and other statistical models in the framework of the thermodynamic method which was developed for studying the critical state [2,3], was built starting from the first principles, and does not contain any hypothesis.

The method is based on introducing the constructive definition of the critical state by means of the systems of linear and nonlinear homogeneous equations and researching the stability conditions for the critical state. It gives rise to a variety of manifestations of the critical state nature. This variety can serve as the reason for explaining some critical features of the models under investigation.

The researches, whose results are reported in this work, were carried on in two directions. The research of the stability of the statistical models has been fulfilled

for the first time. These models correspond adequately to the critical behavior of real (anti)ferromagnets and real (anti)ferroelectrics. In addition, the consideration carried out is of interest for the theory of the critical state, because it illustrates the capabilities of the method [2,3], using these so interesting models as examples.

Now, let us consider the basic principles of the thermodynamic method, as well as the terminology, which will be used below.

2. Thermodynamic Method for Studying the Critical State

The main quantities, which characterize the stability of a thermodynamic system, are the adiabatic parameters (APs) $\left(\frac{\partial T}{\partial S}\right)_x$, $\left(\frac{\partial T}{\partial x}\right)_S$, and $\left(\frac{\partial X}{\partial x}\right)_S$ and the isodynamic parameters (IPs) $\left(\frac{\partial T}{\partial S}\right)_X$, $\left(\frac{\partial T}{\partial x}\right)_X$, and $\left(\frac{\partial X}{\partial x}\right)_T$. The quantities $\left(\frac{\partial T}{\partial S}\right)_x$ and $\left(\frac{\partial X}{\partial x}\right)_S$ are called the adiabatic stability coefficients (ASCs), while the quantities $\left(\frac{\partial T}{\partial S}\right)_X$ and $\left(\frac{\partial X}{\partial x}\right)_T$ the isodynamic stability coefficients (ISCs) [4]. The stability coefficients are connected with the fluctuations of the external system parameters (the first and the second Gibbs lemmas) which grow infinitely in the vicinity of the critical point.

According to works [2,3], the definition of the critical state can be written down in the form of equations

$$\begin{cases} dT = \left(\frac{\partial T}{\partial S}\right)_x dS + \left(\frac{\partial T}{\partial x}\right)_S dx = 0, \\ dX = \left(\frac{\partial X}{\partial S}\right)_x dS + \left(\frac{\partial X}{\partial x}\right)_S dx = 0, \\ \left(\frac{\partial X}{\partial T}\right)_c = -\frac{dS}{dx} = K_c, \end{cases} \quad (1)$$

where K_c is the slope of the phase equilibrium curve at the critical point. For the nontrivial solution of system (1) to exist, the following condition has to be fulfilled along the whole spinodal:

$$D = \left(\frac{\partial T}{\partial S}\right)_x \left(\frac{\partial X}{\partial x}\right)_S - \left(\frac{\partial T}{\partial x}\right)_S^2 = 0. \quad (2)$$

This expression coincides with the known condition of the critical state, $D = 0$, where D is the system stability determinant [4].

The solution of system (1) is the critical slope K_c which can be expressed in terms of the ASCs:

$$-\frac{dS}{dx} = K_c = \left[\text{sign} \left(\left(\frac{\partial T}{\partial x} \right)_S \right) \right] \left(\left(\frac{\partial X}{\partial x} \right)_S \left(\frac{\partial T}{\partial S} \right)_x^{-1} \right)^{1/2}. \quad (3)$$

This definition applied while considering the conditions of the critical state stability [2,3] gives rise to the existence of four alternative types of the critical behavior of thermodynamic systems:

$$\begin{aligned} 1) & \left(\frac{\partial T}{\partial S}\right)_x \neq 0, \left(\frac{\partial X}{\partial x}\right)_S \neq 0, K_c \neq \{0, \infty\}; \\ 2) & \left(\frac{\partial T}{\partial S}\right)_x \neq 0, \left(\frac{\partial X}{\partial x}\right)_S = 0, K_c = 0; \\ 3) & \left(\frac{\partial T}{\partial S}\right)_x = 0, \left(\frac{\partial X}{\partial x}\right)_S \neq 0, K_c = \infty; \\ 4) & \left(\frac{\partial T}{\partial S}\right)_x = 0, \left(\frac{\partial X}{\partial x}\right)_S = 0, K_c = ?. \end{aligned} \quad (4)$$

The behavior type of every specific system is governed by the value of one of the ASCs and the critical slope K_c .

