Self-Duality and Statistical Systems without Internal Energy Scaling Terms at Criticality

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It is argued that self-duality of one system leads to the zero finite-size scaling amplitude of the critical internal energy for all system belonging to the same universality class. For such models, we may expect that condition of equality (up to correction-to-scaling terms) of the internal energies for systems with different sizes will yield more accurate estimates for the critical temperature than the scaling equation for the inverse correlation lengths which is used in the standard phenomenological renormalization-group approach. Analytical and numerical evidences confirming the above conjecture are given for examples of two-dimensional next-nearest-neighbour and spin-1 Ising lattices.

Renormalization-group (RG) theory predicts a general structure of different physical quantities in the vicinity of a phase transition (and references therein): regular part plus scaling terms (resulting from relevant fields) and plus corrections to scaling (connecting with a presence of irrelevant operators, nonlinear scaling fields, etc.). For instance, the inverse correlation length of subsystem with a characteristic linear size \( L \) varies at the bulk phase transition point as

\[
\kappa_L(K_c) = L^{-1}(A_\kappa + aL^{-\omega} + \ldots),
\]

where \( A_\kappa \) is the finite-size scaling (FSS) amplitude of inverse correlation length; \( \omega \) and \( a \) are the correction-to-scaling critical exponent and amplitude, respectively. Taking two subsystems with sizes \( L \) and \( L' \) \( [i.\ e. a\ pair\ (L, L')] \) and neglecting the terms of order \( O(L^{-\omega-1}) \) in eq. (1), one obtains the equation

\[
L\kappa_L(K_c) = L'\kappa_{L'}(K_c),
\]

which serves for estimating \( K_c \) in the phenomenological RG approach [2].

Similarly, the internal energy is written as

\[
u_L(K_c) = u_\infty + L^{-d+1/\nu}(A_u + bL^{-\omega} + \ldots),
\]

where \( d \) is the space dimensionality and \( \nu \) is the correlation-length critical exponent.

For the derivative of inverse correlation length \( \dot{\kappa}_L \equiv \partial\kappa_L/\partial K \) we have

\[
\dot{\kappa}_L(K_c) = L^{-1+1/\nu}(A_\kappa + cL^{-\omega} + \ldots).
\]

From this expansion with an accuracy up to terms of order \( O(L^{-\omega-1+1/\nu}) \), follows the equation

\[
L^{1-1/\nu}\dot{\kappa}_L(K_c) = (L')^{1-1/\nu}\dot{\kappa}_{L'}(K_c).
\]

As shown by Privman and Fisher [3], certain ratios of critical FSS amplitudes are universal quantities. In particular, the ratio \( A_u/A_\kappa \) is universal.

Self-duality relation (itself or in combination with the star-triangle transformation) connects between themselves the values of a partition function by high and low temperatures [4,5]. For example, for Ising model on the isotropic square lattice in the form of \( L \times \infty \) strip with periodic boundary conditions in the transverse direction one has

\[
\lambda_1^{(L)}(K^*) = (\sinh 2K)^{-L}\lambda_1^{(L)}(K).
\]

Here \( \lambda_1^{(L)} \) is the largest eigenvalue of a transfer matrix; note that \( \lambda_1^{(L)} \) equals the partition function of a strip per slice. The dually conjugated value \( K^* \) is connected with the original value \( K \) by the relation

\[
\sinh 2K^* \sinh 2K = 1.
\]
Since the internal energy is a derivative of the free energy \( U_L = \frac{\partial f_L}{\partial K} \) and the free energy per site is equal to \( f_L = L^{-1} \ln \lambda_1(L) \), then one obtains from eqs. (6) and (7) that at the critical point \( K^* = K = K_c \)

\[ u_L(K_c) = u_\infty. \]  

That is, due to self-duality of Ising model on a strip, both the critical FSS amplitude and all correction-to-FSS ones are zero \( (A_\mu = 0 \text{ and all } a = 0) \). This is valid also for other isotropic statistical systems which are invariant under the duality transformations.

As \( A_\mu / A_k \) is the universal quantity, the equality of the amplitude \( A_\mu \) to zero automatically means the absence of the leading finite-size term in the internal energy for all systems (of the same form and with the same boundary conditions) entering to the universality class of the self-dual system. In such a case, neglecting the terms of order \( O(L^{-\nu + d + 1/\nu}) \) in the expansion we come to the equation

\[ u_L(K_c) = u_L'(K_c). \]  

One can expect that this equation will yield estimates of \( K_c \) with high accuracy for different systems in the universality class of which there is a self-dual model.

