Global optimization of tensor renormalization group using the corner transfer matrix

Satoshi Morita* and Naoki Kawashima
Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan
(Dated: September 8, 2020)

A tensor network renormalization algorithm with global optimization based on the corner transfer matrix is proposed. Since the environment is updated by the corner transfer matrix renormalization group method, the forward-backward iteration is unnecessary, which is a time-consuming part of other methods with global optimization. In addition, further approximation reducing the order of computational cost of contraction for calculation of the coarse-grained tensor is proposed. The computational time of our algorithm in two dimensions scales as the sixth power of the bond dimension while the higher-order tensor renormalization group and the higher-order second renormalization group methods have the seventh power. We perform benchmark calculations in the Ising model on the square lattice and show that the time-to-solution of the proposed algorithm is faster than that of other methods.

I. INTRODUCTION

Tensor network methods attract much attention as powerful tools for computing strongly correlated many-body problems. The partition function of classical statistical systems and low-energy states in quantum systems can be represented by tensor networks, in which exponentially large information is compressed efficiently. However, contraction of a large tensor network still requires huge computational cost. Combination of tensor networks and real-space renormalization group ideas resolves this problem. Tensor renormalization group (TRG) method provide a way to calculate coarse-grained tensor based on the singular value decomposition. Truncation of smaller singular values avoids divergence of tensor size. The higher-order tensor renormalization group method (HOTRG) is another method applicable to higher-dimensional systems.

Both the methods do information compression by solving local optimization problems. Approximations in these methods are locally optimal but not so for contraction of the whole tensor network. Therefore, the global optimization is necessary. Since the global optimization problem is defined by using the whole network, we need to introduce other approximations. The whole network is split into two parts, a small system and an environment surrounding it, and then the latter is approximated in an appropriate way. The second renormalization group method (SRG) and the higher-order SRG method (HOSRG) represent an environment as one tensor, which is called the environment tensor. Recently automatic differentiation technique is proposed to calculate the environment tensor. Although these methods drastically improve accuracy, calculation of the environment tensor requires performing the forward-backward iterations.

In this paper, we propose another approximation of the environment. We replace the environment tensor with the corner transfer matrices (CTM) and the edge tensors, which we call the CTM environment. It can be updated by using the CTM renormalization group (CTMRG) instead of the backward iteration. The computational cost of CTMRG is smaller than the backward iteration. The former scales as $O(\chi^6)$ against the bond dimension $\chi$ while the latter has $O(\chi^7)$ scaling. In addition, we introduce additional decomposition, whose key idea is information compression with the environment. This approximation reduces computational cost of tensor contraction for the coarse-grained tensor. Finally, our algorithm achieves computational cost scales as $O(\chi^6)$ while HOTRG and HOSRG has $O(\chi^7)$ cost in two-dimensional systems.

In the next section, we introduce our improved algorithm, which we call CTM-TRG. In the third section, benchmark results performed in the two-dimensional Ising model are shown. We will show that our algorithm has smaller time-to-solution than HOTRG and HOSRG. The last section is devoted to discussions and conclusions.

II. ALGORITHM

Let us consider contraction of a tensor network on the square lattice,

$$Z = \text{Cont} \left( \prod_i T_i \right).$$

A local tensor $T_i$ located at each site $i$ has four indices and connects with other tensors on the nearest-neighbor sites. We assume that each index of $T$ runs from 1 to $\chi$ at most. In other words, the bond dimension of $T$ is equal to $\chi$. For classical systems, $Z$ is the partition function and the Boltzmann weight determines elements of $T_i$. In quantum systems, such a contraction commonly appears as an inner product of a wave function so called the tensor network state or the projected entanglement paired state.

The HOTRG algorithm approximates this contraction by introducing the operator which merges two bonds into a single bond. In the original paper of HOTRG, this bond-merging operator is obtained by the higher-order
singular value decomposition (HOSVD) of a tensor,
\[ M_{(x_1, x_2)}y(x'_1, x'_2)y' \equiv \sum_i T_{x_1 y x'_1} T_{x_2 y x'_2}. \]  
Another solution of the bond-merging operator is the oblique projector \( PQ \) which minimizes
\[ \| M M - M P Q M \| \]  
with keeping the bond dimension between \( P \) and \( Q \) to \( \chi \). Its graphical representation is shown in Fig. 1(a). The algorithm for calculation of \( PQ \) is well known\(^{12-15} \) and its computational cost scales as \( O(\chi^6) \)\(^{15} \). After inserting bond-merging operators, the coarse-grained tensor is defined by contraction
\[ T_{x y x' y'} = \sum_{x_1, x_2, x'_1, x'_2} M_{(x_1, x_2)}y(x'_1, x'_2)y' P_{(x_1, x_2)}x Q_{x' (x'_1, x'_2)} \]  
The computationally heaviest part in HOTRG is this tensor contraction (Fig. 1(b)), which scales as \( O(\chi^7) \).