3. Baxter Eight-vertex Model

The Baxter two-dimensional eight-vertex model [5–7] was proposed as a generalization of the ice-type models with eight permitted vertex configurations and describes the behavior of ferro- and antiferroelectrics. It can also be regarded as a combination of two Ising models (each on its own sublattice) with the interaction between nearest neighbors and coupled by the four-spin interaction. In this case, the model corresponds to a ferromagnet. In the absence of the external field, the Baxter model is solvable exactly. The critical indices of this model are equal to

$$\begin{aligned} \alpha = \alpha' &= 2 - \frac{\pi}{\mu}, \\ \beta &= \frac{\pi}{16\mu}, \quad \gamma = \frac{7\pi}{8\mu}, \quad \delta = 15, \\ \beta_e &= \frac{\pi - \mu}{4\mu}, \quad \gamma_e = \frac{\pi + \mu}{2\mu}, \quad \delta_e = \frac{3\pi + \mu}{\pi - \mu}. \end{aligned} \quad (5)$$

Here, the subscript e denotes the electric critical indices; the indices β , γ , and δ are relevant to the ferromagnet; the index α is identical for the ferromagnet and the ferroelectric; and μ is the parameter of interaction, its values falling within the range $(0, \pi)$. Therefore, one can see that the critical indices depend continuously on the interaction parameter, which contradicts the universality hypothesis. This result distinguishes the Baxter model among other two-dimensional exactly solvable models. From this standpoint, one should

expect that the type of the critical behavior according to the thermodynamic classification and the value of the critical slope would change depending on the interaction parameter. Now, we will demonstrate it.

In the case of the ferromagnet, the asymptotes of the ASCs look like $(\frac{\partial T}{\partial S})_M \sim t^{2-\frac{\pi}{\mu}}$ and $(\frac{\partial H}{\partial M})_S \sim t^{\frac{7\pi}{8\mu}}$, where $t = (T - T_c)/T_c$. It should be noted that, provided the external field is absent, the behavior of the IPs is the same as that of the APs. Within the range $0 < \mu \leq \frac{\pi}{2}$, the index α is negative, and the index γ is positive, i.e. $(\frac{\partial T}{\partial S})_M \neq 0$ and $(\frac{\partial H}{\partial M})_S = 0$, so that $(\frac{\partial T}{\partial M})_S = 0$, $K_c = 0$, and the second type of the critical behavior is realized. If $\frac{\pi}{2} < \mu < \frac{15\pi}{16}$, the fourth type of the critical behavior comes true, the index α increases ($0 < \alpha < \frac{14}{15}$), the index γ falls down ($\frac{7}{4} > \gamma > \frac{14}{15}$), $\alpha < \gamma$, $(\frac{\partial T}{\partial S})_M = 0$, and $(\frac{\partial H}{\partial M})_S = 0$, so that $(\frac{\partial T}{\partial M})_S = 0$. In this case, all the quantities tend to zero, the quantities $(\frac{\partial H}{\partial M})_S$ and $(\frac{\partial H}{\partial M})_T$ faster than the others. The critical slope $K_c = 0$. The case $\mu = \frac{15\pi}{16}$ also corresponds to the fourth type of the critical behavior, but $\alpha = \gamma = \frac{14}{15}$, all the quantities come to zero following the same law, the critical slope $0 < K_c < \infty$. Within the range $\frac{15\pi}{16} < \mu < \pi$, the fourth type of the critical behavior is realized again, $\frac{14}{15} < \alpha < 1$, $\frac{14}{15} > \gamma > \frac{7}{8}$, and $\alpha > \gamma$. All the quantities tend to zero, the quantities $(\frac{\partial T}{\partial S})_M$ and $(\frac{\partial T}{\partial S})_H$ faster than the others. The critical slope $K_c = \infty$.

Thus, the analysis carried out above shows that, if $0 < \mu \leq \frac{\pi}{2}$, the critical behavior of the Baxter model corresponds to the second type of the thermodynamic classification [2, 3] with $K_c = 0$ and, if $\frac{\pi}{2} < \mu < \pi$, to the fourth type which is characterized by three possible values of $K_c - K_c = 0$, $0 < K_c < \infty$, or $K_c = \infty$ — depending on the value of μ from the indicated interval.

