PHYSICAL REVIEW E VOLUME 59, NUMBER 6 JUNE 1999

Universal asymptotic eigenvalue distribution of density matrices and corner transfer matrices in the thermodynamic limit

Kouichi Okunishi, Yasuhiro Hieida, and Yasuhiro Akutsu

Department of Physics, Graduate School of Science, Osaka University, Machikaneyama-cho 1-1, Toyonaka, Osaka 560-0043, Japan

(Received 8 March 1999)

We study the asymptotic behavior of the eigenvalue distribution of the corner transfer matrix ($M_{\rm CTM}$) and the density matrix ($M_{\rm DM}$) in the density-matrix renormalization group. We utilize the relationship $M_{\rm DM}=M_{\rm CTM}^4$, which holds for noncritical systems in the thermodynamic limit. We derive the exact and universal asymptotic form of the $M_{\rm DM}$ eigenvalue distribution for a class of integrable models in the massive regime. For nonintegrable models, the universal asymptotic form is also verified by numerical renormalization group calculations. [S1063-651X(99)50806-4]

PACS number(s): 05.50.+q, 05.20.−y, 11.30.−j, 75.10.Jm

The density matrix renormalization group (DMRG) invented by White [1] is one of the most important numerical methods developed recently. Due to the remarkable success, the method has now become one of the standard methods for studying one-dimensional (1D) quantum systems [2] and two-dimensional (2D) classical statistical systems [3]. In spite of the success, little has been understood about the foundation of the method. Studies clarifying the ''origin'' of efficiency of the method are important because they lead to various (including higher-dimensional [4]) extension of the method. One example is the work of Ref. [5], where a relationship between the density matrix ($M_{\rm DM}$) and Baxter's corner transfer matrix ($M_{\rm CTM}$) [7–9] is pointed out and a new algorithm (CTMRG) is devised. Another example is the work of Ref. [10], where it is pointed out that the DMRG (at its thermodynamic limit) is a variational method using the matrix-product-ansatz (MPA) wave function as a trial wave function. This leads to a direct variational method that does not need the $M_{\rm DM}$ [10], and the product-wave-function RG (PWFRG), which fully utilizes the MPA form of the DMRG-fixed-point wave function [6].

The central object in the DMRG is the $M_{\rm DM}$, which is made from the ground-state wave function (respectively maximal eigenvalue wave function) of quantum Hamiltonian (respectively transfer matrix) by tracing out information of one half of the system. Keeping up to a cut-off-eigenvalue eigenstate of the $M_{\rm DM}$, we have a truncated basis set consisting of a finite number (conventionally denoted by m) of bases to describe the remaining half of the system.

Since the accuracy of the DMRG is determined by the cut-off eigenvalue, it is crucially important to investigate the eigenvalue spectrum $\{\omega_m\}$, in particular, its asymptotic ($m\to\infty$) behavior, which has not been known precisely. In this Rapid Communication, we present the *exact asymptotic form* of the $M_{\rm DM}$ eigenvalue distribution for a class of (noncritical) integrable models, and further, make the first systematic study for nonintegrable systems employing the CTMRG and the PWFRG by which we can efficiently obtain the ''fixed point'' (thermodynamic limit of the system) of the DMRG.

Let us first discuss the integrable cases. In these cases, 1D quantum problems are equivalent to 2D classical statistical problems: the Hamiltonian of the former can be derived by a log-derivative of the transfer matrix of the latter, and the ground-state wave function of the former is identical to the maximal-eigenvalue eigenfunction $\Psi_{\rm max}$ of the latter [9]. Hence, we discuss only 2D classical cases below.

As has been pointed out by Baxter [9], the wave function (WF) $\Psi_{\rm max}$ is interpreted as a product of two CTMs, in the thermodynamic limit. Since the $M_{\rm DM}$ is just a square $\Psi_{\rm max}^2$ (with $\Psi_{\rm max}$ being regarded as a ''wave function matrix''), this interpretation leads to a relationship [5] between the $M_{\rm DM}$, the WF, and the $M_{\rm CTM}$ for 2D classical systems (at least the noncritical case, where the boundary effect is negligible), which is symbolically written as

$$\begin{aligned}\Psi_{\rm max}&=(M_{\rm CTM})^2,\\ M_{\rm DM}&=(M_{\rm CTM})^4.\end{aligned}\tag{1}$$

For integrable models, the diagonal form of the $M_{\rm CTM}$ is easily known, from which we can obtain, for example, the exact one-point function (spontaneous magnetization, etc.) [9]. Due to the relationship (1), the diagonal form is also useful to obtain the exact eigenvalue spectrum of the $M_{\rm DM}$.

