Application of the Density Matrix Renormalization Group Method to a Non-Equilibrium Problem

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(Received )

We apply the density matrix renormalization group (DMRG) method to a non-equilibrium problem: the asymmetric exclusion process in one dimension. We study the stationary state of the process to calculate the particle density profile (one-point function). We show that, even with a small number of retained bases, the DMRG calculation is in excellent agreement with the exact solution obtained by the matrix-product-ansatz approach.

KEYWORDS: asymmetric exclusion process, ASEP, density matrix renormalization group, DMRG, non-equilibrium phenomena, quadratic algebra

§1. Introduction

Many phenomena in the vast realm of non-equilibrium physics can be viewed as the asymmetric (simple) exclusion process (ASEP for short). Models of the ASEP in one spatial dimension have been extensively studied since a remarkable paper appeared, which proposed the so-called matrix product ansatz (MPA). For a class of models, the exact stationary probability distributions have been obtained by the MPA. However, there are many models whose stationary probability distributions cannot be obtained by using the MPA. Alternative approaches are required to study general models of the ASEP.

There are two types of models for the ASEP: discrete-time models and the continuous-time models. The discrete-time models which we treat in this paper are more general than the continuous-time ones because the latter are realized by taking suitable limits of the parameters in the former.

The density-matrix renormalization group (DMRG) method invented by S. R. White is an approximate numerical scheme for diagonalization of Hamiltonians, which has been applied to various one-dimensional quantum systems, with results demonstrating its surprising efficiency. As pointed out by T. Nishino, the DMRG is also applicable to two-dimensional lattice statistical models for

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diagonalization of the transfer matrices. Since the time-evolution operator in the discrete-time ASEP can be regarded as a transfer matrix, we can naturally expect applicability of the DMRG also to the ASEP. In the actual implementation, however, we should consider the following two points. First, we should treat a non-symmetric transfer matrix. Second, the role of the wave function $\psi$ is different; in the ASEP not $|\psi|^2$ but $\psi$ itself is the probability distribution.

In this paper, by properly incorporating the above two points, we apply the DMRG to a model of the ASEP to show that the DMRG is an efficient numerical approach also to non-equilibrium problems.

§2. Model

Let us explain the model which we treat. It is the model of stochastic process of hopping particles on a chain of size $N$. For technical simplicity, we will assume $N$ to be $4 \times \text{integer} + 2$. The time is taken to be discrete. Each site can have two states: either empty or occupied. Particles hop to the right-nearest site with probability $p$ and to the left-nearest site with probability $q$. The chain are coupled to particle reservoirs at the both ends: if the leftmost site is empty (resp. occupied), a particle is added (resp. removed) with probability $\alpha$ (resp. $\gamma$); if the rightmost site is empty (resp. occupied), a particle is added (resp. removed) with probability $\delta$ (resp. $\beta$).

Time evolution of the model consists of the following two steps.

[A-1]
For all odd-even pairs of sites $\{(2j-1, 2j)\}$ ($j = 1, 2, 3, ..., N/2 - 1$) their states are updated simultaneously. States of the leftmost and the rightmost sites are updated in this step.

[A-2]
For all even-odd pairs of sites $\{(2j, 2j+1)\}$ ($j = 0, 1, 2, ..., N/2 - 1$) their states are updated simultaneously.

We introduce a transfer matrix $T$ which describes the discrete-time evolution of the probability distribution. Corresponding to the two steps of the time evolution of the model, $T$ consists of two transfer matrices $T_1$ and $T_2$:

\[ T = T_2T_1 , \]  

(1)

where $T_1$ and $T_2$ correspond to the first step [A-1] and second step [A-2] of the time evolution, respectively. Explicitly,

\[
T_1 = L \otimes T_{1,2} \otimes T_{3,4} \cdots T_{N-3,N-2} \otimes R
\]

\[
T_2 = T_{0,1} \otimes T_{2,3} \cdots T_{N-2,N-1} ,
\]  

(2)
where \( L \) and \( R \) are the left boundary transfer matrix and the right boundary transfer matrix, respectively and \( T_{i,i+1} \) is a local transfer matrix acting on the pair of the sites \( i \) and \( i + 1 \).

