Efficiency of Symmetric Targeting for Finite-T DMRG

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Two targeting schemes have been known for the density matrix renormalization group (DMRG) applied to non-Hermitian problems; one uses an asymmetric density matrix and the other uses symmetric density matrix. We compare the numerical efficiency of these two targeting schemes when they are used for the finite temperature DMRG.

KEYWORDS: DMRG, Finite Temperature, Targeting

§1. Introduction

The density matrix renormalization group (DMRG) established by White[1)] has been successfully applied to various problems in condensed matter physics.[2)] A recent technical progress in DMRG is its applications to non-Hermitian problems, such as asymmetric exclusion process,[3,4)] reaction-diffusion process,[5)] and quantum Hall effect.[6)]

For these non-Hermitian problems, left eigenvectors of the Hamiltonian are not equal to the complex conjugates of the right eigenvectors. Two different targeting schemes have been used for DMRG under the situation. One is to use an asymmetric density matrix, which is a partial trace between the left and the right eigenvectors.[7)] This scheme has been used for the DMRG applied to classical systems[8)] and the finite temperature (finite-T) DMRG.[9–11)] The other scheme is to use a symmetric density matrix, which is created by targeting both left and right eigenvectors as two individual vectors.[1,2,5,6)]

The purpose of this paper is to compare the numerical efficiencies of these two schemes, by observing the cut-off error of the renormalization group (RG) transformation applied to the finite temperature Heisenberg spin chain. In the next section we define the cut-off errors as a function of projection operator, that represents the freedom restriction by the RG transformation. The two targeting schemes are briefly reviewed in §3, and these schemes are compared by calculating the cut-off error numerically. Conclusions are summarized in §4.

§2. Cut-off Error in RG Transformation

The finite-T DMRG[9–11)] estimates the free energy of one-dimensional quantum systems by way of a precise approximation for the largest eigenvalue λ of the quantum transfer matrix[12)] (QTM) $\mathcal{T}$. As an example of QTM, we consider that of the $S = 1/2$ Heisenberg chain. (See Fig.1.) We express the matrix element of the QTM as $\mathcal{T}_{i'j',\,ij}$, where i (i') and j (j') represents the upper-part (U-part) and the lower-part (D-part[13)]) of the column spin, respectively. It has been known that the partition function of N-site system can be approximated by that of the Trotter[14)] decomposed two-dimensional classical system; $Z = \mathrm{Tr}\,\mathcal{T}^N$. When N is sufficiently large, Z is well approximated as

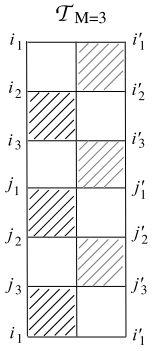

Fig. 1. Quantum transfer matrix $\mathcal{T}_{i'j',\,ij}$ of the $S = 1/2$ Heisenberg spin chain, where the Trotter number M is 3, and both i (i') and j (j') consists of three $S = 1/2$ spin variables.

$$\mathcal{T}^N \simeq \mathbf{V}^{\mathrm{R}} \lambda^N \left(\mathbf{V}^{\mathrm{L}}\right)^T \ , \tag{1}$$

where $\mathbf{V}^{\mathrm{L}}$ and $\mathbf{V}^{\mathrm{R}}$ is, respectively, the left and the right eigenvector of $\mathcal{T}$, that satisfies the eigenvalue relation

$$\sum_{i'j'} V^{\mathrm{L}}_{i'j'}\, \mathcal{T}_{i'j',\,ij} = V^{\mathrm{L}}_{ij} \lambda$$

$$\sum_{ij} \mathcal{T}_{i'j',\,ij} V^{\mathrm{R}}_{ij} = \lambda V^{\mathrm{R}}_{i'j'} \ . \tag{2}$$

We have used the normalization $\left(\mathbf{V}^{\mathrm{L}}, \mathbf{V}^{\mathrm{R}}\right) = \sum_{ij} V^{\mathrm{L}}_{ij} V^{\mathrm{R}}_{ij} = 1$ in Eq.1. It should be noted that $\mathbf{V}^{\mathrm{L}}$ is not equal to $\mathbf{V}^{\mathrm{R}}$ in general, because of the asymmetry $\mathcal{T} \neq \mathcal{T}^T$.

