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Numerical renormalization group at criticality

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Abstract

We apply a recently developed numerical renormalization group, the corner-transfer-matrix renormalization group (CTMRG), to 2D classical lattice models at their critical temperatures. It is shown that the combination of CTMRG and the finite-size scaling analysis gives two independent critical exponents.

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The renormalization group is a basic concept in statistical physics [1,2]. The real-space renormalization group (RSRG) has been applied widely to critical phenomena [1,3]. A recent progress in RSRG is the development of the density-matrix renormalization group (DMRG) by White [4,5]. The DMRG was originally formulated for one-dimensional (1D) quantum models, and was shown to be applicable to 2D classical systems as well [6]. Recently, Östlund and Rommer found a variational principle hidden in the DMRG [7]. They showed that the ground state wave function obtained by DMRG has the form of a matrix product [8–10]. This variational background enables us to accelerate the numerical calculation of DMRG [7,11]. Quite recently Martín-Delgado and Sierra have obtained a unified analytic formulation of conventional RSRG and DMRG [12,13].

Baxter established another RSRG for 2D classical systems by using the corner transfer matrix (CTM) [14–16]. His method is known as a natural extension of variational methods, such as Kramers–Wannier approximation [17], Kikuchi's approximation [18], and the cluster variational method [19]. It should be noted that Baxter's method and White's DMRG method have many features in common. In particular, both are RSRG-based on a variational principle. On the basis of this fact, Nishino and Okunishi have formulated a new renormalization group procedure for 2D classical lattice models [20,11], which we will refer to as "corner-transfer-matrix renormalization group" (CTMRG) in the following. It has been confirmed that the CTMRG precisely determines thermodynamic functions of 2D classical systems in the thermodynamic limit. For example, the calculated internal energy of the square-lattice Ising model is -0.70704 at T_c [20], whose numerical precision is comparable to a recent Monte Carlo result [21].

In this Letter, we show that the CTMRG method determines not only the one-point functions, but also critical exponents of 2D classical spin systems. We apply

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CTMRG to finite-size systems at their critical temperatures, and calculate one-point functions at the center of the system. The finite-size corrections to these one-point functions are found to obey the finite-size scaling (FSS) behaviors determined by two independent critical exponents [22,23].

The CTMRG is a numerical method which can evaluate the partition function of finite-size systems. Consider a square cluster of a classical spin system whose linear dimension N is an odd integer. The cluster consists of four sub-clusters of the size $(N+1)/2$, which are named "corners" according to Baxter; The partition function is calculated as the trace of a matrix $\rho_{(N+1)/2} = (A_{(N+1)/2})^4$, where $A_{(N+1)/2}$ is the so-called "corner transfer matrix" (CTM), which transfers column spins into row spins [16]. It, however, is difficult to deal with $A_{(N+1)/2}$ exactly for large N, because the dimension of the matrix increases rapidly with N. *The point of CTMRG is, that the matrix ρ is identical to the density matrix that appears in White's DMRG* [4,5]. This correspondence enables us to transform $A_{(N+1)/2}$ into a renormalized one $\bar{A}_{(N+1)/2}$. We determine the dimension m of the reduced matrix $\bar{A}_{(N+1)/2}$, so that we can deal with $\bar{A}_{(N+1)/2}$ in realistic numerical calculations. By using a recursive relation between $\bar{A}_{(N+1)/2}$ and $\bar{A}_{(N+3)/2}$, we can increase the linear size of the corner one by one, and obtain $\bar{A}_{(N+1)/2}$ from $N = 3$ to ∞ one after another; this recursive procedure corresponds to the "infinite chain method" in DMRG [4,5]. The renormalized CTM $\bar{A}_{(N+1)/2}$ thus obtained gives the approximate partition function as $\bar{Z}_N = \mathrm{Tr}\,\bar{A}_{(N+1)/2}$. Because of the variational nature of the CTMRG, $\bar{Z}_N$ gives a lower-bound for the exact partition function $Z_N = \mathrm{Tr}\,A_{(N+1)/2}$.