We discuss the simplest case where the diagonal form of the $M_{\rm CTM}$ is given by a single infinite tensor product [9]; due to Eq. (1), diagonal form of the $M_{\rm DM}$ has the same infinite-tensor-product form with redefined parameter. For definiteness let us consider two cases (type I and type II) where the exact diagonal form of the $M_{\rm DM}$ is given by

$$\rho^{(\rm diag)}=\bigotimes_{n=1}^{\infty}\begin{pmatrix}1&0\\0&z^{c_n}\end{pmatrix},\tag{2}$$

with $c_n=n$ for type I models (e.g., transverse-field Ising chain, six-vertex model, eight-vertex model, XXZ chain and XYZ chain) and $c_n=2n-1$ for type II models [e.g., the square-lattice Ising model in the conventional (not eight-vertex) representation] [9]. The parameter z ($0<z<1$) represents the ''degree of noncriticality'' (i.e., $z\to 1$, on approaching the critical point), and how it relates to ''physical'' parameters depends on the model. Note that the $M_{\rm DM}$ (2) is unnormalized. It is ''normalized'' in such a way that its maximal eigenvalue ω_0 is unity; we should divide it by $\mathrm{Tr}\,\rho^{(\mathrm{diag})}$ for conventional normalization.

Due to the tensor-product structure (2), each eigenvalue of $\rho^{(\mathrm{diag})}$ has the form z^n, with n ($\geqslant 0$) being an integer. Further, each eigenvalue z^n may have degeneracy $p(n)$. To study the degeneracy structure of the M_{DM}, it is convenient to consider $\mathrm{Tr}\,\rho^{\mathrm{diag}}$,

$$\mathrm{Tr}\,\rho^{\mathrm{diag}}=\prod_{n=1}^{\infty}(1+z^{c_n})=\sum_{n=0}^{\infty}p(n)z^n, \tag{3}$$

where the degeneracy $p(n)$ is precisely the coefficient of z^n in the infinite series. We should note that, taking the degeneracy into account, the number of retained bases m in the DMRG should be

$$m=m(n)=\sum_{k=0}^{n}p(k), \tag{4}$$

which means that the cut-off eigenvalue of (unnormalized) M_{DM} is z^n and that we should retain all the degenerate bases belonging to this cut-off eigenvalue.

Our problem is to obtain the large-n behavior of $m=m(n)$. For this purpose, we should know the asymptotic behavior of $p(n)$. The partition theory of integers, which has played an important role in studies of integrable interaction-round-a-face models, is helpful again [11]. By $r(n)$ we denote the number of partitions of a positive integer n under a restriction "r." Consider the generating function $f(q)$ associated with the restricted partition problem. It has been known [11] that for a wide class of partition problems, $f(q)$ can also be given in an infinite-product form,

$$f(q)\equiv\sum_{n=0}^{\infty}r(n)q^n=\prod_{n=0}^{\infty}(1-q^n)^{-a_n}, \tag{5}$$

where each a_n is a non-negative real number. For the type I case, we have $a_n=1$ for n odd, and $a_n=0$ otherwise.

The asymptotics of the generating function of the form (5) is calculated by the saddle point method; $r(n)$ for $n\gg 1$ is then given by Meinardus's theorem (cited in Ref. [11], page 89),

$$r(n)=An^{\kappa}\exp(Bn^{\alpha/(1+\alpha)})+(\text{less dominant terms}), \tag{6}$$

where α is the real part of the pole of the Dirichlet series,

$$D(s)\equiv\sum_{n=1}^{\infty}\frac{a_n}{n^s}, \tag{7}$$

and κ is given by

$$\kappa=\frac{D(0)-1-\alpha/2}{1+\alpha}. \tag{8}$$

Explicit forms of A and B which we have omitted in the above are also given by Meinardus's theorem. For the type I models, we have $\alpha=1$ and $\kappa=-3/4$,

