Biorthonormal transfer-matrix renormalization-group method for non-Hermitian matrices

Yu-Kun Huang*

Department of Electrical Engineering, Nan Jeon Institute of Technology, Tainan 73746, Taiwan

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A biorthonormal transfer-matrix renormalization-group (BTMRG) method for non-Hermitian matrices is presented. This BTMRG produces a dual set of biorthonormal bases to construct the renormalized transfer matrix with only half the dimensions of the matrix of a conventional transfer-matrix renormalization group (TMRG). We show that under generic conditions, such biorthonormal bases always exist. Based on a special E·S·E scheme (where S and E represent the system and environment blocks, respectively, and the two dots in between represent two additional physical sites), the BTMRG method can achieve zero truncation of any reduced state in describing both current left and right Perron states so as to reach a high degree of efficiency and accuracy. We believe that the BTMRG constitutes a more powerful and robust tool than conventional TMRG for non-Hermitian matrices and that it would allow us to better understand the collective behaviors and emerging phenomena of strongly correlated many-body systems. We also show that this scheme is particularly adapted to the calculation of the two-site correlation function of a one-dimensional quantum or two-dimensional classical lattice model.

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I. INTRODUCTION

Since its inception in 1992 by White, the density-matrix renormalization group (DMRG) [1] has proven to be one of the most powerful and versatile methods in modern computational physics. The transfer-matrix renormalization group (TMRG) [2] inherits the basic idea of the DMRG and extends DMRG studies to a wide variety of fields—for instance, strongly correlated classical systems [2], the thermodynamics of one-dimensional (1D) quantum systems at finite temperature [3], the stochastic transfer matrix of a cellular automaton [4], nonequilibrium systems in statistical physics [5], and the general Markov random field in image modeling [6]. Despite the success of the TMRG in these fields, there has long been a suspension problem that seems to degrade the quality of the TMRG results. Unlike the Hermitian Hamiltonian in DMRG, the TMRG always concerns the Perron root (maximum eigenvalue) of a *non-Hermitian* transfer matrix, which adds a complication at the level of having distinct left and right Perron states (eigenvectors) and leads to the problem of having no properly prescribed selection of the *density matrix*. A number of choices of the density matrix have been proposed (see Enss and Schollwock in [4]), but it seems that most of these choices are heuristic and lack a solid foundation. One of the main concerns of this paper is to settle this debate among TMRG practitioners, working from a fairly solid foundation.

The principal idea of DMRG is a systematic projection of the full-dimension Hamiltonian onto a small subspace $\widehat{H}$ of the Hilbert space that can accurately describe the ground state of the strongly correlated quantum system. In DMRG, the density matrix is used to obtain the *reduced* (*renormalized*) *orthonormal basis* that spans the subspace $\widehat{H}$. In view of the distinct left and right Perron states for non-Hermitian matrices, the construction of the density matrix becomes ambiguous. In a recent paper [6], the authors presented a special E·S·E scheme (where S and E represent the system and environment blocks, and the two dots in between represent two additional physical sites; see the following context) and a new method for selecting the renormalized basis, which exhibits a high degree of robustness and accuracy. In this paper, we introduce a modified TMRG method that employs a dual set of *biorthonormal bases* to build the renormalized transfer matrix without the explicit concept of density matrices. Based on this scheme, we demonstrate that the *biorthonormal TMRG* (BTMRG) further dramatically improves on previous TMRG performance by reducing by half the dimension of the renormalized transfer matrix and reaching even higher accuracy. The important implication of this work is that the BTMRG, combined with the E·S·E scheme, constitutes a more powerful and robust tool than conventional TMRG and can be used in investigations of all of the above-mentioned fields. By precise simulations, it allows us to obtain a crucial understanding of the collective behaviors and emerging phenomena of strongly correlated many-body systems. Moreover, we also show that this scheme is particularly adapted to the calculation of the two-site correlation function of a 1D quantum or a two-dimensional (2D) classical lattice model.

