Spatial reflection and renormalization group flow of quantum many-body systems with matrix product state representation

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Abstract – The property of quantum many-body systems under spatial reflection and the relevant physics of the renormalization group (RG) procedure are revealed. By virtue of the matrix product state (MPS) representation, various attributes for translational invariant systems associated with spatial reflection are manifested. We demonstrate subsequently a conservation rule of the conjugative relation for reflectional MPS pairs under RG transformations and illustrate further the property of the fixed points of RG flows. Finally, we show that a similar rule exists with respect to the target states in the density matrix renormalization group algorithm.

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Exploration of quantum many-body systems, particularly the translational invariant systems defined on lattices, is one of the most important topics in quantum physics and statistical physics. Nevertheless, to our observation, the intrinsic attribute of the system under spatial reflection and the relevant physics have less been disclosed so far. In particular, a question whether or not the species of quantum many-body states with matrix product construction possess inherently a reflection symmetry [1] is yet to be answered unambiguously. Here, we are motivated to reveal various categories of quantum many-body systems under spatial reflection and to explore the related property under the renormalization group (RG) procedure.

The RG theory, including the seminal proposal of real-space renormalization by Wilson [2] and its renewed development of the density matrix renormalization group (DMRG) method [3], is one conceptual pillar of quantum many-body physics and particularly constitutes a key theoretical element to quantum critical phenomena. A theoretical picture of the standard DMRG algorithm could be formulated in terms of variational optimization within the representation of matrix product states (MPSs) [1,4]. In fact, the generality of this mathematical representation for quantum many-body states, incorporating with the fact that the ground state of most quantum systems could be well approximated by a low-dimensional MPS, accounts unambiguously for the origin of the power of the DMRG algorithm. Recently, it was indicated that the MPS representation has a close connection with the concept developed in the field of quantum information, leading to significant progress, e.g., algorithms for periodic boundary conditions [5], finite temperature [6], and simulating quantum systems of real-time evolution [7]. Meanwhile, it was shown that a general RG procedure can be established upon the quantum state itself via MPS representation with properly defined coarse-graining transformations [8]. With respect to the Wilsonian RG scheme on Hamiltonians, this proposal suggests a specific rescaling approach to realize the scale separation for quantum many-body states.

The main contribution of this paper are as follows. Firstly, by invoking the spatial-reflection transformation, we show that apart from the symmetric states, the translational invariant MPSs could have different attributes, that is, locally inequivalent to their reflectional counterparts or differing from their reflectional counterparts only by local unitary transformations. Subsequently, we show that the conjugative relation of the reflectional MPS pair is preserved along the recurrent coarse-graining transformations. Thus a rule on the conservation of the reflective relation for RG flows is indicated and the property of the leading fixed points is further investigated. Finally, we demonstrate elaborately that a similar law exists with respect to the target states in the numerical DMRG procedure regarding its variational nature of performance.

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Let us begin with the notation of the one-dimension translational invariant MPS:

$$|\Psi\rangle = \frac{1}{\sqrt{W}} \sum_{s_1, \ldots, s_N} \text{Tr}(A^{s_1} \cdots A^{s_N})|s_1, \ldots, s_N\rangle,$$

(1)

where the set of $D \times D$ matrices $\{A^s, s = 1, \ldots, d\}$ parameterize the $N$-spin state with the dimension $D = d^{N/2}$. The normalization factor is obtained as $W = \text{Tr}E^N$, where $E = \sum_{s=1}^d A^s \otimes A^s$ is the so-called transfer matrix with the bar denoting complex conjugation. We now introduce a new state defined by a spatial reflection on $|\Psi\rangle$, that is, $|\Psi_{rfl}\rangle \equiv \mathcal{P}_N|\Psi\rangle$ where $\mathcal{P}_N$ is the parity operator for the $N$-body system depicted by the action $\mathcal{P}_N|s_1, \ldots, s_N\rangle = |s_N, \ldots, s_1\rangle$. In fact, for the present situation with site-independent matrices $\{A^s\}$, the reflectional counterpart state $|\Psi_{rfl}\rangle$ is just an MPS represented by the set of matrices $\{A^s_{rfl}\}$, where $A^s_{rfl} \equiv (A^s)^T$ denotes the matrix transposition of $A^s$. This can be easily seen from the equation