In order to represent explicit matrix elements, we introduce a state variable \( i_n \) at each site \( n \) as:

\[
i_n = 0 \quad \text{(empty); \quad} i_n = 1 \quad \text{(occupied).} \tag{3}
\]

Then, the local transfer matrix \( T \) is given by

\[
T_{n,n+1} = \begin{pmatrix}
(0,0) & (0,1) & (1,0) & (1,1) \\
(0,0) & 1 & 0 & 0 & 0 \\
(0,1) & 0 & 1 - q & p & 0 \\
(1,0) & 0 & q & 1 - p & 0 \\
(1,1) & 0 & 0 & 0 & 1
\end{pmatrix} \tag{4}
\]

where the element \( (T_{n,n+1})_{(f_n,f_{n+1}),(i_n,i_{n+1})} \) represents the probability for the transition from the state \( (i_n,i_{n+1}) \) to the state \( (f_n,f_{n+1}) \). The boundary transfer matrices are

\[
L = \begin{pmatrix}
0 & 1 & 0 & 1 \\
1 - \alpha & \gamma & \alpha & 1 - \gamma \end{pmatrix}, \quad
R = \begin{pmatrix}
0 & 1 & 0 & 1 \\
1 - \delta & \beta & \delta & 1 - \beta \end{pmatrix} \tag{5}
\]

The stationary state of the model has three phases: the high density phase, the low density phase and the maximal current phase. They are separated by the boundary-induced phase transitions \( 7, 1, 6 \).

§3. Method

In this article, we concentrate on the density profile (one-point function) \( \langle i_n \rangle \) \( (0 \leq n \leq N - 1) \) in the stationary state, which can be calculated in two steps as follows.

[B-1]
Obtain the right largest-eigenvalue eigenvector \( |P\rangle \) of \( T \) which satisfy

\[
T|P\rangle = \lambda|P\rangle, \tag{6}
\]

with \( \lambda (= 1) \) being the largest eigenvalue of \( T \). This \( |P\rangle \) is the stationary state whose wavefunction \( \langle i_0, i_1, i_2, \cdots, i_n, \cdots, i_{N-2}, i_{N-1}|P\rangle \) gives the stationary probability distribution.

[B-2]
Calculate \( \langle i_n \rangle \):

\[
\langle i_n \rangle = \frac{\sum_{\{i\}} i_n \langle i_0, i_1, i_2, \cdots, i_n, \cdots, i_{N-2}, i_{N-1}|P\rangle}{\sum_{\{i\}} \langle i_0, i_1, i_2, \cdots, i_n, \cdots, i_{N-2}, i_{N-1}|P\rangle}, \tag{7}
\]

where \( \sum_{\{i\}} \) denotes summation over all states \( \{i_0, i_1, \cdots, i_{N-2}, i_{N-1}\} \) of \( N \) sites.
We should note that to calculate the quantity \( \langle i_n \rangle \), we do not use the left largest-eigenvalue eigenvector of \( T \). This contrasts with the case of the classical statistical system, where the one-point function is expressed as \( \langle Q | \hat{i}_n | P \rangle / \langle Q | P \rangle \) with \( \langle Q | \) being the left largest-eigenvalue eigenvector of \( T \) and \( \hat{i}_n \) the local density operator.

Let us explain how we can incorporate the DMRG in these processes \([B-1]\) and \([B-2]\). The method we employ is essentially the finite-system-algorithm version\( \| \) of the “classical” DMRG.\( \} \). However, since our transfer matrix \( T \) is not symmetric, we need a non-trivial modification in the actual application of the algorithm: Unlike the ordinary DMRG, we should deal with “asymmetric density matrix.”\( \| \| \}

To clarify our explanation, we treat a chain of size \( N = 14 \). Suppose that, at some iteration stage in the DMRG, the renormalized transfer matrix \( T \) is expressed as in Fig. 1. For such form of \( T \), we adopt the notation \( T_4^l \times T_8^r \), where \( T_4^l \) is the renormalized left block transfer matrix of 4 sites, “\( \times \)” represents the local transfer matrix and \( T_8^r \) is the renormalized right block transfer matrix of 8 sites. Just as in the original finite-size algorithm of the DMRG, we consider the set \( \{ T_4^l \times T_8^r \}_{k=2,4,...,N-4} \) to refine iteratively the largest-eigenvalue eigenstate.