The rest of this paper is organized as follows. In Sec. II, we briefly review the E·S·E scheme proposed in [6] and discuss its advantages and disadvantages with respect to conventional TMRG algorithms. Since the E·S·E scheme utilizes a single orthonormal basis, as in conventional TMRG methods, we attribute it to the same class as the conventional TMRG algorithm. In Sec. III, we present the details of the proposed BTMRG algorithm. We show that under generic conditions, dual biorthonormal bases always exist for the distinct left and right Perron vectors of non-Hermitian matrices. In particular, these dual bases reduce to a single orthonormal basis for Hermitian cases. Section IV provides BTMRG simulations for a real non-Hermitian transfer matrix of the famous Ising model and compares its accuracy with our previous TMRG calculations [6]. The results show that our BTMRG constitutes a more robust and powerful tool than conventional TMRG methods. Additionally, we also show that the proposed

*ykln@mail.njtc.edu.tw

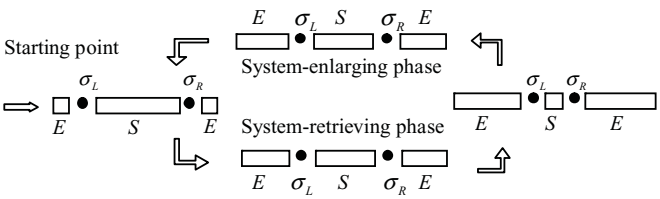

FIG. 1. Finite-TMRG algorithm. A complete cycle of system-retrieving and system-enlarging phases is called a sweep of the finite TMRG.

E·S·E scheme is particularly adapted to the calculation of two-point correlation functions of a 1D quantum or 2D classical lattice model. Finally, in Sec. V, some conclusions are drawn.

II. CONVENTIONAL TMRG FOR NON-HERMITIAN MATRICES

Let us begin with a discussion of the E·S·E scheme proposed in [6] for a 1D spin-1/2 chain as an example. The finite-TMRG algorithm is depicted in Fig. 1. The configuration represents the whole system, which is called the *superblock*, and is divided into two parts: the system block spin (denoted by S and described by the basis $\{|\alpha\rangle\}_{\alpha=1,\ldots,m}$) and the environment block spin (denoted by E and described by the basis $\{|\xi\rangle = |\xi_L\rangle|\xi_R\rangle\}_{\xi=1,\ldots,m}$), with two additional physical spins in between (described by states $|\sigma_L\rangle$ and $|\sigma_R\rangle$, respectively). The renormalization proceeds as follows. Suppose we are currently in the system-enlarging phase. The system block is enlarged by adding two spins accompanied by retrieving the same two spins from the environment block. Suppose that the left and right Perron states $|\psi\rangle$ and $|\varphi\rangle$ are obtained from the Hamiltonian on the basis $\{|\xi\sigma_L\alpha\sigma_R\rangle \equiv |\xi_L\sigma_L\alpha\sigma_R\xi_R\rangle\}$. In Hermitian cases, $|\psi\rangle$ and $|\varphi\rangle$ are identical, and the DMRG obtains the renormalized basis by choosing m eigenstates $\{|\alpha_+\rangle = \sum_{\sigma_L\alpha\sigma_R} A_{\sigma_L\alpha\sigma_R,\alpha_+}|\sigma_L\alpha\sigma_R\rangle\}_{\alpha_+=1,\ldots,m}$ of the (reduced) density matrix $\widehat{\rho}_s = Tr_E|\psi\rangle\langle\psi|$, corresponding to the m largest eigenvalues. This is the principal essence of the DMRG, which keeps those states of the system block that are relevant in describing $|\psi\rangle$ and truncates the other, irrelevant states. In fact, one can show that this is equivalent to performing the *Schmidt decomposition* of $|\psi\rangle$ for a bipartite system, as indicated by our E·S·E setup. Another principal essence of the DMRG is the assumption that the Perron state of the next superblock should be accurately described by the basis $\{|\xi_-\sigma_L\alpha_+\sigma_R\rangle\}$, which is the tensor product of the reduced basis and that of the retrieved environment block and the two spins. (These two principal essences are also the main sources of errors of the DMRG.) In the non-Hermitian case, the left and right Perron states are generally distinct. However, according to the previous description, without the problem of selecting the density matrix, we can treat these two Perron states separately by carrying out the Schmidt decomposition twice, and then combine the two sets of reduced bases by some orthonormalization procedure to form a new *single orthonormal basis* twice as large as the original one. This would produce a more *logical* reduced Hilbert space (than conventional TMRG) able to accurately describe both eigenvectors on the same footing. The reason why this scheme exhibits high efficiency and accuracy is that, in the infinite-TMRG system-enlarging phase, the environment block is kept fixed and small, so that the dimension of the reduced subspace is small. In practical simulations, four environment sites with two sites on each side of the system block are kept, so that $m = 2 \times 2^4$ can be taken. Accordingly, there is *no truncation* of any states in describing the current Perron states. On the other hand, this may yield a relatively large error from the second source, as stated earlier. However, this error will be minimized *variationally* during the finite-TMRG sweeps. In spite of this method's robustness and preciseness, there are two points that appear to degrade the quality of the algorithm for non-Hermitian matrices. First, consideration of both left and right Perron states leads to doubling the size of the renormalized Hamiltonian. Second, in the system-retrieving phase of the first sweep of finite TMRG (see Fig. 1), the attempt at maintaining zero truncation leads to double the number of states of the environment block kept by TMRG. Thus, after several sweeps, the dimension of the renormalized Hamiltonian grows exponentially. However, it is important to note that this scheme can be effectively translated to the Hermitian case, where it will be free of these two unfavorable factors. Nevertheless, fortunately for researchers using non-Hermitian matrices, the employment of a dual set of biorthonormal bases correctly remedies these two drawbacks, allowing researchers to enjoy the same good properties as with Hermitian matrices.