$$|\Psi_{rfl}\rangle = \frac{1}{\sqrt{W}} \sum_{\{s_i\}} \text{Tr}(A^{s_1} \cdots A^{s_N})|s_N, \ldots, s_1\rangle = \frac{1}{\sqrt{W}} \sum_{\{s_i\}} \text{Tr}[(A^{s_1})^T \cdots (A^{s_N})^T]|s_1, \ldots, s_N\rangle.$$  

(2)

Note that the transfer matrix of $|\Psi_{rfl}\rangle$ is related to the one of $|\Psi\rangle$ simply by

$$E_{rfl} = \sum_s A^s_{rfl} \otimes A^s_{rfl} = E^T,$$  

(3)

which indicates that $E$ and $E_{rfl}$ have exactly the same spectrum. This leads clearly to the fact that any MPS has the same correlation length $[9,10]$ with its reflectional counterpart. Furthermore, the overlap of two reflective MPSs is worked out to be

$$\eta \equiv \langle \Psi | \Psi_{rfl} \rangle = \frac{\text{Tr}(E_{T}^2)^N}{\text{Tr}E^N},$$  

(4)

where $E_{T}^2 \equiv \sum_s (A^s)^T \otimes (A^s)^T$. Clearly, eq. (4) suggests a sufficient criterion for an MPS with reflection symmetry, that is, the specified matrix $E_{T}^2$ should have the same spectrum structure with that of the matrix $E$.

The well-known multipartite states in quantum information, typically the Greenberger-Horne-Zeilinger state [11], the cluster state [12] and the MPS of Affleck-Kennedy-Lieb-Tasaki model [13], are shown to be symmetric under spatial reflection. Consider the cluster state as an example. By noting that the state has an MPS representation $\{A^1 = \left( \begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix} \right), A^2 = \left( \begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix} \right)\}$, one can work out that the matrix $E_{T}^2$ has the same spectrum with that of $E$, hence $\eta = 1$ according to eq. (4). More specifically, it is verified that $E_{T}^2 = (I \otimes X)E(I \otimes X^{-1})$, where the matrix $X = \left( \begin{smallmatrix} 1 & 1 \\ 1 & -1 \end{smallmatrix} \right)$ is an invertible transformation connecting the matrix $A^s$ and its transposition: $(A^s)^T \equiv XA^sX^{-1}$. The translational invariant MPS without parity symmetry, as will be shown below, exists in general. In fact, it is of interest to further distinguish two distinct categories for the translational invariant states, namely, those locally inequivalent to their reflectional counterparts and those differing from their reflectional counterparts only by local unitary transformations. Specifically, let us consider a translational invariant MPS $|\Psi\rangle$ represented by

$$A^1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad A^2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad A^3 = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}.$$  

(5)

It is shown that the corresponding transfer matrix $E$ has eigenvalues $-1, -1, (2 + g^2 \pm \sqrt{4 + g^2})/2$ that are distinctly different from those of the matrix $E_{T}^2$ (except the case of $g = 0$). Therefore the specified reflectional MPS pairs $|\Psi\rangle$ and $|\Psi_{rfl}\rangle$ are different according to eq. (4). Moreover, it can be shown that the two MPSs $|\Psi\rangle$ and $|\Psi_{rfl}\rangle$ possess distinct correlation features, hence belong to different equivalence classes, i.e., $|\Psi_{rfl}\rangle \neq U \otimes \cdots \otimes U|\Psi\rangle$ where $U$ stands for local unitary transformations.

