Biorthonormal matrix-product-state analysis for the non-Hermitian transfer-matrix renormalization group in the thermodynamic limit

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Abstract. We give a thorough biorthonormal matrix-product-state (BMPS) analysis of the transfer-matrix renormalization group (TMRG) for non-Hermitian matrices in the thermodynamic limit. The BMPS is built on dual series of reduced biorthonormal bases for the left and right Perron states of a non-Hermitian matrix. We propose two alternative infinite-size biorthonormal TMRG (iBTMRG) algorithms and compare their numerical performances for both finite and infinite systems. We show that both iBTMRGs produce dual infinite-BMPS (iBMPS) which are translationally invariant in the thermodynamic limit. We also develop an efficient wavefunction transformation of the iBTMRG, in analogy with that of McCulloch for the infinite-DMRG (McCulloch, 2008 arXiv:0804.2509), for predicting the wavefunction as the lattice size is increased. The resulting iBMPS allows for probing bulk properties of the system in the thermodynamic limit without boundary effects and allows for reducing the computational cost to be independent of the lattice size; these findings are illustrated by calculating the magnetization as a function of the temperature and the critical spin-spin correlation in the thermodynamic limit for a 2D classical Ising model.

Keywords: classical phase transitions (theory), correlation functions (theory), density matrix renormalization group calculations

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1. Introduction

It has been widely understood that the matrix-product-state (MPS) ansatz constitutes the basis of many numerical algorithms in computational physics, notably the density-matrix renormalization group (DMRG) [1] and the time-evolving block decimation (TEBD) [2]. There are two main variants of the DMRG algorithm. The finite-size algorithm has now been realized to compute variationally the ground state of a strongly correlated 1D quantum system within the class of MPS [3]. While the infinite-size algorithm grows the system by adding iteratively one or more sites and reaches asymptotically, at the fixed point, a translationally invariant MPS state (invariant under translations of some fixed number of lattice sites), it was originally conceived as only for obtaining the initial MPS wavefunction in the thermodynamic limit. Until recently, interest in directly obtaining the translationally invariant MPS wavefunction in the thermodynamic limit was rekindled by the ideas of infinite-TEBD (iTEBD) of Vidal [4] and infinite-DMRG (iDMRG) of McCulloch [5]. Both approaches allow for probing bulk properties of the system in the thermodynamic limit without the influence of boundary conditions and the resulting infinite-MPS (iMPS) can reduce the computational cost of real-time simulation to be independent of the lattice size. The main difference between these two methods lies in the scheme for the local update of the tensors in the MPS. The iTEBD applies a single bond evolution operator to each site simultaneously which amounts to a power method, while the iDMRG obtains the center matrix variationally by using a very efficient local eigensolver.

On the other hand, after nearly two decades of development, the application of DMRG methods has spread over a great variety of fields. One major branch of the DMRG is
the transfer-matrix renormalization group (TMRG) which can be applied to, e.g., the strongly correlated classical systems [6], the thermodynamics of 1D quantum systems at finite temperature [7], the stochastic transfer matrix of a cellular automaton [8], the non-equilibrium systems in statistical physics [9], and the general Markov random field in image modeling [10]. In contrast to the DMRG, the TMRG usually deals with non-Hermitian matrices which involve much more numerical demand in view of the existence of distinct left and right Perron states (i.e., the eigenstates associated with the maximum eigenvalue which we will refer to as the Perron root) of the transfer matrix. This leads to the selection of the reduced density matrix becoming ambiguous. Enss and Schollwöck [8] had provided a comparative discussion on several choices of the density matrix proposed in the literature for the non-Hermitian TMRG. Unfortunately, all of these selections of density matrices cause the conventional TMRG fail to fit the framework of MPS analysis. In a recent paper [11], the author proposed a new TMRG algorithm called the biorthonormal transfer-matrix renormalization group (BTMRG) which employed a dual set of biorthonormal bases to construct the renormalized transfer matrix and reduced the numerical complexity for non-Hermitian matrices to the same as that for the Hermitian case. Numerical simulations for a real non-Hermitian matrix showed that the BTMRG exhibits significant improvement on the efficiency and accuracy over conventional TMRG. Here, dual biorthonormal bases indicate any two sets of vectors \( \{ |\alpha\rangle \}_{\alpha=1,\ldots,m} \) and \( \{ |\beta\rangle \}_{\beta=1,\ldots,m} \) to satisfy \( \langle \alpha | \beta \rangle = \delta_{\alpha\beta} \). In the previous paper, the BTMRG was described in a traditional formulation. In this paper, we will show that the employment of the biorthonormal bases enables the BTMRG to be perfectly reformulated within the framework of MPS analysis where the two Perron states can be represented as dual biorthonormal matrix product states (BMPS). We will propose two alternative methods for building the BMPS. At the same time, two natural questions arise. Does the infinite-size variant of the BTMRG (iBTMRG) create asymptotically dual infinite biorthonormal MPS (iBMPS) that are translationally invariant? Does there exist an efficient transformation in iBTMRG, just like the one in iDMRG [5], for predicting the wavefunction as the lattice size is increased? In this paper, both questions will be answered in the affirmative. Here, instead of the two-site iDMRG where the non-zero truncation of the wavefunction often leads to undesirable effects of the convergence of the iMPS [5], we will use the ‘single-site’ iBTMRG scheme which achieves zero truncation similarly to the single-site iDMRG. In addition, by using a special E · S · E configuration, the critical two-point correlation functions in the thermodynamic limit, especially when the distance between the two points approaches infinity, will be shown to be easily obtained.