Hereafter we use Greek indices to represent the block state. By the power method (i.e., multiplication of \( T \) sufficiently many times), we get the right eigenfunction \( \psi(\mu_3; i_3, i_4, i_5, i_6; \nu_7) \) and the left eigenfunction \( \phi(\mu_3; i_3, i_4, i_5, i_6; \nu_7) \) belonging to the largest eigenvalue of \( T = T_4^l \times T_8^r \). We then form the “density matrix”\( \| \| \| \| \| \| \| \| \| \} \) for the left 5 sites \( \rho_5^l = \{ \rho_5^l(\mu_3, i_3, i_4; \mu_3', i_3', i_4') \} \) as

\[
\rho_5^l(\mu_3, i_3, i_4; \mu_3', i_3', i_4') \equiv \sum_{i_5, i_6, \nu_7} \psi(\mu_3; i_3, i_4, i_5, i_6; \nu_7) \phi(\mu_3'; i_3', i_4', i_5, i_6; \nu_7).
\]  \( (8) \)

Since \( \phi \neq \psi \), in general, for asymmetric \( T \), the matrix \( \rho_5^l \) is also asymmetric: \( \rho_5^l(\mu_3, i_3, i_4; \mu_3', i_3', i_4') \neq \rho_5^l(\mu_3', i_3', i_4'; \mu_3, i_3, i_4) \). As in the ordinary DMRG, we must perform eigenvalue decomposition of \( \rho_5^l \) to choose a truncated basis set for a new 5-site block. In our case, we should obtain both of the right and left eigenvectors for this purpose. Using the obtained transformation matrices for the new block states, we can renormalize the left block transfer matrix of 6 sites \( T_4^l \times \) to get \( T_6^l \). All the necessary block-making procedure can be done in a similar fashion.

By \( \{ L_j^{i_{j-2}, i_{j-1}, \mu_j} \} \) we denote the components of the \( \mu_j \)-th right eigenvector of \( \rho_5^l \) (density matrix for left \( j \) sites) with eigenvalue \( w_{\mu_j}^l \):  

\[
\sum_{\mu_j \sim i_{j-2}, i_{j-1}} \rho_j^l(\mu_j, i_{j-2}, i_{j-1}; \mu_j-2, i_{j-2}, i_{j-1}) L_j^{i_{j-2}, i_{j-1}, \mu_j}(\mu_j-2, i_{j-2}, i_{j-1}, \mu_j) = w_{\mu_j}^l R_j^{i_{j-2}, i_{j-1}, \mu_j}(\mu_j), \]
\( (9) \)

where we set \( \mu_j \equiv i_0 \). For the density matrix \( \rho_j^r \) for right \( j \) sites, we denote its right eigenvector with eigenvalue \( w_{\nu_j}^r \) by \( R_j^r \), whose components \( \{ R_j^{i_{j-2}, i_{j-1}, \nu_j} \} \) satisfy

\[
\sum_{i_{N-j}, i_{N-j+1}, \nu_{j-2}} \rho_j^r(i_{N-j}, i_{N-j+1}, \nu_{j-2}; i_{N-j}, i_{N-j+1}, \nu_{j-2}) R_j^{i_{j-2}, i_{j-1}, \nu_j}(i_{N-j}, i_{N-j+1}, \nu_{j-2}, \nu_j) \]
\( = w_{\nu_j}^r R_j^{i_{j-2}, i_{j-1}, \nu_j}(i_{N-j}, i_{N-j+1}, \nu_{j-2}, \nu_j), \)
\( (10) \)
where we set \(\nu_1 \equiv i_{N-1}\). We can then express the stationary-state vector \(|P\rangle\) in eq. (18) as

\[
\langle i_0, i_1, \ldots, i_{12}, i_{13}|P\rangle = \sum_{\mu_3, i_{11}, i_{12}, i_{13}} L^3_{(i_0, i_{11}, i_{12}), \mu_3} \psi(\mu_3; i_3, i_4, i_5, i_6; \nu_7) R^7_{(i_7, i_8, \nu_5), \nu_7} R^5_{(i_9, i_{10}, \nu_3), \nu_5} R^3_{(i_{11}, i_{12}, i_{13}), \nu_3}. 
\] (11)

The one-point function \(\langle i_n \rangle\) can be obtained as follows. For concreteness, we explain calculation of \(\langle i_4 \rangle\) and \(\langle i_5 \rangle\).