$$p(n)=\mathrm{const}\times n^{-3/4}\exp(B\sqrt{n}), \tag{9}$$

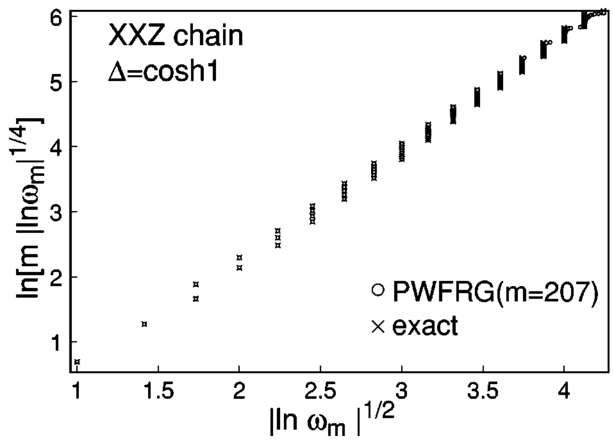

FIG. 1. PWFRG calculation of density-matrix eigenvalues $\{\omega_m\}$ for $S=1/2$ antiferromagnetic XXZ chain and comparison with the exact spectrum. We take the exchange coupling constants to be $|J_x|=|J_y|=1$ and $|J_z|=\Delta=\cosh(1)$. The number of retained bases in the PWFRG calculation is $m=207$.

where $B=\pi/\sqrt{3}$ [11]. For the type II models, a related theorem (Ref. [11], pages 99 and 100, examples 10 and 11) assures the same asymptotic form (9) with $B=\pi/\sqrt{6}$. It is also possible to relate the type II models with Meinardus's theorem (Chapters 1 and 6 in Ref. [11]). We thus have derived the exact asymptotic form of $p(n)$.

Using Eq. (4) and changing the summation into the integration, we finally obtain

$$m\sim n^{-1/4}\exp(B\sqrt{n}), \tag{10}$$

for the type I and II models. How well the DMRG calculation for the $S=1/2$ XXZ chain reproduces the asymptotic behavior (10) is demonstrated in Fig. 1. In the actual calculation, we have employed the quantum version of the PWFRG [12–14], by which we obtain the fixed-point wave function of the DMRG efficiently.

We give a comment on the universality of the asymptotic form (10) among the integrable systems. In the case where $\{a_n\}$ forms a periodic series or the model itself admits a direct partition-theoretic interpretation [15,16], the $\exp(B\sqrt{n})$ behavior is universal (Ref. [11], Chapter 6, examples 1–16). The exponent κ may, however, have possibility of model-dependence [due to $D(0)$], modifying the prefactor $n^{-1/4}$ in Eq. (10).

Let us now proceed to nonintegrable cases, where the exact diagonal form of the M_{CTM} or the M_{DM} is not known. The M_{DM} eigenvalue is no longer given by z^{integer} with single parameter z, or equivalently, $\ln(M_{\mathrm{DM}}$ eigenvalue) does not have equal-spacing distribution. Both the integer n characterizing the M_{DM} eigenvalue, and the quantity $p(n)$, which is essential in the integrable cases lose meaning. Our first task is, then, to translate the result of integrable cases into the one which has meaning also for non-integrable cases.

Writing the mth M_{DM} eigenvalue (including degeneracy) as ω_m, we have $n=\ln\omega_m/\ln z$ in the integrable case. Substituting $n=\ln\omega_m/\ln z$ into Eq. (10), we have

$$m\sim\left(\frac{\ln\omega_m}{\ln z}\right)^{-1/4}\exp\left(B\sqrt{\frac{\ln\omega_m}{\ln z}}\right), \tag{11}$$

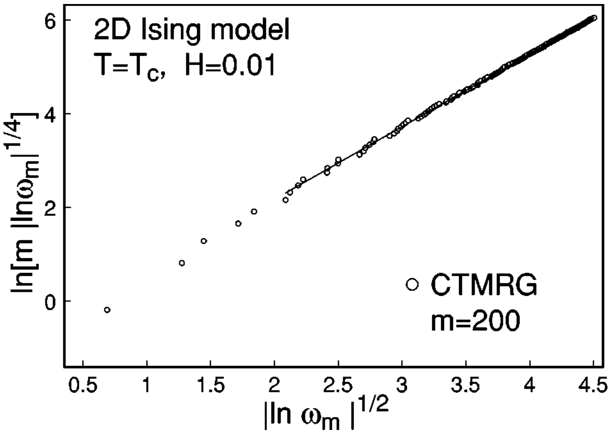

FIG. 2. CTMRG calculation ($m=200$) of the density-matrix eigenvalues $\{\omega_m\}$ for the square-lattice Ising model at a critical temperature T_c in a small external field H. We have also drawn a line corresponding to the universal asymptotic form.