The minimization problem for the bond-merging operator in HOTRG (3) is a local optimization problem. Although such a solution is the best for a \( 2 \times 2 \) cluster, it is not the case for contraction of the whole network. A bond-merging operator obtained from larger clusters like as Fig. 2 will improve accuracy and its limit to infinite cluster size converges to a solution of the global optimization problem which minimizes difference between the whole network with and without a bond-merging operator. However, an optimization problem with larger clusters is intractable because its computational cost rapidly diverges with the cluster size.

Since the global optimization problem involves contraction of the whole network, some approximations are necessary. In the HOSRG algorithm, one local tensor is picked up and the other part is considered as an environment. The environment is represented by a four-index tensor, which we call the environment tensor. More precisely, the local tensor \( T^{(t)} \) and corresponding environment tensor \( \text{Env}^{(t)} \) at each renormalization step \( t \) approximate contraction of the whole network as
\[ Z \simeq \sum_{x, y, x', y'} T_{x y x' y'}^{(t)} \text{Env}_{x y x' y'}^{(t)} . \]  
Calculation of the environment tensor is done by the so-called backward iteration. It is a fine-grained process which updates the environment tensor \( \text{Env}^{(t-1)} \) using information at the \( t \)-th step. On the other hand, a coarse-grained process, called the forward iteration, updates the local tensors and the bond-merging operators. The HOSRG algorithm repeats the forward and backward iterations until convergence.

We note that computational cost of the HOSRG algorithm is scales as \( O(\chi^7) \) as well as HOTRG. Although calculation of the bond density operator defined in Ref.\(^4 \) requires \( O(\chi^8) \) computational cost, it can be avoided by using a similar technique shown in Ref.\(^6 \). Thus both the forward and backward iterations has \( O(\chi^7) \) computational cost.

The environment tensor requires the backward iteration and it causes main difficulty of the HOSRG method. The CTM-TRG employs the corner transfer matrix and the edge tensor since these can be calculated only from the local tensor. The environment tensor is decomposed into four CTMs \( \{ C_{TR}, C_{BR}, C_{BL}, C_{TL} \} \) and four edge tensors \( \{ E_T, E_L, E_B, E_R \} \), which we call the CTM environment in this paper. The subscripts (T, R, B, and L) indicate positions from a local tensor (top, right, bottom and left). For example, the top-right CTM \( C_{TR} \) represents all the tensors in the first quadrant.

The global optimization problem is represented by a
2 × 2 cluster of local tensors and its surrounding CTM environment. The bond-merging operator is calculated as the oblique projector which minimizes difference between two networks shown in the bottom inset. We note that $C_{\text{TL}}$ is decomposed into $c_{\text{TL}}$ and $c_{\text{TL}}'$. (b) A coarse-grained tensor in CTM-TRG is obtained by simultaneous scale transformation along horizontal and vertical directions.

The CTM environment reduces computational cost for calculation of the bond-merging operator to $O(\chi^6)$. However, contraction for the coarse-grained tensor (Fig. 1(b)) still scales as $O(\chi^7)$. To reduce this cost, we introduce an additional approximation (Fig. 4). First, we decompose the local tensor by using the singular value decomposition, $T_{xy} = \sum_{s=1,2} W_{xs} W_{sy} W_{sx} W_{sy}$, and define $t_{\text{TR}} = U \sqrt{\Sigma}$ and $t_{\text{BL}} = V \sqrt{\Sigma}$. Next, we insert truncation operators $p$ and $q$ between $t_{\text{TR}}$ and $t_{\text{BL}}$ to reduce the bond dimension from $\chi^2$ to $\chi'$. These operators are also calculated as oblique projectors which minimize the difference shown in the bottom of Fig. 4(a), where $c_{\text{TL}}$ and $c_{\text{TL}}'$ ($c_{\text{BR}}$ and $c_{\text{BR}}'$) are obtained from SVD of $C_{\text{TL}}$ ($C_{\text{BR}}$). We define $t_{\text{TR}} = t_{\text{TR}p}$ and $t_{\text{BL}} = t_{\text{BL}q}$. In the same manner, we calculate $t_{\text{TL}}$ and $t_{\text{BR}}$. Finally, we obtain the coarse-grained tensor $T^{(t+1)}$ by contraction of the tensor network as shown in Fig. 4(b), where $\tilde{P}$ and $\tilde{Q}$ are the bond-merging operators for vertical bonds. Clearly, computational cost of each step scales as $O(\chi^6)$ at most. In contrast to HOTRG and HOSRG, this method performs scale transformations along horizontal and vertical axes simultaneously.