[C-1]
Perform partial summation

\[
\sum_{\{i\}}^{(4,5)} \langle i_0, i_1, \ldots, i_{N-2}, i_{N-1}|P\rangle = g(i_4, i_5),
\] (12)

where \(\sum_{\{i\}}^{(4,5)}\) means that we do not perform the summation over \(i_4, i_5\).

[C-2]
From the definition of \(\langle i_n \rangle\) (eq. (17)),

\[
\langle i_4 \rangle = \left[ \sum_{i_5} g(i_4 = 1, i_5) \right] / \left[ \sum_{i_4,i_5} g(i_4, i_5) \right],
\] (13)

\[
\langle i_5 \rangle = \left[ \sum_{i_4} g(i_4, i_5 = 1) \right] / \left[ \sum_{i_4,i_5} g(i_4, i_5) \right].
\] (14)

By introducing the following quantities,

\[
\sum_{i_0, i_{11}, i_{12}} L^3_{(i_0, i_{11}, i_{12}), \mu_3} \equiv S^3_3(\mu_3)
\] (15)

\[
\sum_{i_{11}, i_{12}, i_{13}} R^3_{(i_{11}, i_{12}, i_{13}), \nu_3} \equiv S^3_5(\nu_3)
\] (16)

\[
\sum_{i_9, i_{10}, \nu_3} R^5_{(i_9, i_{10}, \nu_3), \nu_5} S^5_3(\nu_3) \equiv S^5_5(\nu_5)
\] (17)

\[
\sum_{i_7, i_8, \nu_5} R^7_{(i_7, i_8, \nu_5), \nu_7} S^7_5(\nu_5) \equiv S^7_7(\nu_7)
\] (18)

we have

\[
g(i_4, i_5) = \sum_{\mu_3, i_{11}, i_{12}, \nu_3, \nu_5, \nu_7} S^3_3(\mu_3) \psi(\mu_3; i_3, i_4, i_5, i_6; \nu_7) S^7_7(\nu_7).
\] (19)

Eq. (19) means that for calculation of \(\langle i_4 \rangle\) and \(\langle i_5 \rangle\) we do not need the full probability distribution; we need only \(S^3_3(\mu_3), S^3_5(\nu_3), S^5_5(\nu_5), S^7_7(\nu_7)\). Accordingly, we need not retain full set of arrays \(\{L^3_{(\mu_3, i_{11}, i_{12}), \mu_3}\}\) and \(\{R^j_{(i_N, i_{N-j+1}, \nu_{j-2}), \nu_j}\}\) in eq. (11) at each iteration.
§4. Results

We present the calculated results for two cases: (A) $p = 0.75, q = 0.25, \alpha = 0.9, \beta = 0.8, \gamma = 0.01, \delta = 0.01$, and (B) $p = 0.75, q = 0.25, \alpha = 0.5, \beta = 0.5, \gamma = 0.4, \delta = 0.9$. The case (A) corresponds to the maximal current phase, and (B) to the high density phase.

In Fig. 2, we compare the DMRG calculation for case (A) with $N = 10$ to the exact results (both by the exact diagonalization and by the program using the MPA), varying the number $m$ of the retained bases. It should be noted that a very small number ($m = 2$) of retained bases gives a quite accurate density profile, implying that the “weight” of the density matrix is “localized” within very small number of bases. The similar behaviors are seen in the DMRG calculation for $N = 102$ in both cases (A) and (B), which are given in Fig. 3 and Fig. 4, respectively. The DMRG calculations with a very small number ($m = 2$) of retained bases are also in excellent agreement with the MPA results.