III. BTMRG FOR NON-HERMITIAN MATRICES

The underlying idea of BTMRG is similar to that of the biorthonormal Lanczos method [7]. Here, by biorthonormality, we mean that $\langle\overline{\alpha}|\overline{\beta}\rangle = \delta_{\alpha\beta}$ for any two sets of vectors $\{|\overline{\alpha}\rangle\}_{\alpha=1,\ldots,m}$ and $\{|\overline{\beta}\rangle\}_{\beta=1,\ldots,m}$. Let $\overline{A} \equiv [|\overline{\alpha}\rangle_{\alpha=1,\ldots,m}]$ and $\overline{B} \equiv [|\overline{\beta}\rangle_{\beta=1,\ldots,m}]$ be matrices formed with a dual set of biorthonormal bases $\{|\overline{\alpha}\rangle\}$ and $\{|\overline{\beta}\rangle\}$ as their columns. Suppose that the left $|\psi\rangle = \sum_\alpha \psi_\alpha|\overline{\alpha}\rangle$ and right $|\varphi\rangle = \sum_\beta \varphi_\beta|\overline{\beta}\rangle$ Perron vectors of the transfer matrix T associated with the Perron root λ can be expressed in terms of these biorthonormal bases. Then we have $|\psi\rangle = \overline{A}|\mu\rangle$ and $|\varphi\rangle = \overline{B}|\nu\rangle$, where $|\mu\rangle$ and $|\nu\rangle$ are two vectors in $\mathbb{C}^m$ formed with the coefficients of $|\psi\rangle$ and $|\varphi\rangle$, respectively, as their elements. Now let the renormalized transfer matrix $\overline{T} : \mathbb{C}^m \to \mathbb{C}^m$ be constructed as

$$\overline{T} \equiv \overline{A}^\dagger T \overline{B} = \sum_\alpha \sum_\beta \langle\overline{\alpha}|T|\overline{\beta}\rangle |e_\alpha\rangle\langle e_\beta|. \tag{1}$$

Accordingly, we have $\langle\mu|\overline{T} = \lambda\langle\mu|$ and $\overline{T}|\nu\rangle = \lambda|\nu\rangle$. This means that if the biorthonormal bases $\{|\overline{\alpha}\rangle\}$ and $\{|\overline{\beta}\rangle\}$ can accurately describe the pairs of Perron vectors of T, then we can obtain T's Perron eigenpairs as $|\psi\rangle = \overline{A}|\mu\rangle$ and $|\varphi\rangle = \overline{B}|\nu\rangle$, where $|\mu\rangle$ and $|\nu\rangle$ are the left and right eigenvectors of $\overline{T}$ associated with the maximum eigenvalue λ. Fortunately, under generic conditions, such bases always exist. Let us return to the system-enlarging phase of finite TMRG, as in Fig. 1. Suppose that we now have dual biorthonormal bases $\{|\overline{\xi}\sigma_L\overline{\alpha}\sigma_R\rangle_L\}$ (to the left of the transfer matrix) and $\{|\overline{\zeta}\sigma_L\overline{\beta}\sigma_R\rangle_R\}$ (to the right of the transfer matrix). By carrying out the Schmidt decomposition for both Perron vectors, we obtain the reduced bases $|\alpha_+\rangle = \sum_{\sigma_L\overline{\alpha}\sigma_R} A_{\sigma_L\overline{\alpha}\sigma_R,\alpha_+}|\sigma_L\overline{\alpha}\sigma_R\rangle_L$ and $|\beta_+\rangle = \sum_{\sigma_L\overline{\beta}\sigma_R} B_{\sigma_L\overline{\beta}\sigma_R,\beta_+}|\sigma_L\overline{\beta}\sigma_R\rangle_R$ for the left and right

