Improved Transfer-Matrix Schemes of Phenomenological Renormalization

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Different phenomenological RG transformations based on scaling relations for the derivatives of the inverse correlation length and singular part of the free-energy density are considered. These transformations are tested on the 2D square Ising and Potts models as well as on the 3D simple-cubic Ising model. Variants of RG equations yielding more accurate results than Nightingale’s RG scheme are obtained. In the 2D case the finite-size equations which give the exact values of the critical point or the critical exponent are found.

1. Introduction

The phenomenological renormalization-group (RG) method is a powerful tool for the investigation of critical phenomena. As it is known, phenomenological RG can be constructed by using not just the correlation length as it is done in Nightingale’s approach, but using any other quantity with a power-law divergence at criticality. Binder suggested a phenomenological renormalization scheme by using the order-parameter moments (cumulants) which are, on the one hand, related to the higher susceptibilities and, on the other hand, immediately suitable for the Monte Carlo simulations. Recently Itakura extended Binder’s cumulant crossing method taking linear combination of several different reduced moments.

In this report, I discuss various RG transformations which follow from general scaling functional equations. These equations are evaluated in terms of the eigenvalues and eigenvectors of the transfer matrices. By large transverse sizes of partly finite subsystems, all those transformations must yield the same results. However, for the small sizes which normally are used in practice, different RG equations lead to estimates with distinct accuracies. My aim is to find the best strategies of a phenomenological renormalization group method. This is especially important for 3D systems.

2. Phenomenological RG Equations

Let us write the finite-size scaling equations for the derivatives of the inverse correlation length $\kappa_L$ and the singular part of the reduced free-energy density $f_L^s$:

$$\kappa_L^{(m,n)}(t, h) = b^{my_t + ny_h - 1}\kappa_L^{(m,n)}(t', h'),$$  \hspace{1cm} (1)

$$f_L^s(m,n)(t, h) = b^{my_t + ny_h - d}f_L^s(m,n)(t', h'),$$  \hspace{1cm} (2)

where $z^{(m,n)}(x, y) = \partial^{m+n}z/\partial x^m\partial y^n$ (z is $\kappa_L$ or $f_L^s$), $t = K - K_c$ is the deviation from critical coupling, $h$ is a normalized external field, $y_t$ and $y_h$ are, respectively, thermal and magnetic critical exponents of the system, $d$ is the space dimensionality, $L$ is a characteristic size of a subsystem and $b = L/L'$ is the rescaling factor.

In the phenomenological approach proposed by Nightingale, eq. (1) with $m = n = 0$ is combined with the ordinary expression for the inverse correlation length $\kappa_L = \ln(\lambda_1^{(L)}/\lambda_2^{(L)})$, in which $\lambda_1^{(L)}$ and $\lambda_2^{(L)}$ are the largest and second-largest eigenvalues, respectively, of the associated
transfer matrix. In the absence of a symmetry breaking field, the critical coupling \( K_c \) is estimated from the equation

\[
L \kappa_L(K_c) = (L - 1) \kappa_{L-1}(K_c).
\]

(4)

In writing this equation, one sets \( L' = L - 1 \).

Another possible way to produce a phenomenological renormalization group is obtained by using eq.(2) with \( m = n = 0 \). The fixed point is given by the relation

\[
L^d f^*_{L}(K_c) = (L - 1)^d f^*_{L-1}(K_c).
\]

(5)

The dimensionless free-energy density, \( f_L = f_\infty + f^*_{L} \), of a subsystem \( L^{d-1} \times \infty \) is calculated by the formula

\[
f_L = L^{1-d} \ln \lambda_1^{(L)}
\]

(6)

and the “background” \( f_\infty \) is introduced as an extra parameter.

Besides eqs. (4) and (5), in this paper I also consider the following RG equations (resulting from the relations (1) and (2)):

\[
\kappa_L^{(n)}(L) = \kappa_{L-1}^{(n)}(L) - \frac{d \ln \lambda_1^{(L)}}{(L-1)^d \lambda_1^{(L-1)}} \kappa_c,
\]

(7)

where \( \chi_L^{(n)} = \frac{\partial^2 f_L}{\partial h^2} \big|_{h=0} = f^{(0,2)}_L(K_c) \) is the zero-field susceptibility and \( \chi_L^{(4)} = \frac{\partial^4 f_L}{\partial h^4} \big|_{h=0} = f^{(0,4)}_L(K_c) \) is a nonlinear susceptibility (eq.(3) corresponds to Binder’s phenomenological renormalization group);

\[
L^{2-d} \kappa^{(1)}_L/\chi_L = (L - 1)^{2-d} \kappa^{(1)}_{L-1}/\chi_{L-1}; \quad (8)
\]

\[
L^{1-d} \kappa^{(2)}_L/\chi_L = (L - 1)^{1-d} \kappa^{(2)}_{L-1}/\chi_{L-1}; \quad (9)
\]

\[
L^{1-2d} \kappa^{(4)}_L/\chi_L^2 = (L - 1)^{1-2d} \kappa^{(4)}_{L-1}/\chi_{L-1}^2. \quad (10)
\]

Here, \( \kappa^{(n)}_L = \partial^n \kappa_L/\partial h^n \big|_{h=0} = \kappa^{(n,0)}_L(K_c) \). Expressions for the derivatives of the inverse correlation length and the free energy with respect to \( h \) in terms of eigenvalues and eigenvectors of the transfer matrix are available in [8].