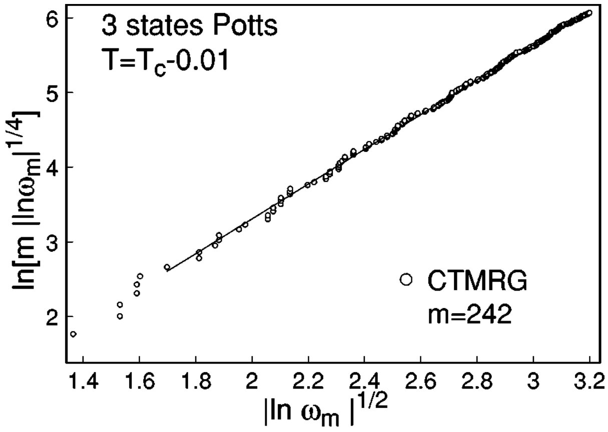

FIG. 3. CTMRG calculation ($m=242$) of the density-matrix eigenvalues $\{\omega_m\}$ for the three-state Potts model slightly below the critical temperature. We have also drawn a line corresponding to the universal asymptotic form.

or equivalently,

$$\ln\left[m\left(\frac{\ln\omega_m}{\ln z}\right)^{1/4}\right]=B\sqrt{\frac{\ln\omega_m}{\ln z}}. \tag{12}$$

From Eq. (12), we obtain the leading asymptotic form

$$\omega_m\sim\exp[-\text{const}\times(\ln m)^2], \tag{13}$$

where const$=|\ln z|/B^2$ for the integrable cases. Clearly, expressions (11)–(13) do not contain the parameter n, which is specific to the integrable models.

There arises an intriguing conjecture: the asymptotic forms (11)–(13) would also apply to nonintegrable systems with B and z being suitably redefined. In the ''neighborhood'' of an integrable model with small nonintegrable perturbations added, we may well expect this conjecture to be true: In spite of the nonintegrable perturbations, the ''stairway structure'' (or degeneracy) in the $M_{\rm DM}$ eigenvalue spectrum still remains in a somewhat smeared-out way, leaving the ''envelope'' of the ω_m-m curve essentially unchanged. As a check of the universality for the nearly integrable cases, we made the CTMRG calculations for two systems: the square-lattice Ising model at the critical temperature in finite external field and the three-state Potts model slightly below the critical temperature (see Figs. 2 and 3). We see clear agreements between the CTMRG calculations and the ''universal asymptotic form.''

As a test of the universality of (11)–(13) for systems far from the integrability, we take the $S=1$ antiferromagnetic Heisenberg spin chain. For calculation of the $M_{\rm DM}$ eigenvalue spectrum, we employ the quantum version of the PWFRG [12,13]. The results are given in Fig. 4, which support the universal asymptotic form.

We have made similar calculations for the $S=1$ bilinear-biquadratic spin chain at $\beta=-0.5$ with the Hamiltonian $\mathcal{H}=\Sigma\vec{S}_i\cdot\vec{S}_{i+1}+\beta\Sigma(\vec{S}_i\cdot\vec{S}_{i+1})^2$, whose result (not shown in this paper) also supports the universality of the asymptotic form.

To summarize, we have discussed the asymptotic distribution of the density-matrix ($M_{\rm DM}$) eigenvalues for noncritical systems (one-dimensional quantum and two-dimensional classical), which controls the accuracy of the density-matrix renormalization group. Based on the equivalence between the $M_{\rm DM}$ and the corner transfer matrix ($M_{\rm CTM}$), we derived the exact asymptotic form of the $M_{\rm DM}$ eigenvalue distribution for a class of integrable models. The resulting expression has been rewritten in a ''universal'' form that does not contain quantities specific to integrable models. Numerical-renormalization-group calculations using the CTMRG and the product-wave function RG have been performed for nonintegrable models, which shows that the nonintegrable models actually have the same asymptotic form of the $M_{\rm DM}$-eigenvalue distribution, in strong support of the universality of the asymptotic form.