Perron vectors. Let $A \equiv [|\alpha_+\rangle_{\alpha=1,\ldots,m}]$ and $B \equiv [|\beta_+\rangle_{\beta=1,\ldots,m}]$ be matrices formed with the basis vectors $\{|\alpha_+\rangle\}$ and $\{|\beta_+\rangle\}$ as their columns. Since $A^\dagger B$ always has a singular-value decomposition (SVD) $A^\dagger B = U\Lambda V^\dagger$, we can readily obtain $(AU)^\dagger(BV) = \Lambda$. If all the singular values $\{\Lambda_{\alpha_+}\}$ of $A^\dagger B$ are nonzero, then we can form a dual set of biorthonormal bases as $\overline{A} \equiv [|\overline{\alpha}_+\rangle_{\alpha=1,\ldots,m}] = AU\Lambda^{-1/2}$ and $\overline{B} \equiv [|\overline{\beta}_+\rangle_{\beta=1,\ldots,m}] = BV\Lambda^{-1/2}$. The biorthonormal bases can be written explicitly as

$$\begin{cases} |\overline{\alpha}_+\rangle = \sum\limits_{\sigma_L\overline{\alpha}\sigma_R} \overline{A}_{\sigma_L\overline{\alpha}\sigma_R,\overline{\alpha}_+}|\sigma_L\overline{\alpha}\sigma_R\rangle, \\ |\overline{\beta}_+\rangle = \sum\limits_{\sigma_L\overline{\beta}\sigma_R} \overline{B}_{\sigma_L\overline{\beta}\sigma_R,\overline{\beta}_+}|\sigma_L\overline{\beta}\sigma_R\rangle, \end{cases} \tag{2}$$

where $\overline{A}_{\sigma_L\overline{\alpha}\sigma_R,\overline{\alpha}_+} = \Lambda_{\overline{\alpha}_+}^{-1/2}\sum_{\alpha_+} A_{\sigma_L\overline{\alpha}\sigma_R,\alpha_+}U_{\alpha_+,\overline{\alpha}_+}$ and $\overline{B}_{\sigma_L\overline{\beta}\sigma_R,\overline{\beta}_+} = \Lambda_{\overline{\beta}_+}^{-1/2}\sum_{\beta_+} B_{\sigma_L\overline{\beta}\sigma_R,\beta_+}V_{\beta_+,\overline{\beta}_+}$. Since range$(\overline{A})$ = range(A) and range$(\overline{B})$ = range(B), the biorthonormal bases in Eq. (2) completely describe both Perron vectors.