It has been known that for a set of parameters, the algebra associated with the MPA admits finite-dimensional representations. In the $n$-dimensional case, the DMRG with $n$ retained bases should be exact. The parameters in the present two cases (A) and (B) do not correspond to such finite-dimensional cases, which means that infinite $m$ in the DMRG is required for exact calculation. Our results show that even for such “infinite-dimensional cases”, DMRG calculation with a very small number of $m$ serves as an excellent approximation.

§5. Summary

In this paper, we have applied the density matrix renormalization group (DMRG) to asymmetric (simple) exclusion process (ASEP) which is a non-equilibrium many-body problem of hopping particles in one dimension. We have calculated the density profiles (one-point function) in the stationary states, which are in excellent agreement with exact solution. We have found that only a very small number of retained bases in the DMRG is necessary to attain the close-to-exact results. We have thus verified that the DMRG is an efficient method to study the ASEP.

We should comment on possible extensions of the present work.

1. Although we have considered only the one-point function in this paper, we can easily calculate 2-point function $\langle i_m i_n \rangle$, and, in principle, general $n$-point function in the stationary state. This is because, DMRG allows us to obtain the full distribution function in the stationary state.

2. The ASEP can be generalized in many different ways. For these generalized models stationary solutions cannot always be obtained by the matrix-product-ansatz approach. The DMRG approach used in the present paper can be easily generalized to these models. For instance,
   - Models including the processes such as coagulation, decoagulation, (pair-)creation, and (pair-)annihilation (We can incorporate this generalization in eq.(4).)
   - Models of site-dependent parameters of probability $p(n), q(n)$, where $n$ represents a site in
the system
• Models with $N$-species particles ($N \geq 2$).
• Models of hopping particles on a ring with a defect. (The DMRG can deal with 1-dimensional system with periodic boundary condition.)

Some of the above are now undertaken, whose results will be given in future publications.

Acknowledgments

The author would like to thank Y. Akutsu, K. Okunishi, T. Nishino, M. Kikuchi, T. Nagao and S. Yukawa for valuable discussions and encouragement. Part of numerical computation in this work was carried out at the Yukawa Institute Computer Facility.

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Fig. 1. A form of the transfer matrix $T = T_4^z \times T_K^x (N = 14)$. According to Nishino’s diagram, $\bigcirc$, $\square$ and $\Diamond$ represent a single site, a 3-site block and a 7-site block, respectively.

Fig. 2. The density profile of the model in the maximal current phase ($N = 10, p = 0.75, q = 0.25, \alpha = 0.9, \beta = 0.8, \gamma = 0.01, \delta = 0.01$)

Fig. 3. The density profile of the model in the maximal current phase ($N = 102, p = 0.75, q = 0.25, \alpha = 0.9, \beta = 0.8, \gamma = 0.01, \delta = 0.01$)

Fig. 4. The density profile of the model in the high density phase ($N = 102, p = 0.75, q = 0.25, \alpha = 0.5, \beta = 0.5, \gamma = 0.4, \delta = 0.9$)
\[ i_n : \text{matrix product ansatz} \]

\[ m = 2, p = 0.75, q = 0.25 \]

\[ \alpha = 0.90, \beta = 0.80 \]

\[ \gamma = 0.01, \delta = 0.01 \]

\[ + : \text{exact diagonalization} \]

\[ \circ : \text{matrix product ansatz} \]

\[ \times : m = 2 \]

\[ \square : m = 10 \]

\[ \triangle : m = 20 \]

\[ \diamondsuit : m = 32 \]
0.2

0.4

0.6

0.8

n


| O : matrix product ansatz |
| X : DMRG ( m = 2 ) |
| p = 0.75  q = 0.25 |
| α = 0.90  β = 0.80 |
| γ = 0.01  δ = 0.01 |
\( \text{matrix product ansatz} \)

\( \text{DMRG (} m = 2 \text{)} \)

\( p = 0.75 \quad q = 0.25 \)

\( \alpha = 0.50 \quad \beta = 0.50 \)

\( \gamma = 0.40 \quad \delta = 0.90 \)