The rest of this paper is organized as follows. In section 2, we present a brief review of the MPS analysis of the standard DMRG in finite systems and reformulate the BTMRG algorithm with the E · S · E configuration proposed in [11] entirely in terms of the BMPS language. In section 3, we propose two alternative methods for building the BMPS of the left and right Perron states for non-Hermitian matrices and develop an iBTMRG algorithm for obtaining asymptotics of the dual iBMPS wavefunctions that are translationally invariant. We also develop an efficient wavefunction transformation in iBTMRG for predicting the BMPS as the lattice size is increased. Section 4 compares the numerical performances of our iBTMRG algorithms in finite systems for a real
non-Hermitian matrix of an anisotropic Ising model. The magnetization as a function of the temperature and the critical two-point correlation function of an isotropic Ising model in the thermodynamic limit are also plotted. Finally, in section 5, some conclusions are drawn.

2. Biorthonormal MPS analysis of BTMRG in finite systems

The connection between DMRG and MPS was first found by Östlund and Rommer [12] who identified the thermodynamic limit of DMRG with a position-independent matrix product wavefunction. The discovery of the MPS on which the DMRG operates has placed the algorithm on a firm footing, provided a deeper understanding, and allowed a concrete and easy to manipulate description of the DMRG. The standard DMRG and MPS formulation was established on a series of reduced orthonormal bases. However, when considering both left and right Perron states of non-Hermitian transfer matrices, the MPS must be built on dual series of reduced biorthonormal bases which we will refer to as biorthonormal matrix product states (BMPS). In this section, we briefly review the finite-size BTMRG algorithm proposed in [11] but reformulate it entirely in terms of a BMPS language. For further information about MPS, see [13].

2.1. MPS formulation of DMRG in finite systems

Let us start with the MPS formulation of the standard DMRG in finite systems. Throughout this paper, we focus on the MPS for open boundary conditions. A spin chain can be bi-partitioned into two parts: the system block where the spins are labeled with \( s_i \), and the environment block where the spins are labeled with \( \varepsilon_i \). Then we denote an MPS on an \( L \)-site lattice by the form

\[
|\psi\rangle = \sum_{s_1,\varepsilon_1} A_1^{s_1} \cdots A_p^{s_p} \Lambda E_q^{\varepsilon_q} \cdots E_1^{\varepsilon_1} |s_1 \cdots s_p \varepsilon_q \cdots \varepsilon_1\rangle
\]  

(1)

where \( p + q = L \) and each matrix at each site has dimension \( m \times m \) with the exception that the end matrices \( A_1^{s_1} \) and \( E_1^{\varepsilon_1} \) are a row vector and a column vector respectively. The \( A \) matrices (\( E \) matrices) satisfy the left-normalization (right-normalization) condition \( \sum_{s_i} A_i^{s_i \dagger} A_i^{s_i} = I \) (\( \sum_{\varepsilon_i} E_i^{\varepsilon_i \dagger} E_i^{\varepsilon_i} = I \)). It is very useful to express an MPS in a tensor network representation (see Schollwöck [13]) as in figure 1(a). For example, the set of matrices \( A_p^{s_p} \) at the \( p \)th site of the system block corresponds to a tensor \( (A_p)^{s_p}_{\alpha_{p-1},\alpha_p} \) with two bond indices \( \alpha_{p-1} \) and \( \alpha_p \) and one physical index \( s_p \). The bond index labels the reduced orthonormal basis state of the system block at different lengths and the physical index labels the state of the spin. Thus the center matrix \( \Lambda \) represents in fact the wavefunction of the superblock in the reduced orthonormal basis \( \{|\alpha_p \varepsilon_q\rangle\}_{\alpha,\xi=1,\ldots,m} \) (see figure 1(a)). The essential notion of the MPS formulation of the finite-size variant of DMRG is that of local updates; that is, we free one matrix, say \( E_p^{s_p} \), at a time while keeping the others fixed, update it using \( A_p^{s_p+1} \) through an efficient optimization of the total energy, and shift the center matrix to the right by one site. When all matrices in the MPS have been updated once, this is called a sweep. Repeat the sweeps until convergence is reached.
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Figure 1. (a) The tensor network representation of the MPS in the standard $S \cdot E$ configuration. (b) The tensor network representation of the MPS in our special $E \cdot S \cdot E$ configuration.

2.2. The $E \cdot S \cdot E$ scheme and the related BMPS representation

Now consider a special bi-partitioning of the chain as indicated by the notation $E \cdot S \cdot E$ where the system block is taken as a consecutive segment of sites around the center of the chain and the environment block is taken as two equal separate segments surrounding the system block. The superblock is updated at a certain time by freeing (or adding) two spins in between the two subsystems, so the matrices of the MPS must be associated with two distant sites. This special configuration is shown to be particularly adapted to the calculation of two-point correlation functions of 1D quantum systems or 2D classical lattice models [11]. Actually, the MPS for this $E \cdot S \cdot E$ scheme can be formulated equivalently to the MPS for the standard DMRG. By folding the spin chain from the center so that the two subsystems and the two free spins are aligned, every two aligned spins can be regarded as a single big spin and the resulting new chain has the same configuration as the more standard $S \cdot E$ scheme. To avoid the notation getting too involved, it is convenient and comprehensive to represent this MPS as a tensor network as in figure 1 (b) where the tensor $(A_p)_{\alpha_{p-1}, \alpha_p}$, now, with two physical indices representing the states of the two spins.