Let us consider a formal decomposition of these vectors

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into the products of matrices

$$V^{\rm L}_{ij} \to \sum_{\xi\eta} O^{\rm L}_{i\xi}\, v^{\rm L}_{\xi\eta}\, Q^{\rm L}_{j\eta}$$

$$V^{\rm R}_{ij} \to \sum_{\xi\eta} O^{\rm R}_{i\xi}\, v^{\rm R}_{\xi\eta}\, Q^{\rm R}_{j\eta} \qquad (3)$$

according to the convention in DMRG,[2] where $O^{\rm L/R}$ and $Q^{\rm L/R}$ satisfy the orthogonal (or duality) relations

$$\sum_i O^{\rm L}_{i\xi} O^{\rm R}_{i\xi'} = \delta_{\xi\xi'}$$

$$\sum_j Q^{\rm L}_{j\eta} Q^{\rm R}_{j\eta'} = \delta_{\eta\eta'}\ , \qquad (4)$$

and ξ and η represent the block spin variables. The matrices $O^{\rm L/R}$ and $Q^{\rm L/R}$ play the role of renormalization group (RG) transformations, when the freedom restriction $1 \le \xi, \eta \le m$ is considered for for both $\mathbf{V}^{\rm L}$ and $\mathbf{V}^{\rm R}$ in Eq.3. Under the restriction, $v^{\rm L}_{\xi\eta}$ and $v^{\rm R}_{\xi\eta}$ are m-dimensional matrices that represent the renormalized states.

In DMRG applied to classical system or finite temperature quantum system, the RG transformations $O^{\rm L/R}$ and $Q^{\rm L/R}$ are determined so that the cut-off error of the partition function

$$\delta Z = {\rm Tr}\,(1-P)\mathcal{T}^N = \left(\mathbf{V}^{\rm L},\, (1-P)\mathbf{V}^{\rm R}\right)\lambda^N \qquad (5)$$

is suppressed, where P is the projection operator

$$P_{i'j',ij} = P^{\rm U}_{i'i}\, P^{\rm D}_{j'j} = \sum_{\xi}^{m} O^{\rm R}_{i'\xi} O^{\rm L}_{i\xi} \ \sum_{\eta}^{m} Q^{\rm R}_{j'\eta} Q^{\rm L}_{j\eta}\,, \qquad (6)$$

that represents the Hilbert space restriction by the RG transformation; $P^{\rm U}$ and $P^{\rm D}$ is projection operator for U- and D-part, respectively. Since the operator $1-P = 1-P^{\rm U}P^{\rm D}$ in Eq.5 can be factorized as

$$(1-P^{\rm U}) + (1-P^{\rm D}) - (1-P^{\rm U})(1-P^{\rm D})\,, \qquad (7)$$

and the third term is negligible when it is applied to $\mathbf{V}^{\rm L}$ and $\mathbf{V}^{\rm R}$, we can precisely estimate the relative cut-off error $\delta Z/Z$ by calculating the inner product

$$\left(\mathbf{V}^{\rm L},\, (1-P^{\rm U})\mathbf{V}^{\rm R}\right) + \left(\mathbf{V}^{\rm L},\, (1-P^{\rm D})\mathbf{V}^{\rm R}\right) = \left(1-{\rm Tr}\,P^{\rm U}\rho^{\rm U}\right) + \left(1-{\rm Tr}\,P^{\rm D}\rho^{\rm D}\right)\,, \qquad (8)$$

where $\rho^{\rm U}$ and $\rho^{\rm D}$ are the *asymmetric density matrices*

$$\rho^{\rm U}_{i'i} = \sum_j V^{\rm L}_{i'j} V^{\rm R}_{ij}$$

$$\rho^{\rm D}_{j'j} = \sum_i V^{\rm L}_{ij'} V^{\rm R}_{ij} \qquad (9)$$

that satisfy the normalization ${\rm Tr}\rho^{\rm U} = {\rm Tr}\rho^{\rm D} = \left(\mathbf{V}^{\rm L}, \mathbf{V}^{\rm R}\right) = 1$. Let us keep in mind that ${\rm Tr}\,P^{\rm U}\rho^{\rm U}$ and ${\rm Tr}\,P^{\rm D}\rho^{\rm D}$ are essential for the cut-off error of the RG transformation by $P = P^{\rm U}P^{\rm D}$.

§3. Asymmetric and Symmetric Targeting

Two different targeting scheme have been used to determine the RG transformation matrices $O^{\rm L/R}$ and $Q^{\rm L/R}$. One is to obtain them by diagonalizing the asymmetric density matrices[7, 8, 10, 11] in Eq.9

$$\rho^{\rm U}_{i'i} \to \sum_{\xi} O^{\rm R}_{i'\xi} w_\xi O^{\rm L}_{i\xi}$$

$$\rho^{\rm D}_{j'j} \to \sum_{\eta} Q^{\rm R}_{j'\eta} w_\eta Q^{\rm L}_{j\eta}\,, \qquad (10)$$

