FIRST-ORDER PHASE TRANSITIONS IN FINITE SYSTEMS II: WEAK BOUNDARY CONDITIONS

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Summary We continue in our brief review of rigorous results on the finite-size effects near first-order phase transitions with a two-phase coexistence. We again consider the large class of statistical mechanical models in (hyper)cubic volumes and at low temperatures that can be analyzed with the help of the Pirogov-Sinai theory. This time, however, we consider a more realistic case of weak fixed boundary conditions. A universal behavior of the asymptotic smoothing of the phase transition discontinuities as well as the determination of the transition point from the finite-size data is presented.

Abstrakt Pokračujeme v našom krátkom prehľade rigoróznych výsledkov o efektoch konečného objemu blízko fázových prechodov prvého druhu s koexistenciou dvoch fáz. Opäť uvažujeme veľkú triedu modelov štatistickej mechaniky v (hyper)kubických objemoch a pri nízkych teplotách, ktoré sa dajú analyzovať pomocou Pirogovej-Sinajovej teórie. Avšak tentoraz uvažujeme realistickejší prípad slabých okrajových podmienok. Je uvedené univerzálne chovanie asymptotického vyhladenia nespojitostí fázových prechodov ako aj určenie bodu prechodu z konečnoobjemových dát.

1. INTRODUCTION

First-order phase transitions are characterized by discontinuities of extensive macroscopic observables (like the internal energy or magnetization) in the thermodynamic limit when the size of the system tends to infinity. Nevertheless, in real, finite systems the jumps are smoothed out and, possibly, shifted with respect to the infinite-volume transition point. In this paper we briefly discuss the rigorous results obtained in Ref. [1] on these finite-size effect for d-dimensional cubic systems of size L^d, where $d\geq 2$. Instead of the general coexistence of several phases studied in Ref. [1], we will restrict ourselves to the case of just two coexisting phases.

The details of the finite-size effects depend crucially on the choice of the boundary conditions that, in turn, depend on the considered physical situation. The simplest case are periodic boundary conditions. However, free boundary conditions, constant boundary conditions, and, more generally, boundary conditions with boundary fields are physically more realistic, although more difficult to analyze. Yet, in the case of fixed constant boundary conditions, where it is necessary to examine the balancing effect of the boundary conditions versus the opposite driving force (like an external magnetic field), the rigorous analysis has been carried out by Borgs and Kotecký.[1] Still, they had to assume the boundary conditions to be sufficiently weak ("close" to the free boundary conditions). It is this case of boundary conditions that we will be considering in this short survey.

The analysis from Ref. [1] is based on the Pirogov-Sinai theory[2,3] of first-order phase transitions, and the results are therefore applicable to all the models tractable by the theory. The models include, in particular, spin lattice models with a finite number of ground states and finite-range interactions (such as the Ising model) at sufficiently low temperatures and the q-state Potts models with q sufficiently large. An important feature of the analysis is that it can deal with both the field- as well as temperature-driven phase transitions within the same framework. Here we will have in mind the former case. An instance of a temperature-driven transition was investigated in Ref. [4].

In the next secion we will present and discuss the results on the finite-size effects from Ref. [1]. The paper is closed with several concluding remarks in Section 3.

2. SURVEY OF RESULTS

Let us consider the Pirogov-Sinai type of a statistical mechanical model, that is, a model whose partition function is equivalent to that of a hard-core gas of boundaries, called contours, that separate the model's ground states (this covers a remarkably large class of models), see the Introduction and Ref. [5] for more details. The system is confined to a d-dimensional cube of side L and is allowed to interact with its surroundings in such a way that this interaction does not strongly prefer any of the ground states inside the cube ("weak" boundary conditions).[1][1]

The model is assumed to have two ground states with the degeneracies $n_1, n_2 \geq 1$ and with the energies E_L^1 and E_L^2, respectively. The energies are smooth functions of a parameter h (say, an external magnetic field), and it is possible to write bulk-surface expansions for them (at least for large L). Namely, there are the bulk energy densities

[1] Mostly, this requirement means that the strength of the boundary interactions is small enough compared to the strength of the bulk interactions (the boundary conditions are close to the free ones), but it may not be quite so.[4]

$e_i(h)$, i=1,2, of the two ground states and their surface energy densities $s_i(h)$ such that

$$E_L^i(h) = e_i(h)L^d + s_i(h)L^{d-1} + O(L^{d-2}), \quad (1)$$

where the symbol $O(x)$ stands here and below for an error term that can be bounded by x with the constant depending only on the dimension d (the bounds are uniform in β, L, and h).