There remains many important problems left for future studies. A more ''physical'' explanation to justify the universal asymptotic form is desired. How universal the obtained asymptotic form itself remains a question to be answered; there may well be different ''universal classes'' of the $M_{\rm DM}$. In fact, the valence-bond-solid (VBS) models [17] have only finite-dimensional $M_{\rm DMs}$, which sharply contrast to the ones studied in this paper. The relation between the

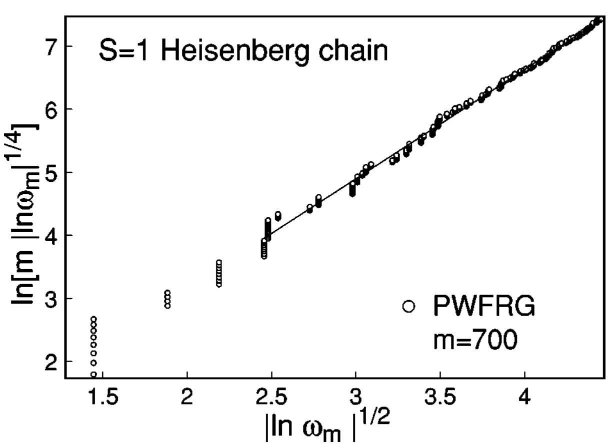

FIG. 4. PWFRG calculation ($m=700$) of density-matrix eigenvalues $\{\omega_m\}$ for $S=1$ antiferromagnetic Heisenberg chain. We have also drawn a line corresponding to the universal asymptotic form.

$M_{\rm DM}$-eigenvalue distribution and the finite-*m* (where *m* is the number of retained bases) behavior of physical (observable) quantities is not known, although there have been a few works discussing the ''finite-*m* scaling''(2D classical [18], transverse-field XXZ chain [19]). The behavior of the $M_{\rm DM}$ for critical system is also an important subject of study [20,21]. Our study made in the present paper may be a first step for clarification of these problems [22].

This work was partially supported by the Grant-in-Aid for Scientific Research from Ministry of Education, Science, Sports and Culture (Grant No. 09640462), and by the ''Research for the Future'' program of the Japan Society for the Promotion of Science (Grant No. JSPS-RFTF97P00201). One of the authors (K. O.) is supported by JSPS, and Y. H. is partly supported by the Sasakawa Scientific Research Grant from The Japan Science Society.

[1] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10 345 (1993).

[2] S.R. White and D.A. Huse, Phys. Rev. B **48**, 3844 (1993); S.R. White, Phys. Rep. (to be published). See also G.A. Gehring, R.J. Bursill, and T. Xiang, Acta Phys. Pol. A **91**, 105 (1997), and references cited therein.

[3] T. Nishino, J. Phys. Soc. Jpn. **64**, 3598 (1995).

[4] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **67**, 3066 (1998).

[5] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **65**, 891 (1996); **66**, 3040 (1997).

[6] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **64**, 4084 (1995).

[7] R.J. Baxter, J. Math. Phys. **9**, 650 (1968); J. Stat. Phys. **19**, 461 (1978).

[8] R.J. Baxter, J. Stat. Phys. **15**, 485 (1976); **17**, 1 (1977).

[9] R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Accademic Press, New York, 1982).

[10] S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995); Phys. Rev. B **55**, 2164 (1997).

[11] G.E. Andrews, *The Theory of Partitions* (Addison-Wesley, Reading, MA, 1976).

[12] Y. Hieida, K. Okunishi, and Y. Akutsu, Phys. Lett. A **233**, 464 (1997).

[13] K. Okunishi, Y. Hieida, and Y. Akutsu, Phys. Rev. B **59**, 6806 (1999).

[14] R. Sato and Y. Akutsu, J. Phys. Soc. Jpn. **65**, 1885 (1996).

[15] R.J. Baxter and P.A. Pearce, J. Phys. A **15**, 897 (1982); **16**, 2239 (1983).

[16] G.E. Andrews, R.J. Baxter, and P. Forrester, J. Stat. Phys. **35**, 193 (1984).

[17] I. Affleck, T. Kennedy, E.H. Lieb, and H. Tasaki, Phys. Lett. A **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).

[18] T. Nishino, K. Okunishi, and M. Kikuchi, Phys. Lett. A **213**, 69 (1996).

[19] Y. Hieida (unpublished).

[20] M. Andersson, M. Boman, and S. Ostlund, e-print cond-mat/9810093.

[21] T.T. Troung and I. Peschel, Z. Phys. B **69**, 385 (1987); **75**, 119 (1988); B. Davies and P. Pearce, J. Phys. A **23**, 1295 (1990).

[22] After completion of the present work, a preprint verifying the relation $M_{\rm DM}=M_{\rm CTM}^4$ (asymptotic behavior is not discussed) for the transverse-field Ising chain appeared in I. Peschel, M. Kaulke, and Ö. Legeza, e-print cond-mat/9810174.