Efficient simulation of Grassmann Tensor Product States

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Recently, the Grassmann-tensor-entanglement renormalization group (GTERG) approach was proposed as a generic variational approach to study strongly correlated boson/fermion systems. However, the weakness of such a simple variational approach is that it provides a unified description of generic Grassmann tensor product states (GTPS) with large inner dimension D will contain a large number of variational parameters and must be determined through usual minimization procedures. In this paper, we first introduce a standard form of GTPS which significantly simplifies the representations. Then we describe a simple imaginary-time-evolution algorithm to efficiently update the GTPS based on the fermion coherent state representation and show the algorithm developed for usual tensor product states (TPS) can be implemented for GTPS in a similar way. Finally, we study the environment effect for the GTERG approach and propose a simple method to further improve its accuracy. We demonstrate our algorithms by studying a simple 2D free fermion system on honeycomb lattice, including both off-critical and critical cases.

Keywords:

I. INTRODUCTION

Since the discovery of fractional quantum hall effect (FQHE) and high \(T_c\) cuprates, it has been realized that a large class of phases and phase transitions cannot be described by Landau symmetry breaking theory. Enormous efforts have been made to understand the underlying physics for these new systems during the last two decades. It has been realized that the strongly correlated nature plays an essential role for these new classes of quantum matter. The most successful and powerful approach to study these new systems is based on new classes of variational wave functions. For example, the famous Laughlin wave function successfully explains the quantized nature of Hall conductance at rational filling. It turns out such a new state is very different from a symmetry breaking state and it can describe new orders of quantum matter-topological order. Although the essential physics of high-\(T_c\) is still under controversy, it is believed the relevant low energy physics is controlled by a class of metastable states—the resonating-valence-bond (RVB) states. A quantitative description for the RVB states is based on the projective wave function approach, which was first proposed to satisfy the no-double-occupancy constraint for (repulsive)Hubbard model in the strong coupling limit. It turns out this new class of states can also describe new phases of matter with topological order or quantum order. Later, those projective functions are widely used to describe the novel phenomena in strongly correlated systems, including frustrated magnets as well as the lattice fractional quantum Hall states.

Despite the success of projective states, they are specially designed to describe states with particular topological order or quantum order and it is very difficult to study the competing effect between different orders. Thus, it is very important to establish a unified frame work to encode different orders of quantum matter. In Ref.¹, a natural generalization of the projective states, the Grassmann tensor product states (GTPS) have been proposed as generic variational wave functions to study interacting boson/fermion systems.

However, only local GTPS (GTPS with short range bonds) can be efficiently simulated approximately. As a result, it is also very important to understand what kind of states can be faithfully represented in a local way. For spin systems, Refs.¹⁰,¹¹ have shown that the ground states of non-chiral topological phases, the so-called string-net condensates, admit a local tensor product states (TPS) representation. Later, the fermionic version of string-net states was proposed in Ref.¹³ and it has been shown they can describe non-chiral topological orders (e.g., fractional topological insulators) in fermion systems. Similar as the bosonic string-net states, their ground states can also be faithfully represented as GTPS since the parent Hamiltonians for these new classes of phases can be described as summations of (fermionic)commuting projectors. In a recent work, it has been shown even for systems with chiral topological orders, all the physical quantities still admit a local GTPS representation despite that their ground states wave functions contain long range bonds. Thus, best to our knowledge, the GTPS variational approach can in principle describe all kinds of gapped local boson/fermion systems in 1+2D. Clearly, the advantage of this new variational approach is that it provides a unified description for many different orders of quantum matter and allows us to study the competing effect between these different orders.

On the other hand, from the quantum information and computation perspective, it has been shown that ground states of gapped local Hamiltonians obey so-called area laws. For local boson/spin systems with translational invariant, states satisfy such a property can be efficiently represented by the class of so-called matrix product states (MPS) in one dimension and tensor...
inherent state representation, all the algorithms developed to solve this problem. Thus, it is natural to generalize this algorithm into GTPS.

In this paper, we will show based on the fermion coherent state representation, all the algorithms developed for usual TPS can be easily generalized into GTPS. The paper is organized as following: In section II, we represent a standard form of GTPS, which only contains one specie of Grassmann variable for each inner index and significantly simplifies the representation for numerical calculations. In section III, we first give a brief review about the concept of imaginary time evolution algorithm for TPS and then present the detail implementation of the imaginary time evolution algorithm for GTPS. Finally, we demonstrate the algorithm for a simple spinless fermion system on honeycomb lattice, including both off-critical and critical cases. In section IV, we describe the algorithm for a critical free fermion system on honeycomb lattice, and find a significant improvement. Finally, we briefly summarize our results and discuss possible future developments along this direction.

II. STANDARD FORM FOR GTPS

In this section, we will introduce a standard form to represent GTPS. In the standard form, each link only associates with one Grassmann variable, thus, the representation in the numerical calculations will be simplified significantly.

Let us recall the generic GTPS wavefunctions (defined in the usual Fork basis):

$$\Psi(\{m_i\}) = \sum_{\{a_j\}} P_0 \int \prod_i T_{i; a_i K_{a_i L}} \prod_{i j} G_{ij; a_i a_j}$$  \hspace{1cm} (1)$$

where

$$T_{i; a_i K_{a_i L}} = \sum_{\{l_{i}^{a_i}\} \{l_{i}^{K}\} \{l_{i}^{L}\}} \prod_{l \in a_i} (d\theta^{\alpha_i}_{l})^{l_{i}^{a_i}}$$

$$G_{ij; a_i a_j} = \sum_{\{l_{i}^{a_i}\} \{l_{j}^{a_j}\}} G(\theta_{ij}^{\alpha_i})^{l_{i}^{a_i}}(\theta_{ij}^{\alpha_j})^{l_{j}^{a_j}}$$  \hspace{1cm} (2)$$