where w_ξ is the common eigenvalue for both $\rho^{\rm U}$ and $\rho^{\rm D}$ in the order of decreasing absolute value; normally all the w_ξ are positive. The projection operators $P^{\rm U}$, $P^{\rm D}$, and P created from $O^{\rm L/R}$ and $Q^{\rm L/R}$ in Eq.10 are asymmetric, as $\rho^{\rm U}$ and $\rho^{\rm D}$ are. Let us call such a construction of $P^{\rm U/D}$ as *symmetric targeting*. In this case, the relative cut-off error in Eq.8 can be calculated from the eigenvalues of the asymmetric density matrix as

$$2 - {\rm Tr}\,P^{\rm U}\rho^{\rm U} - {\rm Tr}\,P^{\rm D}\rho^{\rm D} = 2(1 - \sum_{\xi}^{m} w_\xi)\,. \qquad (11)$$

It is possible to choose $O^{\rm L/R}_{i\xi}$ and $Q^{\rm L/R}_{i\eta}$ so that $v^{\rm L}_{\xi\eta}$ and $v^{\rm R}_{\xi\eta}$ become simultaneously diagonal: $v^{\rm L}_{\xi\eta} = v^{\rm R}_{\xi\eta} = \delta_{\xi\eta}\omega_\xi$ where $\omega^2_\xi = w_\xi$. Thus we can interpret the decomposition in Eq.3 as an extension of the singular value decomposition for the dual vectors $\mathbf{V}^{\rm L}$ and $\mathbf{V}^{\rm R}$.[8]

The other targeting scheme is to treat $\mathbf{V}^{\rm L}$ and $\mathbf{V}^{\rm R}$ as individual vectors,[5, 6] as they simultaneously target ground and excited states in DMRG applied to Hermitian quantum systems.[1] In this case, the RG transformations are obtained by first creating the symmetric density matrices

$$\bar\rho^{\rm U}_{i'i} = \frac{1}{2}\sum_j V^{\rm L}_{i'j} V^{\rm L}_{ij} + \frac{1}{2}\sum_j V^{\rm R}_{i'j} V^{\rm R}_{ij}$$

$$\bar\rho^{\rm D}_{j'j} = \frac{1}{2}\sum_i V^{\rm L}_{ij'} V^{\rm L}_{ij} + \frac{1}{2}\sum_i V^{\rm R}_{ij'} V^{\rm R}_{ij} \qquad (12)$$

and then by diagonalizing them

$$\bar\rho^{\rm U}_{i'i} \to \sum_{\xi} O_{i'\xi} \bar w^{\rm U}_\xi O_{i\xi}$$

$$\bar\rho^{\rm D}_{j'j} \to \sum_{\eta} Q_{j'\eta} \bar w^{\rm D}_\eta Q_{j\eta}\,, \qquad (13)$$

where we have dropped the label L and R from $O^{\rm L/R}$ and $Q^{\rm L/R}$, because $O^{\rm L} = O^{\rm R}$ and $Q^{\rm L} = Q^{\rm R}$. In this case, the projection operators

$$\bar P^{\rm U}_{i'i} = \sum_{\xi}^{m} O_{i'\xi} O_{i\xi}$$

$$\bar P^{\rm D}_{j'j} = \sum_{\eta}^{m} Q_{j'\eta} Q_{j\eta} \qquad (14)$$

are symmetric. Let us call such a construction of $\bar P^{\rm U/D}$ as *symmetric targeting*. Unlike the asymmetric targetting, it is impossible to make the m-dimensional matri-

ces $v^{\rm L}_{\xi\eta}$ and $v^{\rm R}_{\xi\eta}$ simultaneously diagonal. This targeting scheme is often used because there is no need to diagonalize the asymmetric density matrix, which requires special numerical care.[15] It should be noted that the relative cut-off error

$$\delta Z/Z = 1 - {\rm Tr}\,\bar{P}^{\rm U}\rho^{\rm U} + 1 - {\rm Tr}\,\bar{P}^{\rm D}\rho^{\rm D} \qquad (15)$$

in the symmetric targeting is not directly related to the eigenvalues of the symmetric density matrices in Eq. 12.

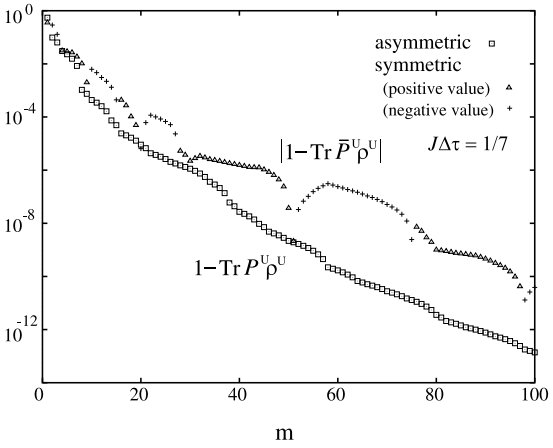

Fig. 2. The relative cut-off error for the asymmetric targeting $1 - {\rm Tr}\,P^{\rm U}\rho^{\rm U}$ in Eq.11 and that for the symmetric targeting $1 - {\rm Tr}\,\bar{P}^{\rm U}\rho^{\rm U}$ in Eq.15 when $J\Delta\tau = 1/7$. For the latter we use triangle mark when it is positive, and use cross mark when negative. The horizontal axis shows the number of states kept.