The error in the partition function $\delta Z_N \equiv Z_N - \bar{Z}_N$ is related to two characteristic length scales. In what follows, we denote the largest and the second-largest eigenvalues of the row-to-row transfer matrix as $\Lambda_0(N,m)$ and $\Lambda_1(N,m)$ respectively, which can be calculated by CTMRG. The first characteristic scale is the correct *correlation length* ξ_N for a finite system defined as follows:

$$1/\xi_N = \log \frac{\Lambda_0(N,\infty)}{\Lambda_1(N,\infty)}. \tag{1}$$

According to the finite-size scaling theory, $1/\xi_N$ is a decreasing function of N as $\sim 1/N$ at the critical temperature $T = T_c$. The other scale is an *effective* correlation length $\xi(m)$ for finite m in the thermodynamic limit,

$$1/\xi(m) = \log \frac{\Lambda_0(\infty,m)}{\Lambda_1(\infty,m)}. \tag{2}$$

This latter scale appears due to the restriction imposed on the size of the matrix $\bar{A}_{(N+1)/2}$. As long as the condition $\xi_N \ll \xi(m)$ is satisfied, $\bar{Z}_N$ is a good approximation for Z_N. But in the opposite case $\xi_N \gg \xi(m)$, $\bar{Z}_N$ will be appreciably smaller than Z_N. Therefore, we expect to observe crossover from the correct system-size dependence of the partition function to finite-m behavior. For the off-critical case, we can make the condition $\xi_N \ll \xi(m)$ satisfied by taking large enough m [20]. For the critical case, on the other hand, we have to deal with the above crossover properly.

In addition to the partition function, we can also calculate the local energy $E(N)$ and the order parameter $M(N)$ at the center of the square clusters of the linear size N [20]. According to the above discussion on the crossover, we expect that the following two-parameter finite-size scaling form [22,23] holds for these thermodynamic functions at T_c: The N dependence of $E(N)$ is

$$E(N) - E(\infty) = N^{1/\nu-d} f(\xi(m)/N), \tag{3}$$

where ν is one of the critical exponents (the correlation length exponent) and $d = 2$ is the spatial dimensionality. In addition to the leading finite-size scaling form $\sim N^{1/\nu-d}$, we introduced an unknown scaling function f which describes the crossover. The asymptotic form of the scaling function will be $f(x \to 0) \sim x^{-1/\nu+d}$ and $f(x \to \infty) \sim$ const. Similarly, the size dependence of the local order parameter $M(N)$ is expected to be

$$M(N) = N^{-(d-2+\eta)/2} g(\xi(m)/N), \tag{4}$$

with another set of critical exponent η (the anomalous dimension of the spin) and a scaling function g introduced. The asymptotic behavior of g will be $g(x \to 0) \sim x^{(d-2+\eta)/2}$ and $g(x \to \infty) \sim$ const. Assuming these two scaling forms, we can estimate two independent critical exponents ν and η as well as $E(\infty)$ from the data given by the CTMRG.

As examples of the 2D classical lattice models, we deal with the Ising model and the 3-state Potts model

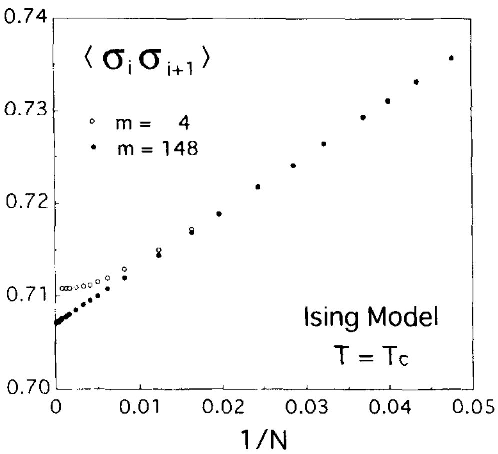

Fig. 1. Nearest-neighbor spin correlation function of the Ising model.