In fact, the singular value Λ_{α_+} of $A^\dagger B$ characterizes the angle between the vectors AU_{α_+} and BV_{α_+} (where U_{α_+} represents the α_+th column vector of U). It may happen that there exist p singular values $\{\Lambda_{\alpha_+}\}_{\alpha_+=m-p+1,\ldots,m}$ that are small or vanishing and thus induce instabilities to our BTMRG method. This means that, for $\alpha_+ = m-p+1,\ldots,m$, the vector AU_{α_+} (and, respectively, BV_{α_+}) is nearly orthogonal to the space spanned by $\{|\beta_+\rangle\}_{\beta=1,\ldots,m}$ (respectively, $\{|\alpha_+\rangle\}_{\alpha=1,\ldots,m}$). To deal with this issue, we may enlarge the space range(A) [respectively, range(B)] by augmenting p redundant vectors $\{|\alpha_+\rangle\}_{\alpha_+=m+1,\ldots,m+p}$ (respectively, $\{|\beta_+\rangle\}_{\beta_+=m+1,\ldots,m+p}$) to the matrix A (respectively, B), such that $\{|\alpha_+\rangle\}_{\alpha_+=m+1,\ldots,m+p}$ (respectively, $\{|\beta_+\rangle\}_{\beta_+=m+1,\ldots,m+p}$) have maximum correlation (i.e., minimum angle) with $\{BV_{\alpha_+}\}_{\alpha_+=m-p+1,\ldots,m}$ (respectively, $\{AU_{\alpha_+}\}_{\alpha_+=m-p+1,\ldots,m}$). The simplest way to accomplish this is to choose $\{|\alpha_+\rangle\}_{\alpha_+=m+1,\ldots,m+p}$ (respectively, $\{|\beta_+\rangle\}_{\beta_+=m+1,\ldots,m+p}$) as the vectors having coefficients [associated with the basis $|\sigma_L\overline{\alpha}\sigma_R\rangle$ (respectively, $|\sigma_L\overline{\beta}\sigma_R\rangle$)] the same as those [associated with the basis $|\sigma_L\overline{\beta}\sigma_R\rangle$ (respectively, $|\sigma_L\overline{\alpha}\sigma_R\rangle$)] of the vectors $\{BV_{\alpha_+}\}_{\alpha_+=m-p+1,\ldots,m}$ (respectively, $\{AU_{\alpha_+}\}_{\alpha_+=m-p+1,\ldots,m}$). Since Perron vectors are concerned, according to the Perron–Frobenius theorem, the left and right Perron vectors, both lying in the first orthant of the Hilbert space, must have a large part of overlap, so that the number of small singular values is small. According to our practical simulations, only very few redundant vectors (about 1 or 2) are needed.

IV. NUMERICAL SIMULATIONS AND DISCUSSION

The paradigmatic isotropic Ising model was used as the test case for evaluating the performance of our BTMRG method based on the E·S·E scheme. The target matrix was $\widetilde{\Pi}_q^N$, where $\widetilde{\Pi}_q$ is the non-Hermitian *fundamental transfer matrix* of the general, local-energy-function-parameterized Markov random field on an infinitely long vertical *twisted cylindrical lattice* with peripheral size N [6,8]. This matrix is intimately related to a 2D Markov additive process and enjoys a very special SVD structure and many fascinating properties [8]. We calculated its free energy per site as a function of temperature ($\widehat{T} = k_BT/J$),

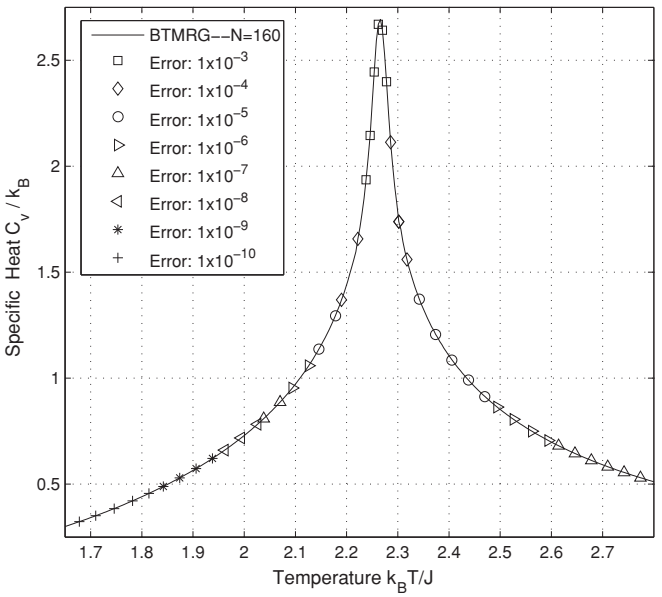

FIG. 2. Specific heat C_v/k_B curve as a function of the temperature k_BT/J of an isotropic Ising model with system size $N = 160$, computed by BTMRG. The number of states kept by BTMRG is $m = 18$.

where, via numerical differentiation, the specific heat (C_v/k_B) curve was plotted and compared to the exact solution [9]. We conducted the simulation for system size $N = 160$, as in Fig. 2, where we kept zero truncation of any states in describing the current Perron states and using two redundant vectors to prevent the small singular value problem ($m = 18$; i.e., the renormalized transfer matrix was of dimension 1 296 × 1 296). In off-critical regions, the BTMRG exhibited a very high degree of efficiency and accuracy. Although in the vicinity of criticality the convergence speed and the accuracy became worse due to the degenerate Perron root and the long-range spin correlation, the BTMRG still exhibited much better performance than our previous TMRG results (see Fig. 8 in [6]). Using the restricted available numerical resources, we further pushed the BTMRG scheme forward to larger values of m at various temperatures $\widehat{T} = 2.126 < \widehat{T}_c$, $\widehat{T} = 2.269 \approx \widehat{T}_c$, and $\widehat{T} = 2.846 > \widehat{T}_c$, and compared its accuracy with that of our previous TMRG scheme, which is regarded as a competitive alternative to conventional TMRG algorithms. As Fig. 3 illustrates, we believe that the BTMRG constitutes, theoretically and numerically, a more powerful and robust tool than conventional TMRG for non-Hermitian matrices in the simulation of strongly correlated many-body systems.