Here $i, j, \ldots$ label different physical sites, $I, J, \ldots$ label different links and $I \in i$ means the link $I$ connects to the site $i$ (See in Fig. 1, any link $I$ uniquely belongs to one physical site $i$). On each link $I$, $a_I$ label the bosonic inner indices, $l_{i}^{a_i} = 0, 1$ label the fermionic inner indices and $a_I$ label different species of Grassmann variables. $m_i$ is the physical index. $\theta^{a_i}_{l_{i}^{a_i}}$ and $\theta^{\alpha_i}_{l_{i}^{a_i}}$ are Grassmann numbers and dual Grassmann numbers that satisfy the standard Grassmann algebra:

$$\theta^{a_i}_{l_{i}^{a_i}} \theta^{\alpha_i}_{l_{i}^{a_i}} = -\theta^{\alpha_i}_{l_{i}^{a_i}} \theta^{a_i}_{l_{i}^{a_i}}, \quad d\theta^{a_i}_{l_{i}^{a_i}} d\theta^{\alpha_i}_{l_{i}^{a_i}} = -d\theta^{\alpha_i}_{l_{i}^{a_i}} d\theta^{a_i}_{l_{i}^{a_i}},$$

$$\int d\theta^{a_i}_{l_{i}^{a_i}} d\theta^{\alpha_i}_{l_{i}^{a_i}} = \delta_{l_{i}^{a_i} l_{i}^{a_i}} \delta_{a_i a_i}, \quad \int d\theta^{a_i}_{l_{i}^{a_i}} 1 = 0.$$  \hspace{1cm} (3)$$

Note that $\Pi_i$ and $\Pi_{i'}$ have opposite orders:

$$\prod_i \theta_i \equiv \theta_1 \theta_2 \theta_3 \ldots \quad \prod_{i'} \theta_i \equiv \ldots \theta_3 \theta_2 \theta_1.$$  \hspace{1cm} (4)$$

The symbol $P_0$ represents a projection of the result of the integral to the term containing no Grassmann variables $\theta^{a_i}_{l_{i}^{a_i}}$.  

FIG. 1: A Graphic representation for the GTPS. The open circle which connects to links $I$ and $J$ represents the Grassmann metric $G_{ij; a_i a_j}$. The filled circle on the physical site $i$ represents the Grassmann tensors $T_{i; a_i K_{a_i L}}$. The Grassmann numbers $\theta^{\alpha_i}_{l_{i}^{a_i}}$ associate with the Grassmann metric $G_{ij; a_i a_j}$ and the dual Grassmann numbers $\theta^{a_i}_{l_{i}^{a_i}}$ associate with the Grassmann tensor $T_{i; a_i K_{a_i L}}$. There are a pair of indices $\{a_i, \{l_{i}^{a_i}\}\}$ live on link $I$. $a_i$ is called the bosonic index while $\{l_{i}^{a_i}\} = 0, 1$ are called the fermionic indices.
For fermion(electron) systems, the physical indices $m_i$ on a local Hilbert space are always associated with a definite fermion parity $P_f(m_i) = \pm 1$. Hence, we can impose the following constraints to issue that Eq. (38) do represent fermion wavefunctions.

\[
\sum_{l} \sum_{\alpha_i} l_{i}^{p} = \text{odd}, \text{ if } P_f(m_i) = -1 \\
\sum_{l} \sum_{\alpha_i} l_{i}^{p} = \text{even}, \text{ if } P_f(m_i) = 1 \\
\sum_{\alpha_i} l_{i}^{p} + \sum_{\alpha_j} l_{j}^{p} = \text{even} \quad (5)
\]

Although the original form Eq.(38) provides us a good physical insight of the state, especially for strongly correlated systems from projective constructions, it is not an efficient representation for numerical simulations. In the following we will derive the standard form of GTPS to simplify the representation.

By using the Grassmann version of singular-value-decomposition(GSVD) method proposed in Ref.1, under the constraint $\sum_{\alpha_i} l_{i}^{p} + \sum_{\alpha_j} l_{j}^{p} = \text{even}$, we can decompose $G_{ij;\alpha_j\alpha_j}$ into:

\[
G_{ij;\alpha_j\alpha_j} = \sum_{p_{i,j}} P_0 \int g_{ij;\alpha_j\alpha_j} S_{i;\alpha_j\alpha_j} S_{j;\alpha_j\alpha_j} \quad (6)
\]

with

\[
g_{ij;\alpha_j\alpha_j} = (1 + d\theta_{f} d\theta_{f}) \delta_{q_i q_j}
\]

\[
S_{i;\alpha_j\alpha_j} = \sum_{\{\ell_{i}^{q}\}} S_{i;\alpha_j\alpha_j}^{\ell_{i}^{q}} \left[ \prod_{\alpha_i} (\theta_{I}^{\alpha_1})^{\ell_{i}^{p}} \right] \theta_{i}^{\ell_{i}^{q}}
\]

\[
S_{j;\alpha_j\alpha_j} = \sum_{\{\ell_{j}^{q}\}} S_{j;\alpha_j\alpha_j}^{\ell_{j}^{q}} \left[ \prod_{\alpha_j} (\theta_{I}^{\alpha_1})^{\ell_{j}^{p}} \right] \theta_{j}^{\ell_{j}^{q}} \quad (7)
\]

and

\[
n_I = n_J = \sum_{\alpha_i} l_{i}^{p} \text{ mod } 2 = \sum_{\alpha_j} l_{j}^{p} \text{ mod } 2, \quad (8)
\]

where $S_{i;\alpha_j\alpha_j}^{\ell_{i}^{q}} = \sqrt{\prod_{n_i} U_{\alpha_i;\ell_{i}^{q}^{n_i} \rightarrow \alpha_i;\ell_{i}^{q}^{n_i}}}$ and $S_{j;\alpha_j\alpha_j}^{\ell_{j}^{q}} = \sqrt{\prod_{n_j} V_{\alpha_j;\ell_{j}^{q}^{n_j} \rightarrow \alpha_j;\ell_{j}^{q}^{n_j}}}$ are determined by the singular-value-decomposition(SVD) for the matrix $M_{\alpha_i;\ell_{i}^{q}^{n_i} \alpha_j;\ell_{j}^{q}^{n_j}} = G_{ij;\alpha_j\alpha_j}^{\ell_{j}^{q}}$ with $M = UAV^T$.