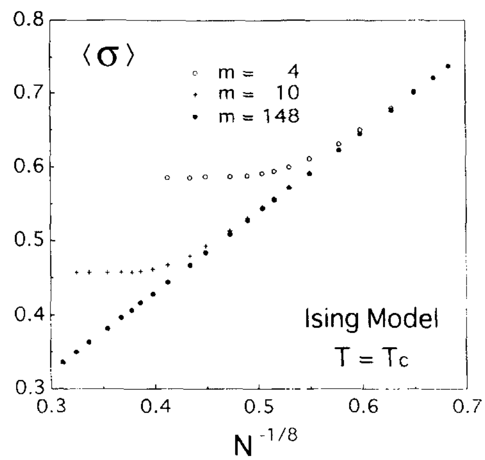

Fig. 2. Spin polarization of the Ising model.

on the square lattice. The exact values of the critical exponents appearing in the scaling forms are $\nu = 1$ and $\eta = 1/4$ for the Ising model and $\nu = 5/6$ and $\eta = 4/15$ for the Potts model. In order to calculate $M(N)$, we impose the ferromagnetic boundary conditions, that is, all the spins at the boundary of the clusters take the same value.

Fig. 1 shows the local energy $E(N) = \langle \sigma_i \sigma_{i+1} \rangle$ of the Ising model against $1/N$ at $T_c = 2.269185314$. We set $m = 148$; the result for $m = 4$ is also shown for comparison. The linear dependence of $E(N)$ on $1/N$ is observed in a wide range of $1/N$, which is consistent with the leading FSS behavior in Eq. (3) with $\nu = 1$. In fact, the least-square fitting of the data in the range $21 \leqslant N \leqslant 401$ to Eq. (3) gives $\nu = 0.993$ and $E(\infty) = 0.70704$, which is close to the exact value $E(\infty) = 1/\sqrt{2} = 0.70711$. Fig. 2 shows the spin polarization $M(N) = \langle \sigma \rangle$ for $m = 4, 10$, and 148. The N dependence is well expressed by $N^{-1/8}$ as we expected. The crossover effect discussed above is clearly seen in the figure: $M(N)$ for different m deviates from $N^{-1/8}$ behavior one by one when N increases. By the least-square fitting in the range $21 \leqslant N \leqslant 401$ we get $\eta = 0.2506$.

Now we check the full two-parameter scaling form for $E(N)$ taking the crossover effect expressed by the scaling function f into account. In Fig. 3 we plot $N(E(N) - E(\infty))$ against $N/\xi(m)$ for $m = 4 \sim 13$; we choose relatively small m in order to observe a small $\xi(m)/N$ region. All the data really collapse

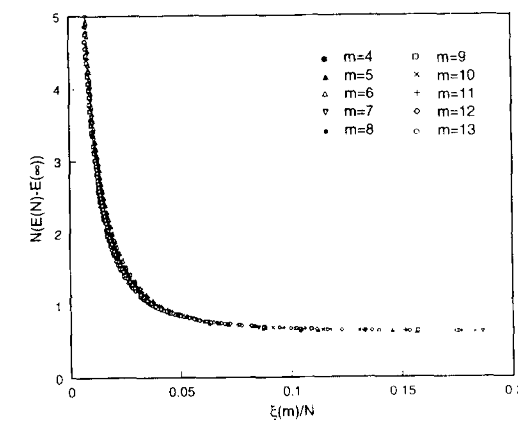

Fig. 3. Two-parameter scaling function $f(\xi(m)/N)$.

into a single curve, and thus the two-parameter scaling assumption, Eq. (3), is justified.

Figs. 4 and 5 show the local energy $E(N) = \langle \delta(\sigma_i \sigma_{i+1}) \rangle$ and the local order parameter $M(N) = \langle \delta(0, \sigma) \rangle$, respectively, of the 3-state Potts model at $T_c = 1.989944809$. Again the expected N dependence, $E(N) - E(\infty) \sim N^{-4/5}$ and $M(N) \sim N^{-2/15}$, are observed. The calculated critical exponent ν is 0.830 in the range $5 \leqslant N \leqslant 31$, and is 0.809 in the range $4 \leqslant N \leqslant 201$. For the exponent η we get 0.266 in the range $5 \leqslant N \leqslant 31$, and 0.267 in the range $5 \leqslant N \leqslant 201$.