In case of the Baxter ferroelectric model, the asymptotes of the stability coefficients look like $(\frac{\partial T}{\partial S})_P \sim t^{2-\frac{\pi}{\mu}}$ and $(\frac{\partial E}{\partial P})_S \sim t^{\frac{\pi+\mu}{2\mu}}$. Provided that $0 < \mu \leq \frac{\pi}{2}$, the index α , similarly to the previous case, is negative, and the index γ is positive. Therefore, $(\frac{\partial T}{\partial S})_P \neq 0$ and $(\frac{\partial E}{\partial P})_S = 0$, so that $(\frac{\partial T}{\partial P})_S = 0$, $K_c = 0$, and the second type of the critical behavior is realized. If $\frac{\pi}{2} < \mu < \pi$, the index α becomes positive within the range $0 < \alpha < 1$, but remains smaller than γ which falls within the range $\frac{3}{2} > \gamma > 1$, and the fourth type of the critical behavior with $K_c = 0$ comes true.

4. Three-spin Model

As was already indicated, the Baxter model can be imagined as two Ising ones, each on its own

sublattice, coupled by four-spin interaction; with only nearest neighbors interacting within each sublattice. The solution of the eight-vertex model has stimulated the interest to models with multispin interactions, especially to the model with three-spin interaction on a triangular lattice.

In this model, every i -th site of the triangular lattice is occupied by a spin σ_i which accepts the value either $+1$ or -1 . The energy of the spin configuration concerned is

$$\mathcal{E} = -J \sum \sigma_i \sigma_j \sigma_k, \quad (6)$$

where the summation is carried on over all the sides of the lattice triangles. The statistical sum looks like

$$Z = \sum_{\sigma} \exp[K \sum \sigma_i \sigma_j \sigma_k], \quad (7)$$

where $K = J/kT$.

While calculating the free energy in the framework of the three-spin model, the results obtained were noticed [1] to coincide exactly with those for the particular case of the eight-vertex model, and the eight-vertex model has the quadruple symmetry of spin configurations in this case. Taking advantage of these properties, Baxter found the operation transforming the three-spin model on the triangular lattice into the eight-vertex model on the square lattice. Therefore, all the results obtained in the framework of the three-spin model are a consequence of the corresponding results obtained in the eight-vertex model.

Since the free energy and the spontaneous magnetization in the three-spin model coincide with the relevant functions of the eight-vertex model if the interaction parameter $\mu = 3\pi/4$, the critical indices of the model look like [8]

$$\alpha = \alpha' = \frac{2}{3}, \quad \beta = \frac{1}{12}, \quad \gamma = \frac{7}{6}, \quad \delta = 15. \quad (8)$$

Proceeding from these data, we have analyzed the asymptotic behavior of the basic thermodynamic characteristics of the stability. While approaching the critical point, all the thermodynamic quantities tend to zero, the quantities $(\frac{\partial H}{\partial M})_S$ and $(\frac{\partial H}{\partial M})_T$ faster than the others. Since $\gamma > \alpha$, the critical slope $K_c = 0$. This corresponds to the fourth type of the critical behavior, which is typical of ferromagnets and ferroelectrics.

This model is most illustrative for the stability conditions of the critical state. It was shown in works [2, 3] that, according to the stability conditions of the critical state, the lowest derivative of the thermal force with respect to the thermal coordinate, which is

distinct from zero, is the derivative of an odd order n . The asymptotic behaviors of the series of such odd derivatives $n = 1, 3, 5, \dots \rightarrow \infty$ are consistent with a series of critical indices $\alpha = 0, \frac{2}{3}, \frac{4}{5}, \dots, \frac{n-1}{n}, \dots \rightarrow 1$. For the derivatives $\left(\frac{\partial T}{\partial S}\right)_x, \left(\frac{\partial^3 T}{\partial S^3}\right)_x, \dots, \left(\frac{\partial^n T}{\partial S^n}\right)_x, \dots$, the corresponding index is the known index of the heat capacity α . In the framework of the three-spin model, $\alpha = 2/3$, which means that the lowest derivative distinct from zero is the derivative of the third order $\left(\frac{\partial^3 T}{\partial S^3}\right)_x$.