(Notice the the constraint $\sum_{\alpha_i} l_{i}^{p} + \sum_{\alpha_j} l_{j}^{p} = \text{even}$ implies a $Z_2$ symmetry for the matrix $M$ and it can be block diagonalized, with each sector labeled as $n_I = n_J = 0$ or 1.) Again, the symbol $P_0$ represents a projection of the result of the integral to the term containing no Grassmann number $\theta_I$. We call $g_{ij;\alpha_j\alpha_j}$ the standard metric for GTPS, which is the Grassmann generalization of the canonical delta function $\delta_{q_i q_j}$.

\[
(a_{i},l_{i}^{p}) \quad G_{ij} \quad (a_{j},l_{j}^{p}) \quad S_{i} \quad g_{ij} \quad S_{j} \quad (a_{i},l_{i}^{p})
\]

\[
\begin{align*}
\text{FIG. 2: A graphic representation of the decomposition Eq. (6). We use double lines(red and blue) to represent the standard metric $g_{ij}$, which is the $Z_2$ graded version of the canonical delta function. The blue line represents the channel with no inner fermion($n_I = n_J = 0$) and the red line represents the channel with one inner fermion($n_I = n_J = 1$) for the standard metric. The arrow of the red line represents the ordering for the dual Grassmann variables $d\theta_I$ and $d\theta_J$. We notice the standard metric $g_{ij}$ only has one specie of Grassmann variable despite the original Grassmann metric $G_{ij}$ contains many species of Grassmann variables on its link $I$ and $J$(labeled by $\alpha_I$ and $\alpha_J$). Here $q_I, q_J$ and $a_I, a_J$ are bosonic indices.}
\end{align*}
\]

Put Eq.(6) into Eq.(38), we have:

\[
\Psi\{\{m_i\}\} = \sum_{\{\alpha_I\};\{\alpha_J\}} P_0 P'_0 \int g_{ij;\alpha_j\alpha_j} \prod_{ij} g_{ij;\alpha_j\alpha_j} \prod_{i} S_{i;\alpha_j\alpha_j} \quad (9)
\]

The Grassmann matrices $S_{i;\alpha_j\alpha_j}$ defined on all links contain even number of Grassmann numbers and they commute with each other. Such a property allows us to regroup them as:

\[
\prod_{i} S_{i;\alpha_j\alpha_j} = \prod_{i} \prod_{l_{i}^{p}} S_{i;\alpha_j\alpha_j}, \quad (10)
\]

We use the fact that each link $I$ uniquely belongs to a site $i$ to derive the above expression. We note $\prod$ defined here have opposite orders according to $\prod$ defined in Eq. (2)

Thus, we can integral out all the Grassmann numbers $\sum_{\{\theta_{I}^{\alpha_1}\}}^{\ell_{i}^{q}^{n_i}}$ and sum over all the bosonic indices $\{\alpha_I\}$ to derive a simplified wave function:

\[
\Psi\{\{m_i\}\} = \sum_{\{\alpha_I\};\{\alpha_J\}} P_0 P'_0 \int g_{ij;\alpha_j\alpha_j} \prod_{i} \frac{T_{i;l_{i}^{p} d\theta_I}}{g_{ij;\alpha_j\alpha_j}} \quad (11)
\]

where the new Grassmann tensor $\tilde{T}_{i;l_{i}^{p} d\theta_I}$... associate with physical site $i$ can be expressed as:

\[
\tilde{T}_{i;l_{i}^{p} d\theta_I} = \sum_{n_K} \tilde{T}_{i;l_{i}^{p} d\theta_I} \prod_{I\in\ell} \theta_{I}^{\ell_{i}^{p}} \quad (12)
\]

with

\[
\tilde{T}_{i;l_{i}^{p} d\theta_I} = \sum_{n_K} \sum_{\alpha_I \alpha_J} \sum_{\ell_{i}^{p} \ell_{j}^{p}} T_{i;l_{i}^{p} d\theta_I} S_{i;l_{i}^{p} d\theta_I} \quad (13)
\]
The fermion number is determined as \( N \). We can further simplify the expression by group the standard metric \( \mathcal{G}_{ij} \) and we use blue(red) line to represent the fermion parity even(odd) indices. If \( P_f(p_i) = -1 \), we associate a Grassmann number \( \theta_i \) with the standard Grassmann tensor \( T^{m_i}_{i;PKL} \) while associate its dual \( d\theta_i \) with the standard metric \( \mathcal{G}_{ij} \). Since the standard metric \( \mathcal{G}_{ij} \) is actually just a Grassmann generalization of the canonical delta function \( \delta_{ij} \), we only need to use an arrow to specify the ordering of the two Grassmann variables \( d\theta_j \) and \( d\theta_i \).

We call Eq.(11) the standard form of GTPS which only contains one spec of Grassmann variable on each link. We can further simplify the expression by group the bosonic index \( qi \) and fermionic index \( ni \) into one super index \( p_i = (qi, ni) \).

\[
\psi(m_i) = \sum_{\{p_i\}} \prod_{ij} \mathcal{G}_{ij};p_i;P \prod_i T^{m_i}_{ij;PKL} \ldots, \quad (14)
\]

with

\[
\mathcal{G}_{ij;p_i;P} = \delta_{P(r)}(d\theta_j)^{N_j(p_j)}(d\theta_j)^{N_j(p_j)}
\]

\[
T^{m_i}_{ij;PKL} \ldots = T^{m_i}_{i;NKQL} \ldots \prod_i \theta_i^{N_i(p_i)} \ldots, \quad (15)
\]

where \( N_j(p_j) = n_j \). Notice the super index \( p_j \) has a definite fermion parity \( P_f(p_j) = \pm 1 \) and the corresponding fermion number is determined as \( N_f = \frac{P_f(p_j) + 1}{2} \).

The new form Eq.(14) is extremely useful in general purpose of numerical calculations. We will use this new form to explain all the details of our algorithms.

### III. THE IMAGINARY TIME EVOLUTION ALGORITHM

In this section, we will give a brief review of imaginary time evolution algorithm of usual TPS first and then generalize all those algorithms into GTPS. Finally, we apply the algorithms to a simple free fermion example on honeycomb lattice.

#### A. A review of the algorithm of TPS

1. **generic discussion**

Let us consider the imaginary time evolution for generic TPS \( |\Psi_0\rangle \).

\[
|\Psi_\tau\rangle = e^{-\tau H}|\Psi_0\rangle
\]

(16)

If we don’t make any approximation, the true ground state can be achieved in the \( \tau \to \infty \) limit.

\[
|\Psi_{GS}\rangle = \lim_{\tau \to \infty} e^{-\tau H}|\Psi_0\rangle = \lim_{N \to \infty} e^{-N\delta \tau H}|\Psi_0\rangle, \quad (17)
\]

where \( N \) is the number of evolution steps and \( \delta \tau = \tau/N \) is a sufficiently tiny imaginary-time slice. However, without any approximation, the inner dimension of TPS will increase exponentially with the number of evolution steps. Hence, we need to find out the best TPS approximation with fixed inner dimension.