Alternatively, following McCulloch [5], such an MPS can be simply expressed as

$$|\psi\rangle = A^1_p \cdots A^p \Lambda E^q_1 \cdots E^q_1.$$  

In this notation, although the ket basis vectors of the MPS are suppressed and the alphabets labeling the states of the aligned spin pairs are simply denoted by two dots, all information is preserved. It is easy to understand that, here, the MPS matrices are local state valued, although this is not explicitly written.

When a non-Hermitian transfer matrix $T$ is considered, the left and right Perron states are generally distinct. Suppose the left $|\psi\rangle$ and right $|\varphi\rangle$ Perron states have MPS as follows:

$$|\psi\rangle = A_1^1 \cdots A_p \Lambda E_1 \cdots E_1 \quad |\varphi\rangle = B_1 \cdots B_p \Gamma F^q_1 \cdots F_1.$$  

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Figure 2. The tensor network representation of the reduced transfer matrix $T$ associated with the dual BMPS of BTMRG on the E·S·E configuration.

When we free the two spins associated with the matrices $E_q$ and $F_q$, we are actually carrying out the local updating by maximizing the quantity $\langle \psi | T | \phi \rangle - \lambda \langle \psi | \phi \rangle$. Hence, if we impose the so-called left- and right-biorthonormal conditions on the MPS matrices

$\sum_{B_i} B_i^\dagger A_i = \sum_{F_i} F_i^\dagger E_i = I \quad (4)$

then the optimization will be equivalent to an eigenvalue problem of the reduced transfer matrix $T$ that can be expressed as a tensor network as in figure 2 (see Schollwöck [13]) where the transfer matrix $T$ is expressed as a matrix product operator (MPO) and $\sigma_L$ and $\sigma_R$ label the states of the free distant spin pair associated with the matrices $E_q$ and $F_q$. The matrix elements of the reduced transfer matrix can be written explicitly as $T_{\alpha_p, \beta_p, \sigma_L, \sigma_R, \xi_{q-1}, \xi_q} = \langle \alpha_p | \sigma_L \sigma_R | \xi_{q-1} \rangle | T | \beta_p | \sigma'_L \sigma'_R | \xi_q \rangle$. If the pair of MPS states of equation (3) satisfies the biorthonormal conditions of equation (4), we refer to the MPS as a dual BMPS. Thus, the BTMRG algorithm can be perfectly fitted into the framework of MPS analysis and enjoy the same numerical complexity as the Hermitian case in DMRG algorithm. In this paper, we will propose two alternative methods for determining the BMPS for the Perron state and compare their numerical performances. The details will be described in section 3.

2.3. The density matrix and the canonical form of BMPS representations

Unlike for the Hermitian Hamiltonian in DMRG, where there is a unique normalized ground state, there are two distinct Perron states in TMRG so the density operator for the Perron state of the system must be taken as $\hat{\rho} = |\varphi \rangle \langle \psi |$ (with proper normalization $\langle \psi | \varphi \rangle = 1$). Thus, from equation (3), we can readily obtain the reduced density operator for the system and environment block as

$\hat{\rho}_S = \sum_{\beta_p, \alpha_p} (\Gamma A)_{\beta_p, \alpha_p} | \beta_p \rangle \langle \alpha_p | \quad \hat{\rho}_E = \sum_{\xi_q, \xi_q} (\Gamma E)_{\xi_q, \xi_q} | \xi_q \rangle \langle \xi_q | \quad (5)$

Note that $\langle \alpha_p | \beta_p \rangle = \delta_{\alpha \beta}$ and $\langle \xi_q | \xi_q \rangle = \delta_{\xi \xi}$ in view of the biorthonormal conditions. However, given a BMPS as in equation (3), we can always construct another BMPS by introducing an arbitrary invertible (non-unitary) transformation of the matrices $E_q$ and $F_q$ (i.e., applying a non-unitary basis transformation $X$ to the current biorthonormal bases
{\ket{\xi_q}} and {\ket{\zeta_q}} such that \( \overline{E}_q = X^{-1}E_q \) and \( \overline{F}_q = X^T F_q \) remain right-biorthonormal. Similar results \( \overline{A}_p = A_p Y^{-1}\) and \( \overline{B}_p = B_p Y \) are obtained by applying a transformation \( Y \) to the current biorthonormal bases \( \{\ket{\alpha_p}\} \) and \( \{\ket{\beta_p}\} \). Thus the varied BMPS turns out to be

\[
|\psi\rangle = \overline{A}_1 \cdots \overline{A}_p \overline{V} \overline{E}_q \cdots \overline{E}_1 \quad |\varphi\rangle = \overline{B}_1 \cdots \overline{B}_p \overline{V} \overline{F}_q \cdots \overline{F}_1
\]

where the new center matrices become \( \overline{X} = Y^\dagger \overline{X} Y \) and \( \overline{Y} = Y^{-1} \overline{Y}^{-1} \) and the new reduced density operators are simply a similar transform of the old density operators: \( \overline{\rho}_S = Y^{-1} \overline{\rho}_S Y \) and \( \overline{\rho}_E = X^{-1} \overline{\rho}_E X \). This implies that if we employ a suitable transformation, we can canonize the form of the BMPS representation.