5. Two-dimensional Potts Model

The Potts model is a generalization of the two-dimensional Ising model. The model is not solvable exactly, but it can be presented as a vertex model with the antiparallel order, and its critical behavior has been investigated quite well.

The Potts model can be formulated for any graph, i.e. for an arbitrary set of vertices (nodes) and edges (lines) that connect those vertices in pairs. Every vertex is associated with a certain quantity σ_i which can accept q values, say, $1, 2, \dots, q$. The feature of this model is that q governs the type of a phase transition. If $q > 4$, the phase transition is of the first kind (with the latent heat of the transformation), and, if $q \leq 4$, it is continuous. We are interested in the latter case. At $q = 1$, the calculated values of the critical indices are

$$\alpha = -\frac{2}{3}, \quad \beta = \frac{5}{36}, \quad \gamma = \frac{19}{18}, \quad \delta = 15. \quad (9)$$

At $q = 2$, the Potts model becomes the Ising one, and the values of the critical indices are

$$\alpha = 0, \quad \beta = \frac{1}{8}, \quad \gamma = \frac{7}{4}, \quad \delta = 15. \quad (10)$$

At $q = 3$,

$$\alpha = \frac{1}{3}, \quad \beta = \frac{1}{9}, \quad \gamma = \frac{13}{9}, \quad \delta = 14. \quad (11)$$

At $q = 4$,

$$\alpha = \frac{2}{3}, \quad \beta = \frac{1}{12}, \quad \gamma = \frac{4}{3}, \quad \delta = 15. \quad (12)$$

In work [1], the critical indices of the Potts model were shown to depend on the interaction parameter, more precisely on $y = 2\mu/\pi$, in a simple manner:

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

$$\delta = \frac{15-8y+y^2}{1-y^2}. \quad (13)$$

For $q = 1, 2, 3$, and 4 , the corresponding values of the parameter y are $\frac{2}{3}, \frac{1}{2}, \frac{1}{3}$, and 0 .

For $q = 1$, the ASCs look like $\left(\frac{\partial T}{\partial S}\right)_M \sim t^{-2/3}$ and $\left(\frac{\partial H}{\partial M}\right)_S \sim t^{19/18}$, i.e. the second type of the critical behavior with $K_c = 0$ comes true. If $q = 2$, the magnitudes of the critical indices $\alpha = 0$ (the logarithmic singularity) and $\gamma = \frac{7}{4}$ bring about the fourth type of behavior with $K_c = 0$. At $q = 3$, the asymptotic behaviors of the stability coefficients are $\left(\frac{\partial T}{\partial S}\right)_M \sim t^{1/3}$ and $\left(\frac{\partial H}{\partial M}\right)_S \sim t^{13/9}$, while, at $q = 4$, $\left(\frac{\partial T}{\partial S}\right)_M \sim t^{2/3}$ and $\left(\frac{\partial H}{\partial M}\right)_S \sim t^{4/3}$. In both cases, the fourth type of the critical behavior with $K_c = 0$ is realized.

6. Critical Behavior of the Ashkin–Teller Model

The Ashkin–Teller model has been proposed as a generalization of the Ising model onto a four-component system [9].

Let us consider the behavior of the ASCs in this model [12]. For the “magnetic” Ashkin–Teller model, the ASC asymptotes are $\left(\frac{\partial T}{\partial S}\right)_M \sim t^{\frac{2-2y}{3-2y}}$ and $\left(\frac{\partial H}{\partial M}\right)_S \sim t^{\frac{2y}{3-y}}$. At $1 < y < \frac{4}{3}$, which corresponds to $\frac{\pi}{2} < \mu < \frac{2\pi}{3}$, the index α becomes negative, and the index γ positive, i.e. the second type of the critical behavior with the critical slope $K_c = 0$ is realized. The inverse adiabatic and isodynamic susceptibilities, as well as the quantities $\left(\frac{\partial T}{\partial M}\right)_S$ and $\left(\frac{\partial T}{\partial M}\right)_H$, approach zero at the critical point, with the thermal stability coefficients $\left(\frac{\partial T}{\partial S}\right)_M$ and $\left(\frac{\partial T}{\partial S}\right)_H$ being finite. If $y = 1$, the critical indices are $\alpha = 0$, $\beta = \frac{1}{8}$, and $\gamma = \frac{7}{4}$, which coincides with the results for the two-dimensional Ising model [10] and corresponds to the fourth type of the critical behavior with $K_c = 0$. Provided $0 \leq y < 1$ ($0 \leq \mu < \frac{\pi}{2}$), the index α becomes positive, and $\alpha < \gamma$, so that the fourth type of the critical behavior with the critical slope $K_c = 0$ is realized. At $y = 0$, the values of the indices are $\alpha = \frac{2}{3}$, $\beta = \frac{1}{12}$, and $\gamma = \frac{4}{3}$, which coincide with the critical indices in the three-spin model [8]. The fourth type of the critical behavior with $K_c = 0$ is also realized in this case.