WLOG, we use the honeycomb lattice geometry to explain the details here and for the rest parts of the paper. To illustrate the key idea of the algorithm, let us consider a simple case that the model Hamiltonian \( H \) only contains a summation of nearest neighbor two-body terms:

\[
H = \sum_{ij} h_{ij}, \quad (18)
\]

Let us divide the Hamiltonian into three parts:

\[
H = H_x + H_y + H_z; \quad H_\alpha = \sum_{i \in A} h_{i,i+\alpha} \quad (\alpha = x, y, z),
\]

(19)

where \( A \) label the sublattices \( A \) and \( x, y, z \) label three different nearest neighbor directions. By applying the Trotter expansion, we have:

\[
e^{-\delta \tau H} = e^{-\delta \tau H_x}e^{-\delta \tau H_y}e^{-\delta \tau H_z} + o(\delta \tau^2) \quad (20)
\]

Notice each \( H_\alpha \) only contains summation of commuting terms, hence we can decompose them without errors:

\[
e^{-\delta \tau H_\alpha} = \prod_i e^{-\delta \tau h_{i,i+\alpha}} \quad (21)
\]
Let us expand $|\Psi_0\rangle$ under the physical basis:

$$|\Psi_0\rangle = \sum_{\{m_i, m_j\}} \sum_{\{a, a'\} \in A} \prod_{i \in A} T_{iabc}^{m_i} \prod_{j \in B} T_{jabc}^{m_j} \prod_{ij} \delta_{aa'}\{|m_i, m_j\},$$

(22)

Here $A, B$ denote two different sublattice in a unit cell and $m_{ij}$ denote the physical indices on site $i(j)$, e.g., $m_{ij} = \uparrow, \downarrow$ for a spin 1/2 system. The canonical delta function $\delta_{aa'}$ defined on link $ij$ can be regarded as the metric associated with tensor contraction, which can be generalized to its Grassmann variable version for fermion systems. After acting one evolution operator $e^{-\delta H_{ij}}$ onto the corresponding link $ij$, we can expand the new state $e^{-\delta h_{ij}}|\Psi_0\rangle$ as:

$$e^{-\delta h_{ij}}|\Psi_0\rangle = \sum_{\{m_i, m_j\}} \sum_{\{a, a'\} \in A} E_{m_i m_j}^{m_i m_j} T_{iabc}^{m_i} T_{jabc}^{m_j} \times \prod_{\nu \neq i} T_{\nu'e'df}^{m_{\nu'}, \bar{\nu}'} \prod_{\nu \neq j} T_{\nu'e'df}^{m_{\nu'}, \bar{\nu}'} \prod_{ij} \delta_{aa'}\{|m_i, m_j\},$$

(23)

where $E_{m_i m_j}^{m_i m_j} = (m_i, m_j)|e^{-\delta h_{ij}}|m_i, m_j\rangle$ is the matrix element of the evolution operator on link $ij$. Use the SVD decomposition, we can decompose the rank 6 tensor $T_{ij;m_i, m_j; bcb'} = \sum_m \sum_{m_i', m_j'} E_{m_i m_j}^{m_i' m_j'} T_{iabc}^{m_i} T_{jabc}^{m_j} T_{ij}^{m_i m_j}$ as:

$$T_{ij;m_i, m_j; bcb'} = \sum_{a} \sum_{a'} T_{iabc}^{m_i} T_{jabc}^{m_j} \delta_{aa'},$$

(24)

where $T_{iabc}^{m_i}$ have enlarged inner dimension $Dd^2$ instead of $D$ for their inner dimensions $a$ (the bonds along $x$ direction). Similarly, the dimension of indices $b, c$ (the bonds along $y, z$ directions) will be enlarged to $Dd^2$ after applying $e^{-\delta h_{ij}}$ on $|\Psi_0\rangle$. Thus, it is easy to see that the inner dimension will increase exponentially with increasing evolution steps if we don’t make any truncation.

To solve the above difficulty, we need to find a new set of $\{T_{iabc}^{m_i}\}$ with fixed inner dimension that minimizes the distance with $e^{-\delta H_{ij}}|\Psi_0\rangle$. If we start from $|\Psi_0\rangle$ and evolve it by $e^{-\delta H_{ij}}$ in a sufficient thin time slice, the cost function $f$ takes the form:

$$f(\{T_{iabc}^{m_i}\}) = |||\Psi'_0\rangle - e^{-\delta H_{ij}}|\Psi_0\rangle||$$

$$= \langle \Psi'_0 | \Psi_0 \rangle - \langle \Psi'_0 | e^{-\delta H_{ij}}|\Psi_0\rangle + h.c. \rangle + const.,$$

(26)

where $f$ is a multi-variable quadratic function of $\{T_{i;\nu'; \nu}^{m_i}\}$, hence we can use the sweep method to minimize it. The advantage of the above algorithm is that the Trotter error will not accumulate after long time evolution. However, calculating the cost function $f$ explicitly is an exponentially hard problem and we need further approximations at this stage. Some possible methods have been proposed based on the MPS algorithm, but the calculational cost can still be very large and the method has only been implemented with open boundary condition(OBC) so far.

2. translational invariant systems

Nevertheless, for translational invariant TPS ansatz, it is possible to develop efficient method to simulate the cost function by using the TERG method. We assume $T_i = T_A$ if $i \in A$ and $T_j = T_B$ if $j \in B$. The cost function can be expressed as:

$$f(T_A; T_B) = \rho e^{b'C' \cdot \bar{b}'C'} T_{A;abc}^{m_i} T_{A;abc}^{m_j} T_{B;abc}^{m_j} T_{B;abc}^{m_j} - (e^{b'C' \cdot m_i} T_{A;abc}^{m_i} T_{B;abc}^{m_i} + h.c.) + \text{const.},$$

(28)

where $\rho$ and $e$ (Fig. 5) are the so-called environment tensors. Here we use the convention that all the repeated indices will be summed over and use $T$ to represent complex conjugate of $T$. Strictly speaking, the environment tensors for $\rho$ and $e$ are also dependent on $T_A'$ and $T_B'$, thus $f$ is no longer a quadratic multi-variable function. However, for sufficiently thin slice time, up to $o(\delta^2)$ error (same order as Trotter error), we can replace $T_A, T_B$ by $T_A', T_B'$ when calculating the environment tensor $\rho, e$ can be derived from $\rho$:

$$e^{b'C' \cdot m_i, m_j} = \rho e^{b'C' \cdot \bar{b}'C'} T_{A;abc}^{m_i} T_{A;abc}^{m_j} T_{B;\bar{b}C'}^{m_j} T_{B;\bar{b}C'}^{m_j}$$