The E·S·E scheme and finite TMRG, as depicted in Fig. 1, are particularly adapted to the calculation of the correlation function $G(r)$ between two sites separated by a distance r *along the horizontal row*. Once the finite TMRG has converged, we have the left $|\psi\rangle$ and right $|\varphi\rangle$ Perron vectors for each step during a sweep of the finite TMRG. The correlation between the two spins σ_L and σ_R can then be expressed as

$$\langle\sigma_L\sigma_R\rangle = \langle\psi|\widehat{\sigma}_L\widehat{\sigma}_R|\varphi\rangle = \sum_{\sigma_L\sigma_R}\sigma_L\sigma_R\sum_{\xi=\zeta,\alpha=\beta}\psi^\dagger_{\overline{\xi}\sigma_L\overline{\alpha}\sigma_R}\varphi_{\overline{\zeta}\sigma_L\overline{\beta}\sigma_R}, \tag{3}$$

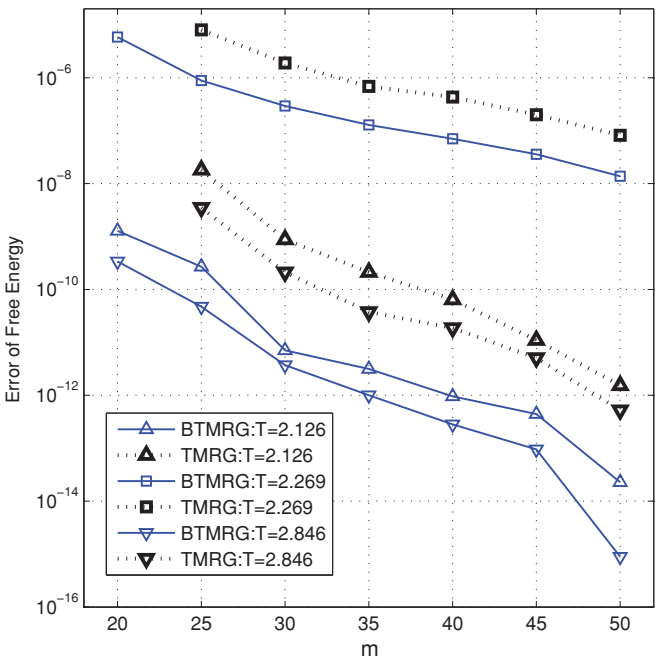

FIG. 3. (Color online) Comparison of accuracy between BTMRG and conventional TMRG algorithms. The error of the free energy of an Ising model is plotted for various m values at three prescribed temperatures: $\widehat{T} = 2.126 < \widehat{T}_c$, $\widehat{T} = 2.269 \approx \widehat{T}_c$, and $\widehat{T} = 2.846 > \widehat{T}_c$.

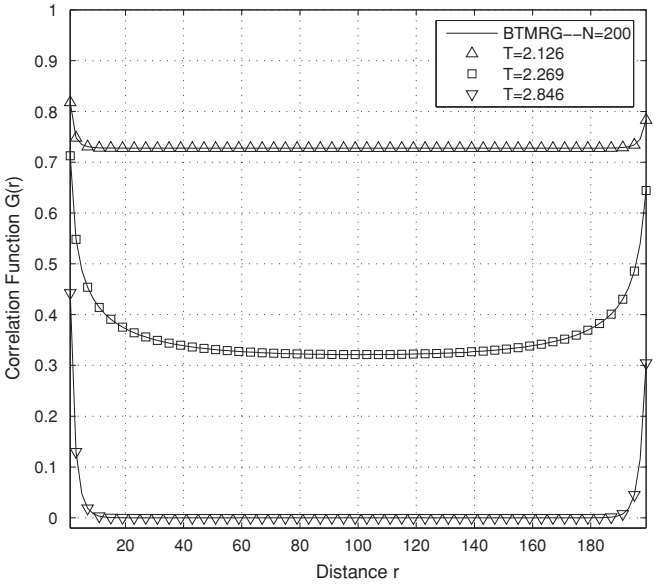

FIG. 4. Correlation function $G(r)$ of the Ising model with system size $N = 200$ at the temperatures given in Fig. 3. The number of states kept by BTMRG is $m = 18$.