Given the BMPS in equation (3), assume that the density matrix \( \rho_S = \overline{1} \overline{X} \) is diagonalizable; then it can be readily obtained that \( \rho_E = \overline{1} \overline{X} Y^{-1} X \overline{D} X^{-1} \) where \( X = \overline{1} \overline{Y}^{-1} \). Since \( X \) and \( Y \) are unique up to a scaling, we can replace \( X \) and \( Y \) by \( \lambda_1 I \) and \( \lambda_2 I \) where \( \lambda_1 \) and \( \lambda_2 \) are two diagonal matrices. Accordingly, we have new center matrices \( \overline{X} = \lambda_1 D \overline{X} = \sqrt{D} \) and \( \overline{Y} = \lambda^{-1}_2 \lambda^{-1}_1 \) on choosing \( \lambda_2 = D^{-1/2} \lambda^{-1}_1 \). Thus the canonical form of BMPS reads

\[
|\psi\rangle = \overline{A}_1 \cdots \overline{A}_p \sqrt{D} \overline{E}_q \cdots \overline{E}_1 \quad |\varphi\rangle = \overline{B}_1 \cdots \overline{B}_p \sqrt{D} \overline{F}_q \cdots \overline{F}_1
\]

and the density matrix bears the canonical form \( \rho_S = \rho_E = D \). Surprisingly, according to our practical simulation, for large enough system size, \( \rho_S = YDY^{-1} \) always exists and the eigenvalues are always real non-negative.

3. Biorthonormal MPS analysis of iBTMRG in the thermodynamic limit

The iDMRG grows the system at a certain time by adding one or two sites at the center of the lattice and produce a fixed point of iMPS that is translationally invariant. By thinking of each aligned spin pair as a big spin, our iBTMRG with the E·S·E configuration can be formulated equivalently to the iDMRG. Throughout this paper, we choose the ‘single-site’ iBTMRG algorithm for the following reasons. First, ‘two-site’ iBTMRG means adding four spins at a time where the dimension of the reduced transfer matrix significantly increases. Second, the inevitable non-zero truncation of the wavefunction of the two-site iBTMRG often leads to a less well converged wavefunction [5]. Third, the single-site iBTMRG can achieve zero truncation of the wavefunction and the problem of being trapped in local minimum can be avoided by introducing White’s correction [14] to the reduced biorthonormal bases.

In this paper, many formulations are derived from a common basic procedure which we will refer to as the Biorthonormalization Procedure. Given two arbitrary bases \( \{\ket{\alpha}\}_{a=1,\ldots,m} \) and \( \{\ket{\beta}\}_{b=1,\ldots,m} \), suppose that \( A \equiv [\ket{\alpha}_{a=1,\ldots,m}] \) and \( B \equiv [\ket{\beta}_{b=1,\ldots,m}] \) are two matrices formed with \( \ket{\alpha} \) and \( \ket{\beta} \) as their columns respectively. By carrying out the singular-value decomposition (SVD) \( A^\dagger B \equiv U \Sigma V^\dagger \), we can readily obtain \( (AP)^\dagger (BW) = I \) where \( P = U \Sigma^{-1/2} \) and \( W = V \Sigma^{-1/2} \). This means that, by applying the non-unitary basis transformation \( P \) and \( W \) to the original bases \( \{\ket{\alpha}\} \) and \( \{\ket{\beta}\} \), we can obtain dual biorthonormal bases \( AP \) and \( BW \).

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3.1. Two alternative iBTMRG algorithms in the thermodynamic limit

We first propose an iBTMRG algorithm for which the main steps are depicted in figure 3. The iBTMRG starts with an initialization procedure (i.e., \( n = 1 \)) which selects a minimum length of the lattice (which depends on the number \( m \) of states kept by BTMRG), obtains the respective reduced bases of the two subsystems from the Perron states, and proceeds to biorthonormalize them. The routine in figure 3 grows the lattice by first adding two sites to the system block and then adding two sites to the environment block, which constitutes a period of the whole algorithm with respect to a repeated fragment of the final iBMPS.

At each time when adding new sites to the lattice, we obtain the Perron states (e.g., \( \psi \)) in the reduced biorthonormal bases, carry out an SVD for the Perron states to obtain the reduced bases of the enlarged block (e.g., \( \psi = A_{n+1} \Lambda_{n+1} \psi \) where \( \sum_{n} A_{n+1}^* A_{n+1} = I \)), and biorthonormalize them to build new biorthonormal bases of the enlarged block (e.g., the right bond states of the tensors \( \overline{A}_{n+1} \) and \( \overline{E}_{n+1} \)). If the lattice size grows large enough, we can additionally canonize the BMPS. This step is convenient for the purpose of checking the convergence of the algorithm. According to the previous description, the biorthonormalization and the canonization procedures are simply applying two successive non-unitary basis transformations to the bases obtained from the SVD; we can combine these transformations together and denote them by \( P, W, Q, R \) with respect to the \( A, B, E, \) and \( F \) matrices respectively (e.g., \( \overline{A}_{n+1} = A_{n+1} P_{n+1} \) and \( \overline{E}_{n+1} = E_{n+1} F_{n+1} \), and thus \( \overline{A}_{n+1} = P_{n+1}^{-1} A_{n+1} Q_{n+1}^{-1} \)). Note that, during the SVD in step 2, we retain zero truncation of the wavefunction when obtaining the reduced basis of the enlarged block. The resulting BMPS read

\[
|\psi\rangle = \overline{A}_1 \cdots \overline{A}_n \overline{\Lambda}_n E_1^c \cdots E_1 \quad |\varphi\rangle = \overline{B}_1 \cdots \overline{B}_n \overline{\Gamma}_n F_1^c \cdots F_1 \tag{8}
\]