Whenever the presence of the contours is energetically sufficiently unfavorable (the Peierls condition[5]), that is, whenever the temperature is low enough, each ground state gives rise to a single phase with a structure very similar to the structure of this ground state. Therefore, assuming the inverse temperature $\beta = \dfrac{1}{k_B T}$ and L sufficiently large, the partition function of the system can be expressed as[1]

$$Z_L(h) = n_1 e^{-\beta F_L^1(h)} + n_2 e^{-\beta F_L^2(h)}. \quad (2)$$

Here F_L^1 and F_L^2 are some "meta-stable" finite-volume free energies smooth in h that, by construction, only little deviate from the corresponding ground-state energies E_L^1 and E_L^2 in the sense that they possess the same kind of a bulk-surface expansion as in Eq. (1),

$$F_L^i(h) = f_i(h)L^d + \tau_i(h)L^{d-1} + O(L^{d-2}), \quad (3)$$

The bulk and the surface "meta-stable" free energy densities satisfy

$$f_i(h) = e_i(h) + O(e^{-const\,\beta}), \quad (4)$$

$$\tau_i(h) = s_i(h) + O(e^{-const\,\beta}) \quad (5)$$

(the error terms $O(e^{-const\,\beta})$ can be explicitly evaluated), and similar relations hold for their derivatives. In addition, the true specific free energy of the model $f(h) \equiv -\dfrac{1}{\beta}\lim_{L\to\infty}\dfrac{1}{L^d}\ln Z_L(h)$ exists and $f(h) = \min\{f_1(h), f_2(h)\}$.

Eqs. (2) to (4) provide a detailed control over the partition function $Z_L(h)$. Notice that the presence of the system's boundary is the main difference with respect to the periodic boundary conditions case: it implies the presence of surface terms in F_L^i (for periodic boundary conditions one simply has[5,6] $F_L^i = f_i L^d + O(e^{-const\,\beta L})$). As a consequence, the degeneracies n_i, i=1,2, are essentially insignificant since they can be absorbed in F_L^i, changing it only by $\dfrac{1}{\beta}\log n_i = O(1)$.

Of course, all the infinite-volume properties of the system are independent of the imposed boundary conditions and remain the same as for periodic boundary conditions.[5] Thus, if there exists a unique point h_0 at which $e_1(h)$ and $e_2(h)$ coincide and the label i=1,2 is chosen in such a way that, say,

$$\frac{\partial}{\partial h}(e_1 - e_2) < 0, \quad (6)$$

there exists a unique point h_t at which $f_1(h)$ and $f_2(h)$ coincide, and $f(h) = f_1(h)$ for $h \geq h_t$, while $f(h) = f_2(h)$ for $h \leq h_t$. Moreover,

$$\frac{\partial}{\partial h}(f_1 - f_2)(h_t) < 0. \quad (7)$$

In other words, h_t is the infinite-volume transition point, and, by Eq. (4), one has $h_t = h_0 + O(e^{-const\,\beta})$ (the error term can be explicitly evaluated).

On the other hand, the behavior of finite-volume quantities is, in a way, quite different. Indeed, let us introduce

$$m_L(h) \equiv \frac{1}{\beta L^d}\frac{\partial}{\partial h}\ln Z_L(h), \quad \chi_L(h) \equiv \frac{1}{\beta}\frac{\partial m_L(h)}{\partial h}, \quad (8)$$

the quantities that represent the first and the second derivative of the finite-volume free energy (such as the specific magnetization and the specific susceptibility of a finite magnetic system). Moreover, let us define the universal (independent of boundary conditions) numbers

$$m_1 \equiv -\frac{\partial f(h_t^+)}{\partial h}, m_2 \equiv -\frac{\partial f(h_t^-)}{\partial h},$$

$$\chi_1 \equiv -\frac{\partial^2 f(h_t^+)}{\partial h^2}, \text{ and } \chi_2 \equiv -\frac{\partial^2 f(h_t^-)}{\partial h^2}.$$

Then the following is true.[1] There is a unique point $h_{\max}(L)$ at which χ_L attains its maximum, and

$$h_{\max}(L) = h_t + \frac{\Delta F_L}{(m_1 - m_2)\beta L^d}[1 + O(L^{-1})]$$

$$+ \frac{\ln\frac{n_2}{n_1}}{(m_1 - m_2)\beta L^d} + \frac{6(\chi_1 - \chi_2)}{(m_1 - m_2)^3 \beta^2 L^{2d}} + O(L^{-3d}), \tag{9}$$

where $\Delta F_L \equiv F_L^1(h_t) - F_L^2(h_t)$. It is the second term on the right-hand side that makes $h_{\max}(L)$ to be different from the periodic boundary condition case, where it is not present.[5] Since $f_1(h_t) = f_2(h_t)$, we have $\Delta F_L = O(L^{d-1})$, and the shift $h_{\max}(L) - h_t$ is of the order L^{-1}. Explicitly,

$$h_{\max}(L) = h_t + \frac{2d\Delta\tau}{(m_1 - m_2)\beta L}[1 + O(L^{-1})], \tag{10}$$

where $\Delta\tau \equiv \tau_1(h_t) - \tau_2(h_t)$ plays the role of a "surface tension" between the two coexisting phases and is usually (for asymmetric models) non-zero. The last two equations enables us to trace the position of the transition point h_t, if finite-size data are given.