For the second example we consider an MPS $|\Psi\rangle$ with

$$A^1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad A^2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad A^3 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$  

(6)

Explicitly, the corresponding transfer matrix $E$ has eigenvalues $1, \pm g^2, g, 0$ and the matrix $E_{T}^2$ has $2g, 1, g^2, 0$, respectively. Therefore, the MPS $|\Psi\rangle$ is different from its reflectional counterpart $|\Psi_{rfl}\rangle$ in view of the fact that the overlap between them is less than unity (apart from two exception points of $g = \pm 1$). Interestingly, in this case the MPSs $|\Psi\rangle$ and $|\Psi_{rfl}\rangle$ differ only by a local unitary transformation, i.e., $|\Psi_{rfl}\rangle = U \otimes \cdots \otimes U|\Psi\rangle$, where $U = \{|1\rangle + |2\rangle + |3\rangle + |4\rangle\}$. Specifically, the present example suggests a special category of translational invariant states that relate to their reflectional counterparts by non-trivial local unitary transformations. In general, the representative matrices of this special sort of MPSs satisfy $(A^s)^T = \sum_j U_j^T (X A^s X^{-1})$, where $U_j^T$ is the representative matrix accounting for the local unitary transformation and $X$ is an invertible matrix, say, it is obtained as $X = \left( \begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix} \right)$ for the present case of eq. (6).

Now let us consider the relation of the reflectional MPS pair under the RG transformation. Following ref. [8], to perform the coarse-graining procedure for the state $|\Psi\rangle$ in eq. (1), one needs firstly to merge the representative matrices for neighboring sites $\tilde{A}^{pq} = ApA^q$. Then, an appropriate representative for the equivalence class can be selected out via the singular-value decomposition

$$\tilde{A}^{(pq)} = \sum_{i=0}^{d'} t^{(pq)}_i \lambda_i V^{(pq)}_i,$$  

(7)

1The difference of the correlation feature between $|\Psi\rangle$ and $|\Psi_{rfl}\rangle$ can be explicitly shown, say, in view of the correlated density matrices $\bar{v} \equiv \rho_{123} - \rho_{12} \otimes \rho_3$ and $\bar{v}^{rfl} \equiv \bar{v}^{rfl} - \rho_{12} \otimes \rho_3$ have different spectrum.
where \((pq)\) and \((\alpha\beta)\) are understood as combined indices, and \(d \leq \min\{D^2, d^2\}\) denotes the number of non-zero singular values of the matrix \(\tilde{A}_{(\alpha\beta)}^{pq}\). The state after one-step RG transformation can therefore be characterized by the new representative matrices

\[
A^p \rightarrow A'^l = \lambda_i V^l.
\]  

(8)

Consider now the specified RG performance on the reflectional counterpart state \(|\Psi_{rfl}\rangle\) represented by \(\{A_{rfl}^q\}\). In view of the relation of the coarse-grained matrices \(\tilde{A}_{rfl}^{(pq)} \equiv A_{rfl}^p A_{rfl}^q = (\tilde{A}^{(qp)})^T\), one has

\[
(\tilde{A}_{rfl})^{(pq)}_{(\alpha\beta)} = \tilde{A}^{(qp)}_{(\beta\alpha)} = \sum_{l=1}^{d'} U_l^{(qp)} \lambda_i V_{(\beta\alpha)}^l.
\]

Hence the RG transformation on \(|\Psi_{rfl}\rangle\) gives rise to

\[
A_{rfl}^p \rightarrow A'_{rfl} = \lambda_i (V^l)^T = (A'^l)^T.
\]

(10)

Clearly, eqs. (8) and (10) show that the relation of spatial reflection is preserved for the reflectional MPS pair under the RG transformation. In fact, the recurrent RG performance indicated by eqs. (7)–(10) suggests an intriguing conjugative structure of RG flow for the translational invariant states. This special flow configuration will continue along the RG procedure until the states reach their fixed points. Furthermore, since the corresponding transfer matrices after one-step RG transformations are given by \(E' = E^2\) and \(E_{rfl}' = (E^T)^2 = (E')^T\), the overlap of the reflectional MPS pair under the recurrent RG performance is obtained explicitly as

\[
\eta \rightarrow \eta' = \frac{Tr\{E^2\}
}{\frac{n}{2} \rightarrow \cdots \rightarrow \frac{n}{2} \frac{Tr\{E^\infty\}}{Tr E^\infty}} \rightarrow \cdots \rightarrow \frac{Tr\{E^\infty\}}{Tr E^\infty},
\]

(11)

where \(n = N/x\) and we have denoted by \(E^\infty\) and \(E_{rfl}^\infty = (E^\infty)\) the transfer matrices of the two reflectional fixed points, i.e., \(E^\infty \equiv \lim_{\rightarrow \infty} E^X\).