The above algorithm builds the biorthonormalized bases from the reduced bases derived from the SVD that are based on other biorthonormal bases. One may notice that there actually exist a lot of possibilities for building the biorthonormal bases. Nevertheless, the process of SVD is critical. We can also jump the SVD and directly biorthonormalize \( \psi^c \) and \( \varphi^c \). But such a numerical procedure will become unstable very quickly. Here, we provide another algorithm which is very different from the above algorithm in nature. The alternative algorithm is depicted in figure 3 with the steps 2–3 enclosed in a rectangle being replaced by the routine depicted in figure 4. In contrast, this algorithm constructs the biorthonormalized bases from the reduced bases derived from the SVD that are based on two orthonormal bases. The first major change lies in step 2 where before performing SVD the Perron states must be restored to being in terms of their own orthonormal bases, e.g., \( \psi^c = P_n \psi Q_n \). The second change lies in step 3 where before performing the biorthonormalization procedure the reduced bases derived from the SVD must be transformed back to being in terms of the previous biorthonormal bases, e.g., \( A_{n+1}^c = P_{n+1}^{-1} A_{n+1} \). As it turns out, two remarkable properties emerge, e.g., \( \overline{A}_{n+1} = P_{n+1}^{-1} A_{n+1} P_{n+1} \) and \( \overline{A}_1 \cdots \overline{A}_n = A_1 \cdots A_n P_{n+1} P_{n+1} \). A similar relation holds for the \( B, E, \) and \( F \) matrices. Accordingly, the BMPS can also be expressed in terms of two series of reduced orthonormal bases:

\[
|\psi\rangle = A_1^c \cdots A_n \Lambda_n E_1^c \cdots E_1 \quad |\varphi\rangle = B_1 \cdots B_n \Gamma_n F_1^c \cdots F_1 \tag{9}
\]

where \( \Lambda_n = P_n \Lambda_n Q_n \) and \( \Gamma_n = W_n \Gamma_n R_n \). For convenience, in this paper, the former algorithm will be referred to as iBTMRG A and the latter as iBTMRG B.
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\[ \cdots \rightarrow A_n \rightarrow \Lambda_n \rightarrow E_n \rightarrow \cdots \]
\[ \rightarrow B_n \rightarrow \Gamma_n \rightarrow F_n \rightarrow \cdots \]

Step 1. Adding two sites to the system block and obtain the Perron states

\[ \cdots \rightarrow A_n \psi \rightarrow E_n \rightarrow \cdots \]
\[ \rightarrow B_n \varphi \rightarrow F_n \rightarrow \cdots \]

Step 2. Perform SVD

\[ \cdots \rightarrow A_n \rightarrow A_{n+1} \rightarrow \Lambda_{n+1} \rightarrow E_n \rightarrow \cdots \]
\[ \rightarrow B_n \rightarrow B_{n+1} \rightarrow \Gamma_{n+1} \rightarrow F_n \rightarrow \cdots \]

Step 3. Perform Biorthonormalization

\[ \cdots \rightarrow A_n \rightarrow A_{n+1} \rightarrow \Lambda_{n-1} \rightarrow E_n \rightarrow \cdots \]
\[ \rightarrow B_n \rightarrow B_{n+1} \rightarrow \Gamma_{n+1} \rightarrow F_n \rightarrow \cdots \]

Step 4. Canonize the BMPS

\[ \cdots \rightarrow \sqrt[\rightarrow A_n \rightarrow A_{n+1} \rightarrow \sqrt[D_{n+1}E_n \rightarrow \cdots \]
\[ \rightarrow B_n \rightarrow B_{n+1} \rightarrow \sqrt[D_{n+1}F_n \rightarrow \cdots \]

Repeat Step 1-4. Adding two sites to the environment block

**Figure 3.** The main steps of iBTMRG A, which grows the lattice by first adding two sites to the system block and then adding two sites to the environment block, constitute a period of the algorithm with respect to a repeated fragment of the final iBMPS.
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Step 2.1  
Restore the bases

\[ \cdots \rightarrow A_n^i \rightarrow P_n \psi_n^i Q_n \rightarrow F_n^i \rightarrow \cdots \]
\[ \cdots \rightarrow B_n^i \rightarrow W_n \varphi_n^i R_n \rightarrow F_n^i \rightarrow \cdots \]

Step 2.2  
Perform SVD

\[ \cdots \rightarrow A_{n+1}^i \rightarrow A_{n+1}^i - \Lambda_{n+1}^i \rightarrow F_n^i \rightarrow \cdots \]
\[ \cdots \rightarrow B_{n+1}^i \rightarrow B_{n+1}^i - \Gamma_{n+1}^i \rightarrow F_n^i \rightarrow \cdots \]

Step 3.1  
Change the bases

\[ \cdots \rightarrow \bar{A}_n^i \rightarrow P_n^{-1} A_{n+1}^i - \bar{\Lambda}_{n+1}^i \rightarrow \bar{E}_n^i \rightarrow \cdots \]
\[ \cdots \rightarrow \bar{B}_n^i \rightarrow W_n^{-1} B_{n+1}^i - \bar{\Gamma}_{n+1}^i \rightarrow \bar{F}_n^i \rightarrow \cdots \]

Step 3.2  
Perform Biorthonormalization

\[ \cdots \rightarrow \bar{A}_n^i \rightarrow \bar{A}_{n+1}^i - \bar{\Lambda}_{n+1}^{\prime} \rightarrow \bar{E}_n^{\prime} \rightarrow \cdots \]
\[ \cdots \rightarrow \bar{B}_n^i \rightarrow \bar{B}_{n+1}^i - \bar{\Gamma}_{n+1}^{\prime} \rightarrow \bar{F}_n^{\prime} \rightarrow \cdots \]

**Figure 4.** The main steps of iBTMRG B are the same as those of iBTMRG A but with the steps 2–3 enclosed in a rectangle in figure 3 replaced by the routine depicted in this figure.

