Referee report on the PhD Dissertation

Scaling properties of phase transitions above the upper critical dimension and the description of DNA denaturation

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The dissertation presents author's results, obtained in collaboration with his advisers, in studying scaling properties of relevant thermodynamic parameters describing critical points of two models: the Ising ferromagnetic model and the DNA denaturation model taken in the form of the Poland-Scheraga model. It consists of four chapters followed by the bibliography comprising 136 items, and by three appendices presenting author's own publications (two published and one accepted journal papers), the list of scientific meetings and similar events where the results were reported, and some basics on Wolff's algorithm used in the work, respectively. The total volume is 109 pages. The dissertation is wtitten in a form standard for such works, the language is mostly correct and understandable, the research tasks and the basics on the starting points of the reseach are explained quite clearly. In my opinion, the subject of the presented research is sufficiently actual and serious that allows one to evaluate the professional level of the author and thus to make a reliable conclusion concerning his correspondence to the degree sought. The aprobation of the results in the form of publications and conference/seminar talks is sufficient. Now let us pass to a more detailed discussion of the work.

It is believed that, for $d < 4$, the critical point properties of the standard nearest-neighbour Ising model on the simple cubic lattice $\mathbb{Z}^d$ essentially differ from those for $d \geq 4$. In view of this, the value $d_c = 4$ is called upper critical dimension. In the dissertation, the author studies these properties numerically in the case $d = 5$ with the help of Wolff's similation technique by applying the Finite-Size-Scaling (FSS) method. The latter means that one simulates the thermodynamic states of a finite portion of spins, the linear size of which is L, subject to certian fixed boundary conditions. Then the divergence/vanishing of the quantities of interest at the critical point is expected to be in the form L^α, $\alpha \in \mathbb{R}$, with the exponents α being the main quantities to be evaluated. The key assumption behind this approach is that, at the citical point, the infinite-volume correlation length ξ diverges, whereas for finite L it behaves as $\xi \sim L^q$ with q possibly different from one. Namely, in the dissertation it is claimed that $q = 1$ for $d \leq d_c$, and $q > 1$ otherwise. The latter possibility corresponds to the so called Q-FSS. In the second chapter, the author presents the results of the mentioned simulations subject to the free boundary conditions, according to which the spins interact only with their neighbours in the bulk, below called *the principal domain*. The similations are carried out in the 'magnetic and 'temperature' sectors, that is, first one fixes $T = T_C$ and varies the values of the external magnetic field h, and then fixes $h = 0$ and varies $T - T_C$. As a result, critical exponents and the corresponding numerical amplitudes for the mean magnetization, the isotermal susceptibility, the internal energy, the heat capacity and some similar parameters are found and discussed. The latter is done in the last section of the second chapter. Here one should positively notice the author's conclusion as to the nature of the scaling, i.e., where it corresponds to the Gaussian type with $q = 1$, or to the Q-FSS with $q > 1$. At the same time, I would welcome a more profound analysis of the whole mass of the results presented in this chapter and their importance for better understanding the nature of the criticality in the studied model.

The third chapter is dedicated to an 'improved' version of the technique developed and used in the preceding chapter, as well as to studying the distribution of the Lee-Yang zeroes of the partition function of the same model at the critical point. The mentioned improvement is related to the fact that the bounded principal domain with the free boundary discussed above in not translation invariant, whereas the infinite volume thermodynamic state at the critical point possesses this symmetry. By taking the periodic boundary condition, one may regain the mentioned invariance for a finite-size system. Similarly as in the infinite volume limit, in this case the total magnetization observable M is just the zero-mode term of the Fourier transform of S_x, $x \in \mathbb{Z}^d$. At the same time, for the bounded principal domain with the free boundary M is the sum of many modes. The key idea of the research under discussion, based on findings known from the literature, is that most of the modes are irrelevant in the vicinity of the critical point and thus may be neglacted. This might essentially reduce the time of calculations of the therodynamic parameters corresponding to the free boundary condition and thereby to study bigger values of L. At this point, I should note that the expressions in eqs. (3.16)–(3.17), page 63, are a bit confusing for me. Here I would expect an explicit description of the considered finite subset of the lattice $\mathbb{Z}^d$ (principal domain) and the corresponding Brilluene zone where the wave vectors are taken from. As mentioned above, along with studying the scaling properties of the magnetization, in this section the author turns to the alocation of the Lee-Yang zeroes. More precisely, it is known that the zeroes of the partition function in the complex plane of values of the external magnetic field h lie on the imaginary axes, and that the gap between the two closest zeroes above and below the origin vanishes at the critical point. In the FSS approach, this corresponds to vanishing of h_1 as $L \to +\infty$, where ih_1 is the zero in the upper half-line closest to the origin. Therefore, in this approach one sets $h_1 \sim L^{-\alpha}$ with $\alpha > 0$ to be evaluated from the simulations, which is done in the mentioned section. Here I found rather incomplete the expessions in eqs. (1.24), page 30, and (3.22), page 68, as it is not indicated what is z and $z_j(L)$ in these formulas. Also one would expect to find here a more extended analysis of the results of this chapter, including of those related to the Lee-Yang zeroes.

The fourth chapter of the dissertation is dedicated to studying the scaling exponents describing the critical point of a complex polymer network that occurs in the DNA thermal denaturation based on the Poland-Scheraga model. Here the author expresses the relavant loop closure exponents through the network exponents. For the latters, ε-expansion results were obtained in papers by Y. Holovatch and co-authors, which then allows the author for obtaining the corresponding expansions also for the mentioned loop closure exponents. After a suitable resummation and setting $\varepsilon = 1$, he thus obtains numerical values of these exponents. Some arguments towards taking into account environmental effects are also employed. The chapter is concluded by comparison of the calculated values with their analogies corresponding to $d = 2$ case. The concluding chapter contains a brief summary of the results obtained in the dissertation.

The dissertation downsides which I decided to mention here may be divided into two types. Those of the first type are rather stylistic, which includes not so numerous typos and uncear parts of the description – both in words and formulas. Among the latters one may name the expression for the partition function $Z_L(h)$ in eq. (1.24) on page 30, where z should be precisely connected with h. I guess it should be $z = e^h$ with an explicit formula for A. Also, in the description of the macromolecules in the capture to Fig. 1.2, page 35, the author mentions points V1, V3, which are not depicted. One may only guess as to the form of the subset of the lattice $\mathbb{Z}^d$ – the principal domain – which is taken in the simulations. Presumably, it is the cube L^d, but this ought to be explicitly stated. I also had problems with understanding formulas (4.26) – (4.27) on page 77. The downsides of the second type characterize the way of presenting the key points of the study. For instance, it is not explained why the author takes the free boundary and the cubic principal domain. Why not to take the periodic boundary condition, which is translation invariant? In that case, one would avoid taking into account multiple Fourier modes in the magnetization M. Another possibility to mitigate the boundary effects could be to take a ball (it has a smaller bound) as the principal domain. Last but not least, one might expect to find in the dissertation how the numerical results obtained herein by means of advanced massive computations contribute to our understanding critical phenomena. Here I should mention, however, that my general impression from reading the dissertation is fully positive, and the criticism expressed in this report is just the usual component of the documents of this type.

To summarize, I claim that the dissertation presents a valuable and reliable research performed by sophisticated methods of modern statistical physics, which undoubtedly shows that **its author Y. I. M. Honchar fully deserves the doctor of philosophy degree in physics**.

Lublin, February 5, 2024 prof. dr hab. Jurij Kozicki