The above-described conservation law of the reflective relation for RG flows is applicable for both the two categories of MPSs: those \(|\Psi\rangle\) differing from \(|\Psi_{rfl}\rangle\) by local unitary transformations and those \(|\Psi\rangle\) locally inequivalent to \(|\Psi_{rfl}\rangle\). For the former case, although \(|\Psi\rangle\) and \(|\Psi_{rfl}\rangle\) are viewed to be equivalent under the coarse-graining transformation, the attribute of spatial reflection is retained along the RG procedure even at the fixed point. In detail, let us examine the MPS of eq. (6). It is direct to calculate that the two reflective fixed points are characterized by \(E^\infty = |\Phi_R\rangle\langle\Phi_R|\) and \(E_{rfl}^\infty = |\Phi_{L}\rangle\langle\Phi_{R}|\), where \(|\Phi_R\rangle = \frac{(|00\rangle + g^2 (|11\rangle)}{(1 + g^2)}\) and \(|\Phi_{L}\rangle = |00\rangle + |11\rangle\). The corresponding representative matrices of fixed-point MPSs \(|\Psi^\infty\rangle\) and \(|\Psi_{rfl}^\infty\rangle\) are obtained, respectively, as

\[
\{A_{\infty}^s\} = \left\{ \begin{array}{c}
[1 \ 0] \\
[0 \ 0] \\
[0 \ 0] \\
[1 \ 0] \\
[0 \ 0]
\end{array} \right\}
\]

(12)

and \(\{A_{\infty}^{s_{rfl}}\} = (A_{\infty}^s)^T, s = 1, \ldots, 4\). It is readily verified that \(|\Psi_{rfl}^\infty\rangle = U \otimes \cdots \otimes U |\Psi^\infty\rangle\) where the local unitary transformation \(U = |1\rangle\langle4| + |4\rangle\langle1|\).

For the situation specified by eq. (5) in which \(|\Psi\rangle\) and \(|\Psi_{rfl}\rangle\) possess a different correlation feature, the corresponding fixed points could be obtained similarly. In detail, since there is no degeneracy in the largest eigenvalue of the transfer matrix \(E\), the fixed points are characterized, up to an irreducible normalization factor, by \(E^\infty = |\Phi_{R}\rangle\langle\Phi_{L}|\) and \(E_{rfl}^\infty = |\Phi_{L}\rangle\langle\Phi_{R}|\), where

\[
\begin{align}
|\Phi_{R}\rangle &= |00\rangle + \frac{k + g^2}{2} |11\rangle \\|\Phi_{L}\rangle &= |00\rangle + \frac{k + g^2}{2} |11\rangle
\end{align}
\]

(13)

One can verify from eq. (4) that for the corresponding fixed-point states \(|\Psi_{rfl}^\infty\rangle < 1\). Notably, it turns out that the state \(|\Psi^\infty\rangle\) differs from \(|\Psi_{rfl}^\infty\rangle\) only by a local unitary transformation\(^2\). Physically, it is understood that all correlation functions decay exponentially along the RG flow and become zero at the fixed point. Therefore the attribute of the fixed point described above is a general feature one exactly expects.

So far, we have revealed various attributes and the relevant physics of RG flows for translational invariant MPSs under spatial reflection. Now, let us consider the DMRG scheme on the specified lattice system. Note that for a system without parity symmetry, i.e., \(H_{rfl} \equiv P(H) \neq H\), there is no reflection relation between the system block and the environment block in the DMRG algorithm any more. On the other hand, it is obvious that the systems \(H\) and \(H_{rfl}\) have corresponding exact ground states related by the reflection transformation. Hence it is interesting to explore whether the performance of the DMRG algorithm could warrant the reflection relation between target states of reflective systems.