### 3.2. Efficient wavefunction prediction and the fixed point of the iBMPS

In both algorithms, the iBTMRG uses a local eigensolver to obtain the Perron vectors. A good initial guess for the eigenvector will significantly improve the performance of the eigensolver. In [5], McCulloch has developed a wavefunction transformation in iDMRG for the prediction of the wavefunction as the lattice size is increased. Such a transformation
can be effectively translated to our iBTMRG. Therefore, at the end of the first half-period of the process in figure 3, the prediction of the next Perron vectors will be

\[
\psi_{\text{trial}} = D_{n+1}^{1/2} D_n^{-1/2} \overline{A}_{n+1} \psi_{\text{current}} = D_{n+1}^{1/2} D_n^{-1/2} \psi,
\]

\[
\varphi_{\text{trial}} = D_{n+1}^{1/2} D_n^{-1/2} \overline{B}_{n+1} \varphi_{\text{current}} = D_{n+1}^{1/2} D_n^{-1/2} \varphi,
\]

where \(D_{n+1}^{1/2}\) and \(\psi\) are the current canonical center matrix and the current Perron vector. Similar results hold for the Perron vector prediction at the end of the second half-period in figure 3:

\[
\psi_{\text{trial}} = \overline{A}_{n+1} D_n^{-1/2} D_n^{1/2} = \psi D_n^{-1/2} D_n^{1/2} = \psi_{\text{current}}
\]

\[
\varphi_{\text{trial}} = \overline{B}_{n+1} D_n^{-1/2} D_n^{1/2} = \varphi D_n^{-1/2} D_n^{1/2} = \varphi_{\text{current}}.
\]

Note that, for finite fixed \(n\), the center matrix \(D_n^{1/2}\) may not be identical for the two half-periods in figure 3, so the center matrices in equations (10)–(11) should use their own \(D_n^{1/2}\). When the size of the lattice is small, the \(D_n^{1/2}\) can be replaced by \(\overline{A}_n\) and \(\overline{B}_n\).

At the fixed point of the iBTMRG, the translational invariant iBMPS should bear the canonical form

\[
|\psi\rangle = \cdots (D_n^{-1/2} \overline{A}_n D_n^{1/2} \overline{E}_n)(D_{n-1}^{-1/2} \overline{A}_{n-1} D_{n-1}^{1/2} \overline{E}_{n-1}) \cdots
\]

\[
|\varphi\rangle = \cdots (D_n^{-1/2} \overline{B}_n D_n^{1/2} \overline{F}_n)(D_{n-1}^{-1/2} \overline{B}_{n-1} D_{n-1}^{1/2} \overline{F}_{n-1}) \cdots
\]

where we take \(n\) to be the iteration step when the convergence criterion is met. At the fixed point, the density matrix would be invariant no matter where the bond is located. This leads to the fixed point criterion \(\sum \overline{A}_n D_n \overline{B}_n^\dagger = D_{n-1}\). Since Tr\((D_n) = 1\) (with proper normalization \(\langle \psi|\varphi\rangle = 1\)), one way of measuring the closeness of the two density matrices \(D_{n-1}\) and \(D_n^* = \sum \overline{A}_n D_n \overline{B}_n^\dagger\) is given by the Kullback–Leibler divergence

\[
D_{KL} = \sum_i D_{n-1}(i) \log \left( \frac{D_{n-1}(i)}{D_n(i)} \right).
\]

In this paper, equation (13) is utilized to check the convergence of our iBTMRG.

### 3.3. Normalization of the iBMPS

The fixed point criterion \(\sum \overline{A}_n D_n \overline{B}_n^\dagger = D_{n-1}\) is equivalent to \(\sum_i (D_n^{-1/2} \overline{A}_n D_n^{1/2})(D_{n-1}^{-1/2} \overline{B}_n D_{n-1}^{1/2})^\dagger = I\) which means that the two matrices \(D_n^{-1/2} \overline{A}_n D_n^{1/2}\) and \(D_{n-1}^{-1/2} \overline{B}_n D_{n-1}^{1/2}\) satisfy the right-biorthonormal condition. Similarly, \(D_n^{1/2} \overline{E}_n D_n^{-1/2}\) and \(D_{n-1}^{1/2} \overline{F}_n D_{n-1}^{-1/2}\) must satisfy the left-biorthonormal condition. Thus, the overlap of the iBMPS in equation (12) must be exactly \(\langle \psi|\varphi\rangle = 1\) at the fixed point. The normalization \(\langle \psi|\varphi\rangle = 1\) is important when we want to apply the iBMPS to the calculation of the expectation value or correlation functions in the thermodynamic limit. However, in practical simulations, the finite number \(m\) of states retained by BTMRG and finite iterations can only reach an approximation of the fixed point, so the iBMPS will not be exactly normalized. In [15], Orús and Vidal have developed a method for the orthonormalization of an iMPS in iTEBD, which can also be effectively translated to our iBTMRG. Define two transfer operators \(T_R\) and \(T_L\) as shown in figure 5. In order to achieve the right-biorthonormal condition, assume that \(\Omega_R\)