(29)

Again, repeated indices need to be summed over here. We notice $\rho$ can be expressed as a tensor trace of double tensors $T_{A} = \sum_m T_{A}^{m} \otimes T_{A}^{m}$ with an impurity tensor $T_{ij}$ on the link $ij$:

$$\rho e^{b'C' \cdot \bar{b}'C'} = t \text{Tr}[T_{ij}^{p} \otimes T_{A} \otimes T_{B} \otimes T_{A} \otimes T_{B} \cdots],$$

(30)

where the impurity double tensor $T_{ij}$ is just a projector:

$$T_{ij; \nu'; \nu}^{b'C' \cdot \bar{b}'C'} = 1; \quad \text{others} = 0$$

(31)

Now it is easy to see we can first decompose the impurity tensor on the link $i,j$ to two rank 3 impurity tensors on
site $i,j$ and then implement the usual TERG algorithm. We can also use a more efficient but complicated way to compute $\rho$ by applying the coarse grain procedures for all sites except sites $i,j$, as introduced in Ref.\textsuperscript{32}.

The above algorithm can be further simplified if we assume the environment tensor $\rho$ has specific forms for certain physical systems. One interesting attempting is proposed in Ref.\textsuperscript{31} by assuming $\rho$ can be factorized as:

$$\rho^{bc'b'c'\bar{b}\bar{b}'c''} = \Lambda_b^{\alpha} \Lambda_c^{\alpha} \Lambda_{b'}^{\alpha} \Lambda_{c'}^{\alpha} \delta_{\bar{b}b}\delta_{c\bar{c}'}\delta_{b'b'}\delta_{c'\bar{c}''},$$

(32)

where $\Lambda^\alpha$ is a positive weight vector defined on links along $\alpha$ direction. The above form can always be true for 1D systems\textsuperscript{35} due to the existence of canonical form of a MPS. Although the above form is not generic enough in 2D, it still works well in many cases, especially for those systems with symmetry breaking order. In this case, the cost function Eq.\textsuperscript{28} can be solved by SVD decomposition and keep the leading $D$ singular values for the following matrix:

$$M_{b'c'mj} = \sum_{a,m',m''} \sqrt{\Lambda_b^{\alpha}} \sqrt{\Lambda_c^{\alpha}} \sqrt{\Lambda_{b'}^{\alpha}} \sqrt{\Lambda_{c'}^{\alpha}} T_{ij,mn} \rho^{bcb'c'mj}$$

$$= \sum_{a,m',m''} \sqrt{\Lambda_b^{\alpha}} \sqrt{\Lambda_c^{\alpha}} \sqrt{\Lambda_{b'}^{\alpha}} \sqrt{\Lambda_{c'}^{\alpha}}$$

$$\times E_{m'm''} T_{bcb'} T_{bc'm'}$$

$$\approx \sum_{a=1}^{D} U_{bcbmajo} V_{b'c'mja} \Lambda_a^{\alpha}$$

(33)

The new tensors $T_A'$ and $T_B'$ can be determined as:

$$T_{A'c'mja}^{m''} = \frac{1}{\sqrt{\Lambda_b^{\alpha} \Lambda_c^{\alpha} \Lambda_{b'}^{\alpha} \Lambda_{c'}^{\alpha}}} U_{bcbmajo}$$

$$T_{B'c'mja}^{m''} = \frac{1}{\sqrt{\Lambda_b^{\alpha} \Lambda_c^{\alpha} \Lambda_{b'}^{\alpha} \Lambda_{c'}^{\alpha}}} V_{b'c'mja}$$

(34)

Similar as in 1D, the environment weight associated with bonds along $x$ direction is updated as $\Lambda^x = \Lambda'$. It is not hard to understand why the above simplified algorithm works very well for systems with symmetry breaking orders, but not in the critical region, since in those cases the ground states are close to product states and the entanglements between $x, y, z$ directions in the environment tensors become pretty weak. However, for topological ordered states, the environment tensors can be more complicated. For example, the $Z_2$ topological ordered state in the toric code model will have an emergent $Z_2$ symmetry and could not be factorized as a product. Hence, for topological ordered states, it is important to calculate the full environment in the imaginary time evolution.
B. Generalize to fermion(electron) systems

In this subsection, we will show how to generalize the above algorithms to GTPS. The key step is to introduce fermion coherent state representation and treat the physical indices also as a Grassmann variable. WLOG, we use a spinless fermion system as a simple example here and for the rest parts of the paper:

\[ |\eta\rangle \equiv \prod_i (1 - \eta_i c_i^\dagger)|0\rangle, \tag{35} \]

where \(\eta_i\) is a Grassmann number.

As already having been discussed in Ref.\(^1\), in this new basis, the GTPS wavefunction Eq.(38) and its standard form Eq.(14) can be represented as:

\[
\Psi(\{\eta_i\}) = \sum_{\{m_i\}} \sum_{\{a_i\}} \int \prod_i \tilde{\eta}_i^{m_i} T_{\alpha;k\alpha;i} \ldots \prod_{ij} \tilde{G}_{ij;a_ia_j} \nonumber \\
= \sum_{\{m_i\}} \sum_{\{p_i\}} \int \prod_i g_{ij;p_i;ij} \prod_i \tilde{\eta}_i^{m_i} T_{\alpha;k\alpha;i} \ldots \nonumber \\
= \sum_{\{m_i\}} \sum_{\{p_i\}} \int \prod_i g_{ij;p_i;ij} \prod_i \tilde{T}_{\alpha;k\alpha;i} \ldots \tag{36} \]

where \(\tilde{\eta}_i\) is the complex conjugate of the Grassmann number \(\eta_i\) and \(\tilde{T}_{\alpha;k\alpha;i}\ldots = \tilde{\eta}_i^{m_i} T_{\alpha;k\alpha;i} \ldots\).