At the beginning of the next step, we need to update the CTM environment by using CTMRG with the local tensor $T^{(t+1)}$. An initial value of the CTM environment at the step $t+1$ can be easily generated from the CTM environment at the previous step $t$. An initial value of $C^{(t+1)}$ is equal to $C^{(t)}$ and that of $E^{(t+1)}$ is calculated from $E^{(t)}$ and the bond-merging operators. For example, the edge tensor on the left edge is initialized as

$$E_{L, xy} = \sum_{x_1, x_2, y_1} E^{(t)}_{L, x_1 y_1} E^{(t)}_{L, x_2 y_2} P^{(t)}_{x_1 x_2}. \quad (6)$$

We note that this contraction has only $O(\chi^5)$ computational cost.

### III. RESULTS

We simulate the Ising model on the square lattice to investigate performance of our proposed algorithm. The initial local tensor at temperature $T = 1/\beta$ is given as

$$T^{(0)}_{xy} = \sum_{s=1,2} W_{xs} W_{sy} W_{sx} W_{sy}, \quad (7)$$

where $W$ is a $2 \times 2$ matrix,

$$W = \begin{pmatrix} \sqrt{\cosh \beta} & \sqrt{\sinh \beta} \\ \sqrt{\cosh \beta} & -\sqrt{\sinh \beta} \end{pmatrix}. \quad (8)$$

The critical temperature is $T_c = 2 / \log(\sqrt{2} + 1)$. The free energy per site is estimated from the coarse-grained tensor $T^{(t)}$ as

$$f = -\frac{1}{\beta N} \log \sum_{xy} T^{(t)}_{xy}, \quad (9)$$

where $t$ is the number of renormalization steps and $N = 2^{2L}$. We perform 20 renormalization steps, which is enough to observe convergence of the free energy even when its relative error is less than $10^{-12}$. Because of the global optimization, the free energy in CTM-TRG converges to its value in the thermodynamic limit much faster than that in HOTRG except in the near-critical region. We note that the free energy can also be estimated from the CTMs. It corresponds to the fixed or open boundary condition, while Eq. (9) assumes the periodic boundary condition. The both should take the same value in the thermodynamic limit and we confirm this fact in our numerical simulations.

In our algorithm, we use the same bond dimension $\chi$ for the local tensor and CTM environment and set $\chi' = 2\chi$ for diagonal decomposition of a local tensor in Fig. 4. In most cases, we use the fixed boundary condition (FBC) for the initial condition of the CTM environment. The initial edge tensor $E^{(0)}$ is a $2 \times 1 \times 1$ tensor and its element is given as $E_{x_1 y_1} = W_{x_1}$, where the first index connects with a local tensor. The initial CTM is a $1 \times 1 \times 1$ identity matrix, that is, $C_{11} = 1$. We first perform 32 CTMRG steps to obtain the CTM environment at $t = 0$ and do 4 CTMRG steps per each update of $T^{(t)}$. Although we observe that 4 is not enough to achieve convergence near the criticality, it is still sufficient for making the whole procedure produce more accurate results.
than HOTRG. We also use the open boundary condition (OBC), which is expected to be better than FBC in the paramagnetic phase. The initial CTM and edge tensor for OBC are defined by using $W$ as well as the initial local tensor $T^{(0)}$, for example, $C_{xy} = \sum W_{sx} W_{sy}$. For comparison, we also perform HOTRG and HOSRG simulations. In HOSRG, we repeat the forward-backward iterations four times because of our observation that it is sufficient for the convergence of the free energy in all the cases.