For the “electric” Ashkin–Teller model, the ASCs look like $\left(\frac{\partial T}{\partial S}\right)_P \sim t^{\frac{2-2y}{3-2y}}$ and $\left(\frac{\partial E}{\partial P}\right)_S \sim t^{\frac{7-4y}{6-4y}}$. At the interaction parameter values $1 < y < \frac{4}{3}$ which correspond to $\frac{\pi}{2} \leq \mu < \frac{2\pi}{3}$, the second type of the critical behavior, in the same manner as in the previous case, is realized. At $0 \leq y < 1$ ($0 \leq \mu < \frac{\pi}{2}$), the inequality $\alpha < \gamma$ always holds true, and the fourth type of the critical behavior with the critical slope $K_c = 0$ is realized. The

case $y = 0$ corresponds to the three-spin model, as it was before.

7. Conclusions

Thus, in this work, the research of the thermodynamic stability of the Baxter, three-spin, Ashkin–Teller, and Potts models has been carried out for the first time, making use of the method developed in works [2,3]. The asymptotic expressions for the complete set of stability characteristics have been found, and the reasons for the universality hypothesis to be violated in some of those models have been revealed.

The Baxter model can realize the second or fourth type of the critical behavior, with the fourth type being presented by three opportunities with three different critical slopes of the phase equilibrium line. The origin of the universality hypothesis violation lies in the fact that each of the indicated types of the critical behavior (the second type, the second and fourth types with $K_c = 0$, the fourth type with $0 < K_c < \infty$, and the fourth type with $K_c = \infty$) is connected with a certain value or a continuous range of values of the interaction parameter μ . From this point of view, the particular cases of the eight-vertex models, where the universality hypothesis is not valid, are the Lieb model ($\mu = 0$) – in which the universality hypothesis is fulfilled, but the scaling law hypothesis is not [11] – and the Ising ($\mu = \frac{\pi}{2}$) and the three-spin model ($\mu = \frac{3\pi}{4}$) – in which both hypotheses are valid. The Ashkin–Teller model, as well as the Baxter one, violates the universality hypothesis; and the second and fourth types, respectively, of the critical behavior prove true for them.

It is interesting to note that the analysis of experimental data carried out for ferroelectrics and ferromagnets revealed that the second and fourth types of the critical behavior are also realized in real crystals, and this circumstance agrees well with the obtained theoretical results.

To summarize, the demonstrated analysis of the critical properties of exactly solvable two-dimensional statistical models is a beautiful illustration of the thermodynamic method applied for studying the critical state [2,3]. The violation of the universality hypothesis, i.e. the dependence of the critical indices on the interaction parameter, has the fundamental origin, namely, a variety of manifestations of the critical

state nature which were obtained while considering the conditions of its stability. It is essential to emphasize once more that the thermodynamic method concerned [2,3] is based on the first principles only and uses no hypotheses.

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ТЕРМОДИНАМІКА МОДЕЛЕЙ З ПОРУШЕННЯМ ГІПОТЕЗИ УНІВЕРСАЛЬНОСТІ

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Резюме

Розглядаються критичні властивості деяких двовимірних точно розв'язуваних моделей статистичної механіки, таких, як восьмивершинна модель Бекстера, триспінова модель, модель Поттса і модель Ешкіна–Теллера. Досліджено поведінку повного комплексу характеристик стійкості цих моделей в околі критичної точки і встановлено типи критичної поведінки. Пояснено порушення гіпотези універсальності в моделях Бекстера і Ешкіна–Теллера.