On honeycomb lattice with translational invariant, we can simplify the above expression as:

\[
\Psi(\{\tilde{\eta}_i\}, \{\tilde{\eta}_j\}) = \sum_{\{m_i\},\{m_j\}} \sum_{\{a_i\},\{a_j\}} \int \prod_i g_{aa'} \prod_i \tilde{T}_{\alpha;i\alpha;ij} \prod_j \tilde{T}_{\beta;ij;\beta'}, \tag{37} \]

with

\[
\tilde{T}_{\alpha;i\alpha;ij} = \tilde{T}_{\alpha;i\alpha;ij} \phi_{\alpha}^N(a) \phi_{\beta}^N(b) \phi_{\gamma}^N(c), \nonumber \\
\tilde{T}_{\beta;ij;\beta'} = \tilde{T}_{\beta;ij;\beta'} \phi_{\beta'}^N(b') \phi_{\gamma'}^N(c'), \nonumber \\
g_{aa'} = \delta_{aa'} \phi_{\alpha}^N(a') \phi_{\alpha'}^N(a'). \tag{38} \]

Comparing with usual TPS, here the link indices \(\{a, a'\}\) always have definite fermion parity \(P_f = \pm 1\). \(N_f = 0\) when \(P_f = 1\) while \(N_f = 1\) when \(P_f = -1\).

Let us start from the simplest case with the assumption the environment can also be approximated by some weight. In this case, the imaginary time evolution for GTPS can be reduced to a SVD problem of Grassmann variables. The Grassmann version of the matrix \(M\) in Eq.(33) can be constructed as following:

(a) Let us first sum over the bond indices \(a, a'\) and integral out the Grassmann variable \(\theta_{\alpha}, \theta_{\alpha'}\):

\[
\int d\theta_{\alpha} d\theta_{\alpha'} \phi_{\alpha}^N(a) \phi_{\beta}^N(b) \phi_{\gamma}^N(c) \phi_{\beta'}^N(b') \phi_{\gamma'}^N(c') = \delta_{\alpha\alpha'} \delta_{\beta\beta'} \delta_{\gamma\gamma'} \phi_{\alpha}^N(a') \phi_{\alpha'}^N(a). \tag{39} \]

Here the sign factor \((-)^{|m_i|+|m_j|} N_f(a) (-)^{|m_j|+|m_j|+N_f(b)+N_f(c)}\) comes from the anti-commuting relations of Grassmann variables.

(b) Next we derive the matrix element of the evolution operator under fermion coherent state representation. Let us first calculate them under the usual Fock basis \((c_i^\dagger)^{m_i}(c_i)^{m_i}|0\rangle\) with \(m_i, m_j = 0, 1\). Let us define:

\[
E_{m_i m_j}^{m'_i m'_j} = \langle 0|(c_i^\dagger)^{m_i}(c_i)^{m_i}|0\rangle e^{-\delta \tau h_{ij}} \langle c_i^\dagger)^{m'_i}(c_i)^{m'_i}|0\rangle \tag{40} \]

Thus, we can expand \(e^{-\delta \tau h_{ij}}\) as:

\[
e^{-\delta \tau h_{ij}} = \sum_{m_i m_j m'_i m'_j} E_{m_i m_j}^{m'_i m'_j} (c_i^\dagger)^{m_j}(c_i)^{m'_j}|0\rangle e^{-\delta \tau h_{ij}} \langle c_i^\dagger)^{m'_i}(c_i)^{m'_i}|0\rangle \tag{41} \]

In the fermion coherent state basis, we have:

\[
\langle \eta_i, \eta_j|e^{-\delta \tau h_{ij}}|\eta_i, \eta_j\rangle = \sum_{m_i, m_j, m'_i, m'_j} E_{m_i m_j}^{m'_i m'_j} (\eta_i^{m_j})(\eta_i^{m'_j})(\eta_j^{m'_i})(\eta_j^{m'_i}) \tag{42} \]

(c) Then we can evolve the state \(\Psi\) to a new state \(\Psi'\):

\[
\Psi'(\{\eta_i', \eta_j\}) = \int d\tilde{\eta}_i d\eta_i d\tilde{\eta}_j d\eta_j (1 + \eta_i \tilde{\eta}_i)(1 + \eta_j \tilde{\eta}_j) \\
\times \langle \eta_i', \eta_j'|e^{-\delta \tau h_{ij}}|\eta_i, \eta_j\rangle \Psi(\{\eta_i \}, \{\eta_j\}). \tag{43} \]

Put Eq.(39) and Eq.(42) into the above equation, it is easy to derive the Grassmann version of the rank 6 tensor \(T_{ij}\) defined on the link \(ij\). We have:
We notice there is an extra sign factor $(-m_j[m_i + N_f(b) + N_f(c)])$ after we reorder these Grassmann variables.

(d) Finally, we can define the Grassmann generalization of the $M$ matrix after putting the environment weight for all the inner indices.

$$M_{b c m_i; b' c' m_j} = M_{b c m_i; b' c' m_j} (-\eta_j)^{m_i} N_j(b) \theta_\gamma N_j(c) \times (-\eta_j)^{m_j} N_j(b) \theta_\gamma N_j(c).$$

where the coefficient matrix $M$ reads:

$$M_{b c m_i; b' c' m_j} = \sum_{a m_i, m_j} \sqrt{\Lambda^a_b \Lambda^c_b \Lambda^a_{c'} \Lambda^c_{c'}} \times (-m_i)[m_i + N_f(b) + N_f(c)] \times (-m_j)[m_j + N_f(b) + N_f(c)] \times E_{m_i, m_j} T_{A; a b c} T_{B; a' b' c'}.$$  

Since $h_{ij}$ is a local fermionic operator, it will always contain even number of fermion operators. As a result, the nonzero elements of $M$ matrix will always contain even number of Grassmann variables and we can apply GSVD as discussed before. We keep the largest $D$ eigenvalues:

$$M_{b c m_i; b' c' m_j} = \sum_{a} U_{b c m_i; a} \Lambda_a V_{b' c' m_j; a}$$

The coefficient matrix $M$ will have a block diagonal structure, hence the new index $a$ will have a definite fermion parity $P_f(a) = P_f(b)P_f(c) = P_f(b')P_f(c')$. Similar as in usual TPS case, the new Grassmann tensors $\mathcal{T}^i$ and $\mathcal{T}^f$ have the form

$$\mathcal{T}^m_{A; a b c} = \sqrt{\Lambda}_a \sqrt{\Lambda}_b \sqrt{\Lambda}_c U_{b c m_i; a} \theta_\alpha N_j(a) \theta_\beta N_j(b) \theta_\gamma N_j(c).$$

$$\mathcal{T}^m_{B; a' b' c'} = \sqrt{\Lambda}_a \sqrt{\Lambda}_b \sqrt{\Lambda}_c V_{b' c' m_j; a'} \theta_\alpha N_j(a') \theta_\beta N_j(b') \theta_\gamma N_j(c').$$

However, due to the reordering of Grassmann variables, extra signs appear in the new tensors $\mathcal{T}^i_A$ and $\mathcal{T}^i_B$.

$$\mathcal{T}^m_{A; a b c} = (-m_j N_f(a) \sqrt{\Lambda}_a \sqrt{\Lambda}_b \sqrt{\Lambda}_c U_{b c m_i; a}.$$}

$$\mathcal{T}^m_{B; a' b' c'} = (-m_j N_f(a') \sqrt{\Lambda}_a \sqrt{\Lambda}_b \sqrt{\Lambda}_c V_{b' c' m_j; a'}.$$}

Again $\Lambda_a$ is used as the new environment weight for all links along $x$ direction.