We compare relative errors in the free energy from the exact solution in the thermodynamic limit (Fig. 5). The method of CTM-TRG shows better accuracy than HOTRG in all cases and compatible to HOSRG. In the ferromagnetic phase, CTM-TRG is more accurate than HOSRG. It is because CTM-TRG performs scale transformations along horizontal and vertical directions simultaneously (Fig. 4(c)). We confirmed that our algorithm without the $O(\chi^6)$ approximation shows the same accuracy as HOSRG. Above the critical temperature, CTM-TRG has slightly larger error than HOSRG, which is caused by the small number of CTMRG iterations. The open boundary condition is more suitable for an initial value of the CTM environment in the paramagnetic phase and it provide more accurate results than HOSRG. We note that results with $\chi = 64$ is much better than the result reported in Ref. 7, which performed one-dimensional renormalization algorithm for large bond-dimension.

Elapsed time of each method is shown in Fig. 6. Our data clearly shows $O(\chi^6)$ scaling of CTM-TRG while HOTRG and HOSRG have $O(\chi^7)$. Although elapsed time of CTM-TRG is longer than HOTRG in the range of bond dimension we calculated, they will switch places around $\chi = 250$. Computational time was measured by simulations in a single core on Intel Xeon E5-2697A (2.60 GHz) with 128 GB memory.

FIG. 5. (Color online) Comparison of relative errors in the free energy. The vertical dashed line indicates the critical temperature.

FIG. 6. (Color online) Elapsed time of 20 renormalization steps as a function of the bond dimension. The dashed lines proportional to $\chi^6$ and $\chi^7$ are guides for eyes.

FIG. 7. (Color online) Relative error in the free energy at $T = T_c/1.01$ (top) and $T_c/0.99$ (bottom) as a function of the elapsed time of 20 steps.
by the dashed line in the bottom plot of Fig. 8, we find superior to the latter in larger bond dimension. As shown almost the same time-to-solution, the former should be icality. Although CTM-TRG and HOTRG seem to have achieves the best performance with large bond dimen-

otic phase as shown in Fig. 5. In the paramagnetic phase (<c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c><c>Fig. 7 shows time-to-solution at $T = T_c/1.01$ and $T_c/0.99$, CTM-TRG always outperform the other methods at $T = T_c/1.01$. It is because the global optimization drastically improves accuracy in the ferromagnetic phase as shown in Fig. 5. In the paramagnetic phase ($T = T_c/0.99$), CTM-TRG has steepest slope and achieves the best performance with large bond dimensions.

In Fig. 8, we show performance of CTM-TRG at criticality. Although CTM-TRG and HOTRG seem to have almost the same time-to-solution, the former should be superior to the latter in larger bond dimension. As shown by the dashed line in the bottom plot of Fig. 8, we find that relative error in the free energy of CTM-TRG is $\varepsilon_f \sim 0.013 \times \chi^{-4.0}$ and CTM-TRG achieves the same accuracy with 20% smaller bond dimension than HOTRG. From these facts and scaling of the computational time, we estimate that the crossing point between CTM-TRG and HOTRG exists about 20000 seconds in the top plot of Fig. 8. The relative error of CTM-TRG and HOTRG is proportional to $\tau^{-0.66}$ and $\tau^{-0.57}$, respectively.

IV. DISCUSSION AND CONCLUSIONS

In this paper, we consider the global optimization of tensor renormalization group and propose the improved algorithm based on the CTM environment. In our proposed algorithm CTM-TRG, the environment tensor of the HOSRG method is replaced by the CTMs and edge tensors. Since the CTM environment can be easily updated by using CTMRG, our algorithm does not require any backward iteration. In addition, we introduce additional approximation by decomposing the four-rank tensor into three-rank tensors which reduces the order of computational cost for tensor contraction without serious reduction in the overall accuracy. Computational cost of each step in CTM-TRG is bounded by $O(\chi^6)$, while HOTRG and HOSRG has $O(\chi^7)$ computational cost. Therefore our algorithm can produce almost the same accuracy as HOSRG within smaller computational time. We also show that time-to-solution of CTM-TRG is shorter than HOTRG and HOSRG in the paramagnetic and ferromagnetic phases.

In the present work, we use the standard CTMRG method to calculated the CTM environment. Recently a variational method based on the uniform matrix product state was proposed and it was applied to contraction of two-dimensional tensor networks. The edge tensors construct an eigenvector of the row-to-row (or column-to-column) transfer matrix represented as a matrix product operator, and the CTM is calculated as a solution of the fixed point equation. This algorithm improves convergence speed of the CTM environment especially near the critical point. Thus usage of such a variational approach instead of CTMRG may improve performance of our proposed algorithm.