In addition, if h is in the interval $|h - h_t| \le \frac{C}{L}$ (the value of the constant C is not essential, just the fact that $h_{\max}(L)$ lies in this interval), then $m_L(h)$ *smoothly* interpolates between the values m_1 and m_2, the interpolation being given by the function tanh, whereas $\chi_L(h)$ has the shape of a spike approximated by the function $\cosh^{-2}$,

$$m_L(h) = \frac{m_1 + m_2}{2} + \frac{m_1 - m_2}{2} \times \tanh[\beta \frac{m_1 - m_2}{2}(h - h_{\max}(L))L^d] + O(L^{-1}), \tag{11}$$

$$\chi_L(h) = (\frac{m_1 - m_2}{2})^2 L^d \times \cosh^{-2}[\beta \frac{m_1 - m_2}{2}(h - h_{\max}(L))L^d] + O(L^{d-1}). \tag{12}$$

The width of rounding of m_L between m_1 to m_2 is of the order L^{-d}, implying that the slope of m_L in this region, that is, the height of the spike exhibited by χ_L, is of the order L^d. This enormous height of χ_L is a result of the presence of the phase transition (one would expect a height of the order[5] $O(1)$).

From Eqs. (9) to (12) we see that the role of the weak boundary conditions is practically limited to the position of the point $h_{\max}(L)$. Thus, a different choice of weak boundary conditions results in a possible move of the functions $m_L(h)$ and $\chi_L(h)$, but their tanh and $\cosh^{-2}$ profiles remain basically unchanged.

Finally, if $|h - h_t| \ge \frac{C}{L}$, then m_L and χ_L are very well approximated by their infinite-volume limits,

$$m_L(h) = -\frac{\partial f(h)}{\partial h} + O(e^{-const\,\beta L}), \tag{13}$$

$$\chi_L(h) = -\frac{\partial^2 f(h)}{\partial h^2} + O(e^{-const\,\beta L}). \tag{14}$$

as in the periodic boundary condition case. Fig. 1 depicts schematically the results contained in Eqs. (9) to (14).

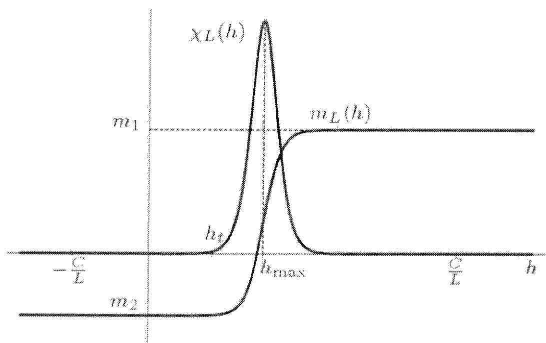

Fig. 1 An infinite-volume observable 1_∞ that is the first derivative of a thermodynamic potential exhibits a jump between m_1 and m_2. However, the jump is smoothed out in its finite-volume version 1. The second derivative of a thermodynamic potential 2 has the shape of a spike in a finite volume, while it has a singularity of the d-function type (not shown). Its maximum position $h_{\max}$ is in general shifted with respect to the infinite-volume transition point h_t.

3. CONCLUDING REMARKS

In this paper we gave a short survey of the rigorous results obtained in Ref. [1] on the finite-size effect near first-order phase transitions for d-dimensional cubic systems with weak boundary conditions. The situation of a field-driven transition with a two-phase coexistence was discussed. We took into account possible degeneracies n_1 and n_2 of the two ground states ($n_1 = n_2 = 1$ in Ref. [1] so that the terms containing $\ln \frac{n_1}{n_2}$ are all equal to zero there). We compared this situation with the case of periodic boundary conditions[5] and demonstrated that the main difference between the rounding of finite-volume observables in the two cases was in the position of the rounding with respect to the infinite-volume transition point. The shift is of the order L^{-1} in the case of weak boundary conditions, while it is only L^{-d} (or L^{-2d} if $n_1 = n_2$) in the case of periodic boundary conditions. For both types of boundary conditions the first derivatives of a thermodynamic potential were in finite volume smoothed out according to the function tanh. The profiles of higher-order derivatives are determined by the corresponding higher-order derivatives of tanh (that is, $\cosh^{-2}$ for the second order, etc.).

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