The full environment tensors can be very similar as in usual TPS case. The Grassmann version of the environment tensor $\rho$ can be efficiently simulated by GTPS. The environment tensor $c$ can be calculated from $\rho$ and $\mathcal{T}^i_j$. The cost function can be derived from Eq.(28) after replacing $\rho$ and $\mathcal{T}^i_j$. We contract the tensor-net and integral out all the Grassmann variables, it can be reduced to a usual multi-variable quadratic minimization problem for the coefficient tensors $\mathcal{T}^i_A$ and $\mathcal{T}^i_B$, we can solve it by using the sweep method. Although the algorithm with full environment is general, it is still very time consuming and a much more efficient method is very desired. Nevertheless, it turns out that the simple updated method works very well in many cases and we will focus on the application of this method in this paper.

### C. A free fermion example

In this subsection, we demonstrate the above algorithm by studying a free fermion model on honeycomb lattice. We consider the following (spinless)fermion Hamiltonian:

$$H = -\Delta \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.) + \mu \sum_i n_i$$

We first test our algorithm in the parameter region where the system opens a gap. For example, we can fix $\mu = 1$ and take different values for $\Delta$ from 0.1 to 0.5. See in Fig. (10), even with the minimal inner dimension $D = 2$, the GTPS variational approach already gives out very good ground state energy. Here and through out the whole paper, we fix the total system size to be $N = 2 \times 3^9$ sites and with PBC.(The GTEG algorithm will allow us to reach huge size in principle, however, for better convergency, we choose relatively large but not huge size.)
We note the agreement for the ground state energy is better for small $\Delta$, which is expected since the system becomes a trivial vacuum state $|0\rangle$ in the limit $\Delta = 0$. In the insert of Fig. 10, we also plot the ground energy as a function of $D_{\text{cut}}$ and it is shown the energy converges for very small $D_{\text{cut}}$ (around $D_{\text{cut}} = 15$, where $D_{\text{cut}}$ is the number of singular values we keep in the GTERG algorithm). We find the relative error can be very small, e.g., 0.4% for $\Delta = 0.2$.

Although we get good results for the above simple example, it is not quite surprising since a trivial gapped fermion system only evolves local physics. A much more challenging and interesting example is at $\mu = 0$, in which case the low energy physics of the system is described by two Dirac cones in the first Brillouin Zone(BZ). Actually, up to a particle-hole transformation on one sublattice, the above fermion paring Hamiltonian is equivalent to the fermion hopping Hamiltonian that describes the novel physics in graphene (the spin less version) where low energy electrons deserve a Dirac like dispersion. In Fig. 10, we plot the ground state energy as a function of $D_{\text{cut}}$ for inner dimensions $D = 2$ and $D = 4$. In this case, the $D = 2$ approach only gives very poor results comparing to the gapped case. However, when we increase the inner dimension to $D = 4$, we find that the ground state energy agrees pretty well with the exact one, with a relative error of 0.6%. Another interesting feature is that such a critical system would require a much larger $D_{\text{cut}}$ (around $D_{\text{cut}} = 70$ for $D = 4$.) for the convergence of the GTERG algorithm. Later, we would discuss a possible improvement for the GTERG algorithm, which allows us to access much larger inner dimension $D$.

Finally, we would like to make some comments and discussions about the above results:

(a) Although a gapless fermion system with Dirac cones is critical, it does not violate the area law because it only contains zero dimensional Fermi surfaces.

(b) The good agreement in ground state energy does not imply the good agreement in long range correlations. Indeed, our conjecture is that for any finite $D$, the variational wave function we derive may be always associated with a finite correlation length which scales polynomially in $D$. We note that an interesting critical fPEPS state with finite inner dimension $D = 2$ was proposed in Ref. 18, however, that model is different from our case since the
Dirac cones in that model contain a quadratic dispersion along some directions in the first BZ.

(c) Although the GTPS variational approach can not describe the above system with finite inner dimension $D$, the variational results will still be very useful. From the numerical side, we can apply both finite and infinite size scalings to estimate the physical quantities in the infinite $D$ and infinite size limit. From the analytic side, the finite correlation length corresponds to a finite gap in the system, which is known as Dirac mass term in the effective theory\textsuperscript{36}. In quantum field theory, a controlled calculation (without singularities in calculating correlation functions) can be performed by first taking the Dirac mass term to be finite and then pushing it to the zero limit.

IV. POSSIBLE IMPROVEMENTS OF THE GTERG APPROACH

In this section, we will discuss possible improvements for the TERG algorithm and its Grassmann generalization. Again, let us start from usual TPS case. Its Grassmann generalization would be straightforward by replacing the complex number valued tensors with those Grassmann valued tensors. We notice the simple SVD method used in TERG algorithm actually implies the following cost function:

$$f_{SVD} = ||T - S \cdot S'||,$$

where the rank four double tensor $T$ is defined as $T_A \cdot T_B$ and $\cdot$ means summing over indices for the connected link, as see in Fig.11 (a). (Actually it is the inner product of two vectors if we interpolate $T_{AB}$ as $D^6$ dimensional vectors, where $D$ is the inner dimension of the TPS.) $||\cdots||$ is the usual 2-norm of a vector. (The rank 4 tensor $T$ and rank 3 tensors $S, S'$ can be viewed as $D^6$ and $D^6$ dimensional vectors.) Such a cost function only minimizes the 2-norm of local error $\delta T = T - S \cdot S'$ for a given cut-off dimension $D_{cut}$ (the dimensional of the link shared by $S$ and $S'$) and could not be the optimal one for minimizing global error. To figure out the optimal cost function, let us divide the system into large patches, as seen in Fig.12. If we trace out all the internal indices inside the patch, we can derive a rank $L$ (the number of sites on the boundary of the patch) tensor $T'$ for the patch and the norm of TPS can be represented as the tensor trace of the new double tensors $T'$. When we perform the TERG algorithm and replace $T$ by $S \cdot S'$, we aim at making a small error for the double tensor $T'$.