In detail, let us look into the DMRG procedure with \(B \bullet B\) configuration for one-dimensional spin chains. The standard DMRG iterative performance could be described as follows. Suppose that the superblock consists of two blocks and two spins in between at a certain step. The system block \(B_L\) contains spins \(1, \ldots, M - 1\), and the environment block \(B_R\) contains \(M + 1, \ldots, 2M - 1\). The states of two spins in between are denoted as \(|s_M\rangle\) and \(|s'_{M}\rangle\), respectively. The target state, i.e., the ground state of the superblock has the following form:

\[
|\Psi\rangle = \sum_{s_M,s'_{M}} \sum_{\alpha,\beta=1}^{D} A_{s_M,s'_{M}}^{\alpha,\beta} |\alpha\rangle_{M-1} |s_M\rangle |s'_{M}\rangle |\beta\rangle_{M-1},
\]

(14)

where the orthonormal bases \(|\alpha\rangle_{M-1}\) and \(|\beta\rangle_{M-1}\) under local transformations could be shown by the fact that there exists an invertible \(X\) such that \(E_{rfl}^\infty = X \otimes X E^\infty (X \otimes X)^{-1}\).
that the target state minimizes the energy. From eq. (14), the reduced density matrices of the left and right half superblock, $B_L\mathbf{e}$ and $\mathbf{e}B_R$, are derived directly by virtue of the following singular-value decomposition:

$$A_{\alpha,\beta}^{s_M,s'_{M}} = (U\Sigma V)^{(s_M,\alpha),(s'_M,\beta)}$$

$$= \sum_{a'} U_{(s_M,\alpha),a'} \Sigma_{a'} V_{a',(s'_M,\beta)},$$

(15)

where $(s_M,\alpha)$ and $(s'_M,\beta)$ are understood as combined indices and $\Sigma$ is a diagonal matrix with elements (singular values) $\Sigma_{a'}$, sorted in decreasing order, accounting for square roots of eigenvalues of the reduced density matrices. Then, a truncation algorithm to achieve new system and environment blocks for the next-step iteration, $B_L\mathbf{e} \rightarrow B_L'$ and $\mathbf{e}B_R \rightarrow B_R'$, is performed by retaining only the following $D$ eigenvectors with the largest eigenvalues:

$$|\alpha\rangle_M^{(s_M)} = \sum_{s_M=1}^{D} U_{(s_M,\alpha),(s_M,\alpha)}^{L} |s_M\rangle_M \otimes |s_M\rangle_M,$$

(16)

$$|\beta\rangle_M^{(s'_M)} = \sum_{s'_M=1}^{D} V_{(s'_M,\beta),(s'_M,\beta)}^{R} |s'_M\rangle_M \otimes |s'_M\rangle_M.$$ 

Here, $U_{(s_M,\alpha),(s_M,\alpha)}^{L}$ and $V_{(s'_M,\beta),(s'_M,\beta)}^{R}$ are just unitary matrices truncated from $U_{(s_M,\alpha),(s_M,\alpha)}^{L}$ and $V_{(s'_M,\beta),(s'_M,\beta)}^{R}$, respectively, and they fulfill the relation

$$I = \sum_{s_M} U_{(s_M,\alpha),(s_M,\alpha)}^{L} U_{(s_M,\alpha),(s_M,\alpha)}^{L\dagger} = \sum_{s'_M} V_{(s'_M,\beta),(s'_M,\beta)}^{R} V_{(s'_M,\beta),(s'_M,\beta)}^{R\dagger}.$$

(17)

In terms of the MPS representation, the target state in the above DMRG iteration procedure can be depicted distinctly as

$$|\Psi\rangle = \sum_{\{s_i\}} T_{\{s_i\}} U_{\{s_i\}}^{M-1} A_{s_M,s'_{M}}^{s_M,s'_{M}}$$

$$\times V_{\{s_i\}}^{M-1,s_{M+1}} \cdots V_{\{s_i\}}^{M-1,s_{M+1}} |s_1 \cdots s_{2M-1}\rangle,$$