where $\psi_{\overline{\xi}\sigma_L\overline{\alpha}\sigma_R}$ and $\varphi_{\overline{\zeta}\sigma_L\overline{\beta}\sigma_R}$ represent the coefficients of the left and right Perron vectors associated with the respective biorthonormal bases and satisfy the condition $\langle\psi|\varphi\rangle = \sum_{\sigma_L\sigma_R}\sum_{\xi=\zeta,\alpha=\beta}\psi^{\dagger}_{\overline{\xi}\sigma_L\overline{\alpha}\sigma_R}\varphi_{\overline{\zeta}\sigma_L\overline{\beta}\sigma_R} = 1$. Three correlation functions are plotted in Fig. 4 for system size $N = 200$ at the above three prescribed temperatures. The numerical errors are all controlled within the order of 10^{-8}. Since we conducted the simulations on an infinitely long vertical twisted cylindrical lattice that has boundary conditions (BCs) similar to *periodic-free BCs* (see [8]), the correlation function tends to be symmetric. As we expected, the upper curve corresponds to *ferromagnetism* with positive spin-spin correlation that increases with deceasing temperature, while the lower curve corresponds to *paramagnetism* with vanishing spin-spin correlation due to thermal fluctuations. (For an exact expression of the correlation function along the direction parallel to the axis of the cylinder for the ferromagnetic and paramagnetic regions, refer to [10].) The middle curve at the transition point is the critical two-point correlation function. To our knowledge, to date no suitable exact expression has been found for the critical correlation function on finite lattices [11]. However, it is well known [12] that at the thermodynamic limit, the critical correlation function of the Ising model behaves like $G(r) \propto r^{-1/4}[1 + O(r^{-2})]$ at large distance r. It is apparent that the result appears to be in accordance with such behavior as $N \to \infty$. Although, in [13], the infinite *time-evolving block decimation* (iTEBD) approach, independent of TMRG, has been proposed to evaluate partition functions of 2D classical models, and also allows for straightforward calculation of the two-point correlation function, we have to emphasize that the BTMRG with E·S·E scheme differs from iTEBD in several respects. First, BTMRG is a variational method, while iTEBD amounts to a power method. Second, BTMRG approaches the thermodynamic limit by extrapolating the finite-system calculation very accurately, while iTEBD directly treats the infinite system from the onset. Third, importantly for the calculation of two-point correlators, the E·S·E scheme obtains the correlation immediately in every single step of the finite-system sweep, without the extra effort of evaluating the tensor network between two points as in iTEBD, especially when the distance r is large (see Fig. 10 in [13]).

Finally, we would point out that within the framework of our BTMRG and the E·S·E scheme, all simulated states exactly enjoy a form of the so-called matrix product state (MPS) [14], which reads, for example, for the left Perron state

$$|\psi\rangle = \sum_{\tau_i\theta_i\sigma_L\sigma_R}\sum_{\xi_1,\alpha_1} \left(\overline{C}_1^{[\tau_1^L;\tau_1^R]}\cdots\overline{C}_t^{[\tau_t^L;\tau_t^R]}\Psi^{[\sigma_L;\sigma_R]}\overline{A}_s^{[\theta_s^L;\theta_s^R]\dagger}\cdots\overline{A}_1^{[\theta_1^L;\theta_1^R]\dagger}\right)_{\xi_1,\alpha_1} |\xi_1\tau_1^L\cdots\tau_t^L\sigma_L\theta_s^L\cdots\theta_1^L\alpha_1\theta_1^R\cdots\theta_s^R\sigma_R\tau_t^R\cdots\tau_1^R\rangle, \tag{4}$$