The obtained exponents ν and η of the 3-state Potts model seem to have lower accuracy than those of the Ising model. The reason may be attributed to that we used the same value of m for both models. Since the

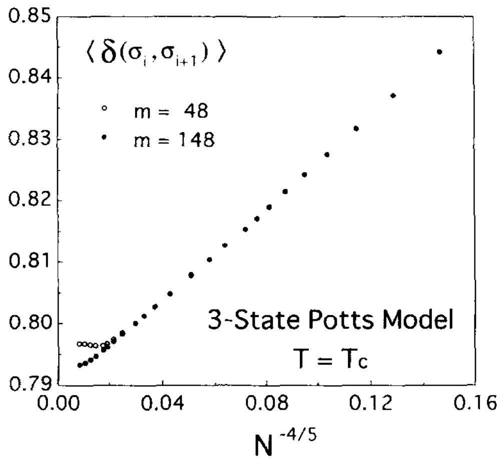

Fig. 4. Nearest-neighbor spin correlation function of the 3-state Potts model.

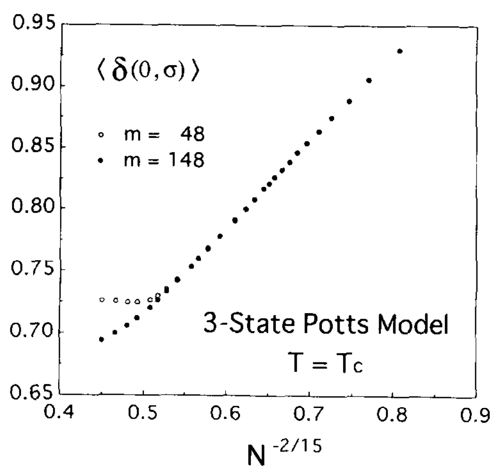

Fig. 5. Spin polarization of the 3-state Potts model.

Potts model has a larger spin degree of freedom than the Ising model, a larger size of matrix may be required to retain the same order of accuracy as in the Ising case.

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References

[1] L.P. Kadanoff, Physics 2 (1965) 263.
[2] K.G. Wilson and J. Kogut, Phys. Rep. 12 (1974) 75.
[3] T.W. Burkhardt and J.M.J. van Leeuwen, Real-space renormalization, Topics in Current Physics, Vol. 30 (Springer, Berlin, 1982), and references therein.
[4] S.R. White, Phys. Rev. Lett. 69 (1992) 2863.
[5] S.R. White, Phys. Rev. B 48 (1993) 10345.
[6] T. Nishino, J. Phys. Soc. Japan 64(10) (1995) 3598.
[7] S. Östlund and S. Rommer, Phys. Rev. Lett. 75 (1995) 3537.
[8] A. Klümper, A. Schadschneider and J. Zittarz, Z. Phys. B 87 (1992) 281.
[9] A. Klümper, A. Schadschneider and J. Zittarz, Europhys. Lett. 24 (1993) 293.
[10] A. Schadschneider and J. Zittarz, Ann. Physik 4 (1995) 157.
[11] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 64(11) (1995) 4084.
[12] M.A. Martín-Delgado and G. Sierra, to appear in Phys. Rev. Lett.
[13] M.A. Martín-Delgado and G. Sierra, to appear in Int. J. Mod. Phys. A.
[14] R.J. Baxter, J. Math. Phys. 9 (1968) 650.
[15] R.J. Baxter, J. Stat. Phys. 19 (1978) 461.
[16] R.J. Baxter, Exactly solved models in statistical mechanics (Academic Press, London, 1980) p. 363.
[17] H.A. Kramers and G.H. Wannier, Phys. Rev. 60 (1941) 263.
[18] R. Kikuchi, Phys. Rev. 81 (1951) 988.
[19] T. Morita, M. Suzuki, K. Wada and M. Kaburagi, eds., Foundations and applications of cluster variation method and path probability method, Prog. Theor. Phys. Suppl. (1994) 115.
[20] T. Nishino and K. Okunishi, Preprint.
[21] A.J.F. de Souza and F.G. Bardy Moreira, Phys. Rev. B 48 (1993) 9586.
[22] M.E. Fisher, in: Proc. Int. School of physics "Enrico Fermi", Vol. 51, ed. M.S. Green (Academic Press, New York, 1971) p. 1.
[23] M.N. Barber, in: Phase transitions and critical phenomena, Vol. 8, eds. C. Domb and J.L. Lebowitz (Academic Press, New York, 1983) p. 146, and references therein.