3. Results and discussions

To represent numerical data in tables, eqs.(4), (5), (7), (8), (9) and (10) will be labeled by symbols \( \kappa^{(n)}_L, f^{(0,2)}_L, \chi^{(n)}_L/\chi^2, (\kappa^{(1)}_L)^2/\chi^2, \kappa^{(2)}_L/\chi^2, \kappa^{(3)}_L/\chi^2 \) and \( \kappa^{(4)}_L/\chi^2 \), respectively.

Table 1

| \( (k) \) | \( (\chi^{(4)}/\chi^2) \) | \( (\kappa^{(4)}/\chi^2) \) |
|---|---|---|
| 0.42236 | 0.43088 | -2.23% |
| 0.42593 | 0.43242 | -1.88% |
| 0.42596 | 0.43243 | -1.87% |
| 0.44324 | 0.44168 | +0.23% |
| 0.44105 | 0.44626 |

In table 1, results for the critical coupling in the Ising model on a square lattice are given. The calculations were carried out for strips \( L \times \infty \) with a periodic boundary condition in the transverse direction. The estimates are shown for the pairs \( (L - 1, L) \) with \( L \leq 5 \). In the case of \( (3, 4) \) pairs, the errors are also given. The type of phenomenological RG equations which have been used are indicated in the first column of the table. In this model \( K_c = \frac{1}{\pi} \ln(1 + \sqrt{2}) \) and \( f_\infty = 2G/\pi + \frac{1}{\pi} \ln 2 \) (G is Catalan’s constant) [8].

It is seen from table 1 that the best lower bound is given by eq.(6). Slightly worse results are obtained by Binder’s phenomenological renormalization-group procedure. This approach which is normally implemented by Monte Carlo simulations was used in the transfer-matrix version in [8]. Nightingale’s renormalization (first line in table 1) which is traditionally used by transfer-matrix calculations has only the third position in accuracy among the lower estimates.

I also found the phenomenological RG equations leading to the upper bounds for \( K_c \) (last two lines in table 1). Among these more accurate results are provided by eq.(3). The magnitude of the error in line four of table 1 is the least among all lower and upper estimates of \( K_c \). Unfortunately, such approach requires a knowledge about the background \( f_\infty \).

Transfer-matrix eigenvalues for the Ising strips are known in analytical form [8]. Using this fact I considered the RG transformation [8] which makes use of the first derivative with respect to \( K \) \( (m = 1, n = 0; h = 0) \). For the fixed point this
K lattice are collected in table 2. For this model ν is that in the 2D eq.(1) with m = 1 + 1/√κ.

The data obtained for the 3-state square Potts model the finite-size corrections to the reduced energy density, and L∞ is the singular part of the transformation gives

$$L^{d-ν} u_L(K_c) = (L - 1)^{d-ν} u_{L-1}(K_c),$$

(11)

where u_L = u_L - u∞ is the singular part of the root of eq.(11) is equal to the exact value of Kc since u_L(Kc) ≡ 0 for all L. In other words, all finite-size corrections to the background u∞(= √2/3) are zero.

Moreover, in the 2D Ising model ∂κL/∂K at K = Kc is also independent of L and, therefore, eq.(11) with m = 1 and n = 0 gives the exact value for the critical exponent: ν = 1/γν = 1.

The table obtained for the 3-state square Potts lattice are collected in table 2. For this model Kc = ln(1 + √3) and f∞ = 4G/3π + ln(2 + √3) + 1/3 ln(2 + √3) [3]. Inspecting table 2 it is seen that eqs.(3) and (4) lead to more qualitative estimates than Nightingale’s approach. Again, the lowest absolute error is yielded by the phenomenological RG equation based on fL.

Numerical calculations on strips L × ∞ show us that in the 2D q-state Potts model the finite-size corrections to the background energy, u∞ = 1 + 1/√κ, are also absent and, consequently, the equation

$$u_L(K_c) = u_{L'}(K_c)$$

(12)

yields the exact value of Kc. Note that this equation has been derived earlier from other considerations [3].

Let us discuss now the results presented in table 2 for the 3D Ising model on a simple-cubic lattice. For this model Kc = 0.2216544(3) [10] and f∞ = 0.77790(2) [11]. Renormalizations were done for the L × L × ∞ parallelepipeds with periodic boundary conditions in both transverse directions. As in the 2D case, the best lower values of Kc are obtained from eq.(10).

In the 3D case the amplitudes of the finite-size corrections to the critical-point energy are not equal to zero. As a result, eq.(12) only yields an approximate value of Kc.

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Table 2

| (κ)   | (2, 3) | (3, 4) | (4, 5) |
|-------|--------|--------|--------|
| 0.96248 | 0.98350 | −2.1% | 0.99467 |
| (κ(1/2)/χ) | 0.99311 | 0.99920 | −0.6% | 1.00380 |
| (f*) | 1.00927 | 1.00667 | +0.2% | 1.00565 |

Table 3

| (κ)   | (2, 3) | (3, 4) | (4, 5) |
|-------|--------|--------|--------|
| 0.21340 | 0.21826 | −1.53% |        |
| (κ(4)/χ) | 0.21823 | 0.22002 | −0.74% |        |
| (κ(4)/χ2) | 0.21824 | 0.22006 | −0.72% |        |
| (f*) | 0.22354 | 0.22236 | +0.32% |        |
| (κ(2)/χ) | 0.22658 | 0.22314 | +0.67% |        |