Using the exact solution for the two-dimensional square Ising lattice, one can establish that in the isotropic case the dependent-L part is absolutely absent not only in the internal energy (what was shown above from duality relation) but also in the temperature derivative of the inverse correlation length:

\[ \kappa_L(K_c) = \text{const upon } L. \]  

Therefore the finite-size equation

\[ \kappa_L(K_c) = \kappa_L'(K_c) \]  

yields the exact value of \( K_c \) for the infinite square Ising lattice from solutions for the strips \( L \times \infty \) of finite widths starting with the pair \( (1,2) \). Moreover, the requirement of agreement of eq. (11) with the scaling relation leads in this model to the exact value for the correlation-length critical exponent: \( \nu = 1 \). Therefore, in the Ising model under discussion

\[ \kappa_L(K_c) = A_k \cdot L^0 \]  

with \( A_k = -2 \). Consequently, in this model all corrections to FSS behaviour in the inverse correlation length derivative \( \kappa_L(K_c) \) are completely compressed.

Let us discuss now the key question, namely the convergence rate of estimates \( K_c \) which follow from eqs. (8) and (11). Take, for instance, models belonging to the two-dimensional Ising universality class.

At first consider the NNN model, i. e. a square Ising lattice with couplings both nearest neighbours (interaction constant is \( J_{NN} \)) and next-nearest neighbours (interaction constant is \( J_{NNN} \)). Estimates of \( K_c \) for this model are done in table 1 within the framework of phenomenological RG approximation with using the eq. (4). For the double \( (L = 2) \) and triple \( (L = 3) \) Ising strips with \( NN \) and \( NNN \) couplings, solutions exist in an exact analytical form. Therefore, we used analytical formulas for the internal energy densities and derivatives of inverse correlation lengths in the case of a pair \((2,3)\). Unfortunately, we should restrict ourselves only by numerical calculations for the strips of larger widths \( L \). The results obtained are collected in table 1 (\( J_{NNN}/J_{NN} = 1 \)) and in table 2 (\( J_{NNN}/J_{NN} = -1/4 \)).

From these tables it is seen that approximate

| \( (L, L + 1) \) | eq.(2) | eq.(9) | eq.(11) |
|----------------|-------|-------|-------|
| (2,3)          | 0.195084 | 0.191796 | 0.194076 |
| (3,4)          | 0.192511 | 0.191193 |       |
| (4,5)          | 0.191374 | 0.190596 |       |
| (5,6)          | 0.190883 | 0.190410 |       |
| (6,7)          | 0.190628 | 0.190217 |       |
| (7,8)          | 0.190484 | 0.190269 |       |
| (8,9)          | 0.190397 | 0.190243 |       |
| \( \infty \)   | 0.19019269(5) |       |       |
Table 2
Estimates of $K_c$ for the 2D NNN Ising lattice by $J_{NNN}/J_{NN} = -1/4$

| $(L, L + 1)$ | eq.(2)  | eq.(9)  | eq.(11) |
|--------------|---------|---------|---------|
| (2, 3)       | 0.628082| 0.687193| 0.684975|
| (3, 4)       | 0.643618| 0.694006|          |
| (4, 5)       | 0.663507| 0.696592|          |
| (5, 6)       | 0.677302| 0.697329|          |
| (6, 7)       | 0.685553| 0.697448|          |
| (7, 8)       | 0.690221| 0.697411|          |
| (8, 9)       | 0.692834| 0.697357|          |
| $\infty$    | 0.697220(5) |        |         |

Values of $K_c$ yielding by eqs. (2), (9) and (11) are upper estimates by $J_{NNN}/J_{NN} = 1$ while by $J_{NNN}/J_{NN} = -1/4$ those are lower ones. By this, the accuracy of estimates following from eqs. (2) and (11) is higher than that given by eq. (2). In turn, from the two best approximations the estimates of $K_c$ which are ensured from the internal energy equation have the highest accuracy. It is important that the exactness of those estimates by fixed sizes of subsystems in a pair $(L, L + 1)$ is higher than that which gives eq. (2) by bigger subsystem sizes, i.e. by larger transfer-matrix orders. For instance, by $J_{NNN}/J_{NN} = 1$ the estimate following from eq. (2) with a pair (2, 3) is better in comparison with the estimate which yields eq. (2) with the larger pair (3, 4). For the next pair (4, 5) the improvement is much larger.

The second model which we will discuss in the given report is the square Ising lattice with NN couplings only but with the spin $S = 1$ (in the previous model the spin was equal to $S = \frac{1}{2}$). Estimates of $K_c$ obtained for such a model within the ordinary phenomenological RG, i.e. from eq. (4), are available in [1]. In table 3 we reproduce these estimates together with those which we obtained by solving eq. (11). From the table one can see that estimates are lower in both cases. By this, higher accuracy is given again by the equation identifying the critical internal energies of subsystems with different linear sizes.

Thus, using in fact only the qualitative information that in the given universality class there is a self-dual system, we can choose more effective strategy by utilizing the subsystem solutions which always are restricted by some maximal size $L_{\text{max}}$.

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