Now let us compare the relative cut-off errors for both asymmetric and symmetric targeting. We choose the $S = 1/2$ isotropic Heisenberg spin chain as the reference system, and fix the Trotter number $M = 7$ so that we can obtain the eigenvector of $\mathcal{T}$; we have to know $\mathbf{V}^{\rm L}$ and $\mathbf{V}^{\rm R}$ exactly in order to evaluate $\delta Z/Z$. We consider the case where U-part contains the same number of spin variables as D-part; this U-D division is normally used for the infinite system algorithm.[1] Since U-part is identical to the D-part, $1 - {\rm Tr}\,P^{\rm U}\rho^{\rm U} = 1 - {\rm Tr}\,P^{\rm D}\rho^{\rm D}$ holds for Eq.11 and $1 - {\rm Tr}\,\bar{P}^{\rm U}\rho^{\rm U} = 1 - {\rm Tr}\,\bar{P}^{\rm D}\rho^{\rm D}$ for Eq.15. Figure 2 shows the relative cut-off errors when the imaginary time step $J\Delta\tau$[11] is equal to 1/7. As it is seen, $1 - {\rm Tr}\,P^{\rm U}\rho^{\rm U}$ decreases monotonically with respect to m, and is always positive. On the other hand, the dumping of $1-{\rm Tr}\,\bar{P}^{\rm U}\rho^{\rm U}$ with respect to m is oscillatory; $1-{\rm Tr}\,\bar{P}^{\rm U}\rho^{\rm U}$ is not always positive,[16] and the calculated partition function is not the variational lower bound. For most of m the error $1 - {\rm Tr}\,P^{\rm U}\rho^{\rm U}$ is smaller than $|1 - {\rm Tr}\,\bar{P}^{\rm U}\rho^{\rm U}|$, that shows the superiority of asymmetric targeting for the finite-T DMRG.

Figure 3 shows the cut-off errors for relatively high temperature $J\Delta\tau = 1/14$. In both Figs.2 and 3, we have to keep twice as large as m for the symmetric targeting in order to keep the same cut-off error of the asymmetric targeting. This may be explained by the fact that the asymmetric projection operator $P^{\rm U/D}$ is created by $2m$ numbers of linearly independent vectors, while the symmetric projection operator $\bar{P}^{\rm U/D}$ is created by m numbers of orthogonal vectors.

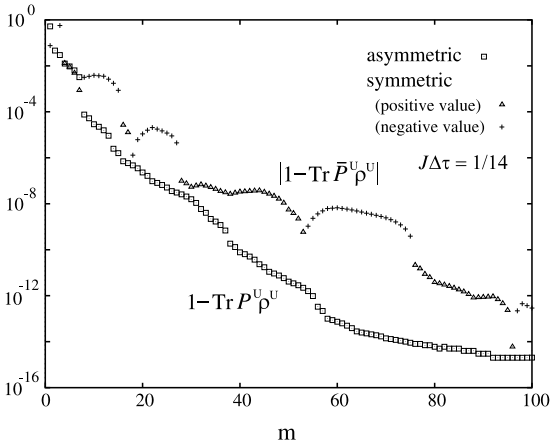

Fig. 3. The relative cut-off errors in relatively high temperature $J\Delta\tau = 1/14$.

§4. Conclusion

We have compared the numerical efficiency of the symmetric and asymmetric targeting schemes when they are applied to the finite temperature DMRG. It is shown that the cut-off error calculated by the symmetric targeting is larger than that of asymmetric targeting; as far as cut-off error is concerned, the asymmetric targetting is superior to the symmetric targetting.

If we keep twice as large as m for the symmetric targeting, we can recover the numerical precision of the asymmetric targeting. Therefore, for the problems that does not require large m for the DMRG calculations, the symmetric targeting is of use, in the sense that it does not require the diagonalization of asymmetric density matrix, and is free from complex eigenvalue problem.[11,15]

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16) Note that the density matrix ρ^{U} is asymmetric, and $\bar{P}^{\mathrm{U}}$ is the symmetric projection operator. In such a case, $1 \geq \mathrm{Tr}\, \bar{P}^{\mathrm{U}} \rho^{\mathrm{U}}$ is not always true.