and the right Perron state has a similar representation with matrices $\overline{B}_i^{[\theta_i^L;\theta_i^R]}$ and $\overline{D}_i^{[\tau_i^L;\tau_i^R]}$. It is interesting to note that $\sum_{\theta_i^L,\theta_i^R}\overline{A}_i^{[\theta_i^L;\theta_i^R]\dagger}\overline{B}_i^{[\theta_i^L;\theta_i^R]} = I$ and $\sum_{\tau_i^L,\tau_i^R}\overline{C}_i^{[\tau_i^L;\tau_i^R]\dagger}\overline{D}_i^{[\tau_i^L;\tau_i^R]} = I$. Thus, our algorithm can be described equivalently in terms of *variational optimization* [15] within the class of MPS: Sweeping forward and backward through the chain, one keeps all matrices $\overline{A}$, $\overline{B}$, $\overline{C}$, and $\overline{D}$ fixed and seeks the coefficients $\psi_{\xi\sigma_L\alpha\sigma_R}$ and $\varphi_{\zeta\sigma_L\beta\sigma_R}$ that *maximize the partition function*.

V. CONCLUSIONS

This work presents a biorthonormal TMRG method for non-Hermitian matrices, which employs dual biorthonormal

bases to build a renormalized transfer matrix with only half the dimensions of a matrix from conventional TMRG. The biorthonormal bases always exist and can be easily accessed. In particular, the dual bases reduce to a single orthonormal basis for Hermitian cases. We propose a solution to the long-standing suspension problem of how to determine the density matrix of TMRG for non-Hermitian matrices. The BTMRG in combination with the E·S·E scheme is very robust and exhibits excellent accuracy, making it a more powerful and robust tool than conventional TMRG amd can be used in the investigation of all related fields. The BTMRG and the E·S·E scheme are also shown to be particularly adapted to the calculation of the two-point correlation function of 1D quantum or 2D classical lattice models.

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[1] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); U. Schollwoeck, Rev. Mod. Phys. **77**, 259 (2005); K. Hallberg, Adv. Phys. **55**, 477 (2006).
[2] T. Nishino, J. Phys. Soc. Jpn. **64**, 3598 (1995); T. Nishino and K. Okunishi, *ibid.* **66**, 3040 (1997).
[3] N. Shibata, J. Phys. A **36**, 381 (2003); A. E. Feiguin and S. R. White, Phys. Rev. B **72**, 220401 (2005).
[4] A. Kemper, A. Schadschneider, and J. Zittartz, J. Phys. A **34**, L279 (2001); T. Enss and U. Schollwock, *ibid.* **34**, 7769 (2001).
[5] E. Carlon, M. Henkel, and U. Schollwock, Phys. Rev. E **63**, 036101 (2001); S. Trebst *et al.*, Phys. Rev. Lett. **96**, 250402 (2006); M. Cramer *et al.*, *ibid.* **101**, 063001 (2008); T. Barthel *et al.*, Phys. Rev. A **79**, 053627 (2009).
[6] Y.-K. Huang and S.-N. Yu, Physica A **390**, 801 (2011).
[7] G. H. Golub and C. F. Van Loan, *Matrix Computations* (Johns Hopkins University Press, Baltimore, 1996).
[8] Y.-K. Huang and S.-N. Yu, Physica A **389**, 736 (2010).
[9] L. Onsager, Phys. Rev. **65**, 117 (1944).
[10] A. I. Bugrij, Theor. Math. Phys. **127**, 528 (2001); A. I. Bugrij and O. Lisovyy, *ibid.* **140**, 987 (2004).
[11] J. Kaupuzs, Comput. Methods Appl. Math. **5**, 72 (2005); Int. J. Mod. Phys. C **17**, 1095 (2006).
[12] H. Au-Yang and J. H. H. Perk, Int. J. Mod. Phys. B **16**, 2089 (2002).
[13] R. Orus and G. Vidal, Phys. Rev. B **78**, 155117 (2008).
[14] S. Ostlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995); M. A. Martin-Delgado and G. Sierra, Int. J. Mod. Phys. A **11**, 3145 (1996); S. Rommer and S. Ostlund, Phys. Rev. B **55**, 2164 (1997); U. Schollwock, Ann. Phys. **326**, 96 (2011).
[15] J. Dukelsky *et al.*, Europhys. Lett. **43**, 457 (1998); T. Nishino *et al.*, Int. J. Mod. Phys. B **13**, 1 (1999); F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004); F. Verstraete, V. Murg, and J. I. Cirac, Adv. Phys. **57**, 143 (2008).