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In this section, we test our iBTMRG A and iBTMRG B algorithms on a 2D classical Ising model. The target matrix is $\Pi_q^N$ where $\Pi_q$ is the non-Hermitian fundamental transfer

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Figure 6. The comparison of the infinite-size (iBTMRG) and finite-size (fBTMRG) variants of three BTMRG algorithms, by plotting the error of the free energy of an anisotropic Ising model with lattice size $N = 160$ at the critical temperature $T_c = 2/\log(1 + \sqrt{2})$.

matrix of the general local energy function-parameterized Markov random field on an infinitely long vertical twisted cylindrical lattice with peripheral length $N$ [10, 16]. (The Ising model is just a special case of a Markov random field.) This matrix is intimately related to a 2D Markov additive process and enjoys a very special SVD structure and many fascinating properties [16].

4.1. iBTMRG in finite systems

Our iBTMRG algorithms can also be applied to the partition function calculation of classical models in finite lattices. The method used to build the reduced biorthonormal bases in iBTMRG A is essentially the same as the previous BTMRG in [11] which we will refer to as iBTMRG C for convenience. However, the system-growing strategy of iBTMRG C is different from that of the single-site iBTMRG. For the same $E \cdot S \cdot E$ configuration, the previous BTMRG grows the system by adding two sites at each iteration to the system block while keeping the environment block fixed and small. To our knowledge, both proposed single-site iBTMRG algorithms had never been tested before. Here, we will compare the performances of our iBTMRG algorithms and the previous one by computing the free energy of the Ising model on a finite 2D lattice. Figure 6 shows the error of the free energy (i.e., the logarithm of the Perron root of the transfer matrix $\Pi_q$) of an anisotropic Ising model ($J_x = -J_y$ where $J_x$ and $J_y$ represent the interaction between horizontally and vertically neighboring spins) at the critical temperature $T_c = 2/\log(1 + \sqrt{2})$ for system size $N = 160$ and various numbers of states $m$ kept by iBTMRG. We also compare the performances of the finite-size variant of BTMRG (fBTMRG) for the three algorithms where the Perron states from the iBTMRG
The fidelity $1 - \langle \psi^{\text{trial}} | \psi^{\text{opt}} \rangle$ between the Perron state predictors and the optimal ones for the anisotropic Ising model at criticality with $m = 40$ states kept in the reduced basis. The inset shows the convergence of the Kullback–Leibler divergence to the fixed point of the iBMPS with respect to the number of iterations.

Figure 7. The fidelity $1 - \langle \psi^{\text{trial}} | \psi^{\text{opt}} \rangle$ between the Perron state predictors and the optimal ones for the anisotropic Ising model at criticality with $m = 40$ states kept in the reduced basis. The inset shows the convergence of the Kullback–Leibler divergence to the fixed point of the iBMPS with respect to the number of iterations.

were used as the initial BMPS states and were further optimized variationally. From figure 6, we can see that iBTMRG A and B exhibit almost identical performances which were further slightly improved by their variational finite-size variants. For iBTMRGs, algorithms A and B give rise to very close results and only outperform algorithm C a little. Although iBTMRG C has the merit of high efficiency, it is interesting to note that its accuracy is far poorer and remains constant for all values of $m$. This is because, in the system-growing stage, the size of the environment block is kept fixed and small, so the entanglements between the two subsystems remain fixed and small irrespective of the reduced basis size $m$.

4.2. iBTMRG in the thermodynamic limit

In iBTMRG, finding the Perron states using an iterative eigensolver is the most time-consuming part, so the overlap between the initial wavefunction and the variational optimum $\langle \psi^{\text{trial}} | \psi^{\text{opt}} \rangle$ will dominate the performance of an iBTMRG algorithm. Figure 7 shows the fidelity $1 - \langle \psi^{\text{trial}} | \psi^{\text{opt}} \rangle$ (see [5]) between the Perron states predictors and the optimal ones for the above anisotropic Ising model at criticality with $m = 40$ states kept in the reduced basis. Before the peripheral size of the system grows larger than $N = 50$, the center matrices in equations (10) and (11) must be replaced by the uncanonized center matrix $\bar{\Lambda}_n$ and $\bar{\Gamma}_n$ since the density matrices cannot be diagonalized to real positive eigenvalues until $N = 50$. From figure 7, the uncanonized center matrices seem inappropriate for the usage of the wavefunction transformation. Once the canonical center matrices are utilized, the fidelity quickly drops down to $10^{-6}$ and continues to decay at a nearly constant rate. Moreover, the two predictions for algorithms A and B have very
similar effectiveness and the right Perron state transformation appears to prevail with respect to the left Perron state transformation. Another important issue concerns the convergence of the translationally invariant fixed point of the iBMPS. In this paper, we use the Kullback–Leibler divergence to monitor the convergence of the algorithm. The inset of figure 7 shows the convergence to the fixed point of the iBMPS with respect to the number of iterations. In view of the degeneracy of the Perron root and the long-range spin correlation at the criticality, the convergence appears to be quite slow. However, in off-critical regions, the convergence can be as fast as reaching $10^{-12}$ as the size exceeds $N = 200$.