We also comment on applicability of CTM-TRG to higher-dimensional systems. Although we have focused on the two-dimensional systems in this paper, the global optimization using the CTM environment can be generalized to higher-dimensions. In three dimension, we need to introduce the face tensor in addition to the CTMs and edge tensors to construct the environment.

It is known that TRG and HOTRG may converge to a fictitious fixed point owning to short-range entanglement and calculation of the scaling dimensions from eigenvalues of the transfer matrix is failed. Even in tensor renormalization methods with the global optimization like as HOSRG, short-range correlations are not removed completely. Such a problem also occurs in our proposed algorithm. Thus, to catch critical phenomena with better accuracy may eventually require introduction of entanglement filtering techniques. Especially, the loop entanglement filtering techniques seem to fit well with network structure appeared in Fig. 4. Moreover, entanglement filtering using the environment may remove short-range correlations more efficiently. However, it is out of the scope of the present work and still remains for future works.
ACKNOWLEDGMENTS

The authors would like to thank K. Harada, and T. Okubo for valuable discussions. The computation in this work is partially executed on computers at the Supercomputer Center, the Institute for Solid State Physics, the University of Tokyo. This research was supported by MEXT as “Exploratory Challenge on Post-K computer” (Challenge of Basic Science—Exploring Extremes through Multi-Physics and Multi-Scale Simulations) and by JSPS KAKENHI Grant Number JP19H01809 and JP20K03780.

* morita@issp.u-tokyo.ac.jp
1 R. Orús, Ann. Phys. 349, 117 (2014).
2 S.-J. Ran, E. Tirrito, C. Peng, X. Chen, L. Tagliacozzo, G. Su, and M. Lewenstein, Tensor Network Contractions: Methods and Applications to Quantum Many-Body Systems (Springer International Publishing, 2020).
3 M. Levin and C. P. Nave, Phys. Rev. Lett. 99, 120601 (2007).
4 Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, Phys. Rev. B 86, 045139 (2012).
5 Z. Y. Xie, H. C. Jiang, Q. N. Chen, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 103, 160601 (2009).
6 H. H. Zhao, Z. Y. Xie, Q. N. Chen, Z. C. Wei, J. W. Cai, and T. Xiang, Phys. Rev. B 81, 174411 (2010).
7 B.-B. Chen, Y. Gao, Y.-B. Guo, Y. Liu, H.-H. Zhao, H.-J. Liao, L. Wang, T. Xiang, W. Li, and Z. Y. Xie, (2019), arXiv:1912.02780.
8 R. J. Baxter, Exactly Solved Models in Statistical Mechanics (Academic Press, London, 1982).
9 T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 65, 891 (1996).
10 T. Nishino and K. Okunishi, Journal of the Physical Society of Japan 66, 3040 (1997).
11 F. Verstraete and J. I. Cirac, “Renormalization algorithms for quantum-many body systems in two and higher dimensions,” (2004), arXiv:cond-mat/0407066.
12 L. Wang and F. Verstraete, (2011), arXiv:1110.4302.
13 P. Corboz, T. M. Rice, and M. Troyer, Phys. Rev. Lett. 113, 046402 (2014).
14 S. Yang, Z.-C. Gu, and X.-G. Wen, Phys. Rev. Lett. 118, 110504 (2017).
15 S. Iino, S. Morita, and N. Kawashima, Phys. Rev. B 100, 035449 (2019).
16 S. Morita, R. Igarashi, H.-H. Zhao, and N. Kawashima, Phys. Rev. E 97, 033310 (2018).
17 V. Zauner-Stauber, L. Vanderstraeten, M. T. Fishman, F. Verstraete, and J. Haegeman, Phys. Rev. B 97, 045145 (2018).
18 M. T. Fishman, L. Vanderstraeten, V. Zauner-Stauber, J. Haegeman, and F. Verstraete, Phys. Rev. B 98, 235148 (2018).
19 T. Nishino and K. Okunishi, Journal of the Physical Society of Japan 67, 3066 (1998).
20 H. Ueda, K. Okunishi, and T. Nishino, Phys. Rev. B 89, 075116 (2014).
21 Z. C. Gu and X. G. Wen, Phys. Rev. B 80, 155131 (2009).
22 L. Ying, Multiscale Model. Simul. 15, 1423 (2016).
23 K. Harada, Phys. Rev. B 97, 045124 (2018).
24 M. Hauru, C. Delcamp, and S. Mizera, Phys. Rev. B 97, 045111 (2018).
25 G. Evenbly, Phys. Rev. B 98, 085155 (2018).