(18)

where we have used the notation $|s_1 \cdots s_{2M-1}\rangle = |s_1 \cdots s_M, s'_M \cdots s_{2M-1}\rangle$ and the summation indices $\{s_i\}$ run over all the $2M$ spins. Note that the MPS here is site dependent, i.e., no longer translational invariant, and we have adopted periodic boundary conditions in eq. (18). The DMRG procedure is now clearly phrased as that once the transformation $A_{s_M,s'_{M}}^{s_M,s'_{M}} \rightarrow (U_{\{s_i\}}^{M-1}, V_{\{s_i\}}^{M-1})$ is derived, then both system and environment blocks increase in length by one site and the algorithm is iterated until some desired final length is reached.

The promising conjugated DMRG flow for the reflected system $H_{refl}$ is outlined below. It turns out that the target state of the superblock for the system $H_{refl}$ relates to the original one (18) merely by an action of the parity operator $|\Psi_{refl}\rangle = \mathcal{P}|\Psi\rangle$. Namely, one has

$$|\Psi_{refl}\rangle = \sum_{\{s_i\}} U_{\{s_i\}}^{M-1} A_{s_M,s'_{M}}^{s_M,s'_{M}} \times V_{\{s_i\}}^{M-1,s_{M+1}} \cdots V_{\{s_i\}}^{M-1,s_{M+1}} |s_1 \cdots s_{2M-1}\rangle,$$

(19)

where the tensors in the last expression are defined by

$$V_{\{s_i\}}^{[k],s_k} = (V_{\{s_i\}}^{[k],s_k})^T, \quad \tilde{U}_{\{s_i\}}^{[k],s_{M+k-1}} = (\tilde{U}_{\{s_i\}}^{[k],s_{M+k-1}})^T, \quad \tilde{A}_{s_M,s'_{M}}^{s_M,s'_{M}} = (A_{s_M,s'_{M}}^{s_M,s'_{M}})^T.$$

(20)

To demonstrate the reflecting forms (18) and (19) of target states are preserved along the DMRG iteration for systems $H$ and $H_{refl}$, we need to prove that i) the formulated states (18) and (19) minimize the energy of the two reflected systems simultaneously; ii) the truncation algorithm of DMRG warrants that the resulted new representative matrices and target states satisfy repetitiously the indicated reflective relation.

Point i) is readily verified since the expected values of the Hamiltonians $H$ and $H_{refl}$ over the states (18) and (19) satisfy faithfully

$$E = \langle \Psi | H | \Psi \rangle / W = \langle \Psi_{refl} | H_{refl} | \Psi_{refl} \rangle / W,$$

(21)

with the normalization factor $W = \langle \Psi | \Psi \rangle = \langle \Psi_{refl} | \Psi_{refl} \rangle$. To demonstrate point ii), we note the following relation:

$$A_{\alpha,\beta}^{s_M,s'_{M}} = (V^T \Sigma U^T)_{\alpha,\beta}^{s_M,s'_{M}}$$

$$= \sum_{\beta'} V_{\beta',\alpha}^{s_M,s'_{M}} V_{\beta',\beta}^{s_M,s'_{M}}.$$ 

(22)

Consequently, by virtue of the specified DMRG truncation prescription one obtains the new representative matrices $V_{\beta',\alpha}^{s_M,s'_{M}}$ and $U_{\beta',\beta}^{s_M,s'_{M}}$, and the corresponding recursive relations (cf. eq. (16)). This completes our proof that the presented forms (18) and (19) of target states are preserved along the DMRG iterative procedure for the two reflective systems.

In conclusion, we have disclosed the property of quantum many-body systems under spatial reflection and revealed a universal conjugative flow structure for both the RG scheme on translational invariant MPSs and the DMRG algorithm. An intriguing extension to high spatial dimensions via projected entangled pair states [14] is awaited for us to explore further.

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