Once we have the translationally invariant iBMPS (after the normalization $\langle \psi \mid \varphi \rangle = 1$), the calculation of the expectation value or the two-point correlator in the thermodynamic limit can be very efficient. For illustration, we take an isotropic ($J_x = J_y = J$) Ising model as an example and calculate its magnetization as a function of the temperature and its spin–spin correlation function at the critical temperature. Now consider equation (16); if we free the unit cells $\psi_{\alpha,\xi}^{\sigma_L,\sigma_R,\sigma_R'} \equiv D_n^{1/2}(D_n^{-1/2}A_{\alpha,\xi}^{\sigma_L,\sigma_R} D_n^{1/2}F_{\sigma_R})$ and $\varphi_{\beta,\zeta}^{\sigma_L,\sigma_R,\sigma_R'} \equiv D_n^{1/2}(D_n^{-1/2}B_{\beta,\zeta}^{\sigma_L,\sigma_R} D_n^{1/2}F_{\sigma_R})$, then we have Perron states in the thermodynamic limit expressed as $\psi_{\alpha,\xi}^{\sigma_L,\sigma_R,\sigma_R'}$ and $\varphi_{\beta,\zeta}^{\sigma_L,\sigma_R,\sigma_R'}$ with respect to dual biorthonormal bases. Note that the spins $\sigma_L, \sigma_R$ are two neighboring spin pairs located on the left side and right side of the system block, and the spins $\sigma_L', \sigma_R'$ are two (infinitely) far distant aligned spins. Therefore, the magnetization in the thermodynamic limit can be calculated by using

$$\langle \sigma_R \rangle = \sum_{\sigma_R} \sum_{\alpha=\beta,\xi=\zeta} \sum_{\sigma_L,\sigma_R'} \psi_{\alpha,\xi}^{\sigma_L,\sigma_R,\sigma_R'} \varphi_{\beta,\zeta}^{\sigma_L,\sigma_R,\sigma_R'}.$$ 

(17)

For an infinite 2D isotropic Ising model, the exact solution for the magnetization is $(1-(\sinh(2J/k_B T))^{-1})^{1/8}$ [17]. Here, we compute the magnetization by using equation (17) and the exact formula as in figure 8 where the inset shows the relative error between the
Figure 9. The scaling behavior of the spin–spin correlator of an isotropic Ising model at the critical temperature obtained from equation (18) which is compared with the exact solution.

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Numerical result and the exact one. Similarly, the spin–spin correlation between two infinitely far distant spins in the thermodynamic limit can be calculated by using

\[
\langle \sigma_L \sigma_R \rangle = \sum_{\sigma_L, \sigma_R} \sum_{\alpha = \beta, \xi = \zeta} \psi_{\alpha, \xi} \phi_{\beta, \zeta} \sigma_L \sigma_R \sigma_L' \sigma_R'.
\]  

(18)

At the critical temperature, the exact spin–spin correlation function scales as \( G(r) \propto r^{-1/4}(1 + O(r^{-2})) \) [18]. Ideally, equation (18) will be zero, but in practice it can only be seen as the correlation of two spins separated by a distance \( r \) equal to half of the system size \( N \) where the fixed point criterion is met. This implies that we can regard equation (18) as the correlation function in the thermodynamic limit as \( r = N/2 \). Figure 9 shows the scaling behavior of the spin–spin correlator compared with the exact solution. It is worthy of note that, in the region at low temperature near criticality, our iBTMRG is quite prone to getting stuck. Fortunately, on introducing White’s correction [14] to the reduced biorthonormalized bases, the algorithm exhibits much improved efficiency and convergence with the correction weight around \( 10^{-3} \)–\( 10^{-4} \). In [15], Orú and Vidal have conducted the same calculation as in figures 8 and 9 by using the iTEBD algorithm for the same Ising model (see figures 11 and 12 in [15]). For the magnetization, although the iTEBD has achieved a better accuracy than iBTMRG, the conditions are not the same. In addition to the main difference already mentioned in section 1, another difference is that the transfer matrix that they have dealt with is Hermitian which is much numerically well conditioned than a non-Hermitian one. More importantly, for the two-point correlation calculation, instead of evaluating a very long tensor network as in [15], we use a very efficient formula, equation (18), and obtain a result that is comparable with respect to the iTEBD.

5. Conclusions

In this paper, we give a thorough biorthonormal matrix-product-state (BMPS) analysis of the transfer-matrix renormalization group (TMRG) for non-Hermitian matrices...
and propose a ‘single-site’ infinite-size biorthonormal TMRG (iBTMRG) algorithm to directly obtain dual infinite-BMPS (iBMPS) which are translationally invariant in the thermodynamic limit. Unlike for the standard DMRG where the MPS was established on a series of reduced orthonormal bases, the BMPS are built on dual series of reduced biorthonormal bases for the left and right Perron states of a non-Hermitian matrix. We propose two alternative methods for the construction of the dual biorthonormal bases and compare their numerical performances for both finite and infinite systems. We also develop an efficient wavefunction transformation of the iBTMRG, in analogy with that of McCulloch [5] for the infinite-DMRG, to predict the wavefunction as the lattice size is increased. The resulting translationally invariant iBMPS not only allows investigating bulk properties of a strongly correlated system in the thermodynamic limit without the boundary effect but also allows the very efficient evaluation of the expectation and two-point correlation function of the system. For illustration, we calculate the magnetization as a function of the temperature and the critical spin–spin correlation function in the thermodynamic limit for a 2D classical Ising model.

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