Now it is clear why the simple SVD method that minimizes local errors could not approximate the patch double tensor $T'$ in an optimal way. Let us rewrite $T'$ as $T' = E \cdot T$. (Notice here we regard the rank $L$ double tensor $T'$ as a $D^{2L}$ dimensional vector, the rank 4 double tensor $T$ as a $D^8$ dimensional vector and the rank $L + 4$ double tensor $E$ as a $D^{2L}$ by $D^8$ matrix.) The double tensor $E$ is called as environment tensor. The cost function which provides the best approximation for $T'$ can be represented as:

$$f = ||E \cdot (T - S \cdot S')||$$

Again, $\cdot$ means the vector inner product and $||\cdots||$ means the usual 2-norm. Comparing with the simple SVD method, the environment tensor gives a complex weight for each component of the local error $\delta T$. Notice the cost function proposed here is very different from the one in Ref.\textsuperscript{32}, which aims at minimizing $\text{Tr} (E \cdot T)$.

Although the environment tensor $E$ is conceptually useful, it is impossible to compute this rank $L + 4$ tensor when the patch size becomes very large. Nevertheless, we
Finally, the weight vector $\Omega^z$ for $x-\text{link}$ can be updated as $\Omega^z = \Omega^\prime$.

In general cases, the assumption Eq.(53) could not be true, however, as long as $\mathbb{E}_{\lambda,pqp'q'}/\sqrt{\Omega_p}\sqrt{\Omega_{q'}}\sqrt{\Omega_{q'}}$ has a much more uniform distribution (up to proper normalization):

$$
\frac{\mathbb{E}_{\lambda,pqp'q'}/\sqrt{\Omega_p}\sqrt{\Omega_{q'}}\sqrt{\Omega_{q'}}}{\sqrt{\Omega_p}\sqrt{\Omega_{q'}}\sqrt{\Omega_{q'}}} \sim 1,
$$

(57)

the above weighted TERG(wTERG) algorithm can still improve the accuracy for fixed $D_{cu}$ with the same cost. This is because the SVD method is the best truncation method if the environment has a random but uniform distribution.

By replacing the complex valued double tensors with Grassmann variable valued double tensors, all the above discussions will be valid for GTPS. However, the definition of the inner product and the corresponding 2-norm $||\cdot||$ should also be generalized into their Grassmann version, which evolves the integration over Grassmann variables for the connected links with respect to the standard Grassam metric. For example, the cost function of the GSVD method discussed in Ref. can be formally written as:

$$
I_{GSVD} = \delta T^f \cdot \delta T^f = ||\delta T^f|| = ||T^f - S^f \cdot S^\dagger f||,
$$

(58)

To explain the meaning of the above expression more explicitly, we consider a simple case that $T^f$ only contains one species of Grassmann variables. We can express $T^f$ as:

$$
T^f_{pqp'q'} = T^f_{pqp'q'} (\theta_\alpha)^N_f (p) (\theta_\gamma)^N_f (q) (\theta_\beta)^N_f (p') (\theta_{\gamma'})^N_f (q'),
$$

(59)

where $T^f_{pqp'q'}$ is the complex coefficient of the Grassmann number valued double tensor $T^f_{pqp'q'}$ and $N_f(p) = p + 1$ is determined by the fermion parity of the inner index $p$. We notice $T^f_{pqp'q'} = \sum_{A:B} T^f_{A:pqp'q'B} = \sum_{A:B} T^f_{A:pqp'q'B}$. If we express the Grassmann number valued double tensors $T^f_{A:B;}_{rqp}$ on sublattice $A(B)$ as:

$$
T^f_{A:B;}_{rqp} = T^f_{A:B;}_{rqp} (\theta_\alpha)^N_f (r) (\theta_\gamma)^N_f (p) (\theta_\gamma)^N_f (q),
$$

(60)

Similarly, we can express $S^f$ and $S^\dagger f$ as:

$$
S^f_{rqp} = S^f_{rqp} (\theta_\alpha)^N_f (r) (\theta_\gamma)^N_f (q) (\theta_\beta)^N_f (p),
$$

$$
S^\dagger f_{r'qp'} = S^\dagger f_{r'qp'} (\theta_\alpha')^N_f (r') (\theta_\gamma')^N_f (q) (\theta_\beta')^N_f (p'),
$$

(61)

Again, $S^f_{rqp}$ and $S^\dagger f_{r'qp'}$ are the complex valued coefficients. Recall the definition of the standard Grassmann metric $g_{rr'}$:

$$
g_{rr'} = \delta_{rr'} \left( \frac{d\theta_\alpha}{N_f(r)} \frac{d\theta_\alpha'}{N_f(r')} \right),
$$

(62)

the inner product $S^f \cdot S^\dagger f$ explicitly means:
\[
\left( \mathbf{S}^f \cdot \mathbf{S}'^f \right)_{pp'q'}^{\mu} = \sum_{r'r'} \mathbf{g}_{rr'} \mathbf{S}_r p q r' q' \left( \theta_{\alpha_r} \right)^{N_f(r)} \left( \theta_{\alpha_r'} \right)^{N_f(r')} \left( \theta_{\beta_r} \right)^{N_f(p)} \left( \theta_{\beta_r'} \right)^{N_f(p')} \left( \theta_{\gamma_r} \right)^{N_f(q)} \left( \theta_{\gamma_r'} \right)^{N_f(q')} \\
= \sum_r \mathbf{S}_r p q r' q' \left( \theta_{\alpha_r} \right)^{N_f(r)} \left( \theta_{\beta_r} \right)^{N_f(p)} \left( \theta_{\gamma_r} \right)^{N_f(q)} \\
\left( \theta_{\beta_r'} \right)^{N_f(p')} \left( \theta_{\gamma_r'} \right)^{N_f(q')} . \tag{63}
\]

Thus, we have:
\[
\delta \mathbf{T}^f_{pp'q'} = \delta \mathbf{T}_{pp'q'} \left( \theta_{\alpha_r} \right)^{N_f(r)} \left( \theta_{\beta_r} \right)^{N_f(p)} \left( \theta_{\gamma_r} \right)^{N_f(q)} \left( \theta_{\beta_r'} \right)^{N_f(p')} \left( \theta_{\gamma_r'} \right)^{N_f(q')} , \tag{64}
\]

with
\[
\delta \mathbf{T}_{pp'q'} = \mathbf{T}_{pp'q'} \left( - \right)^{N_f(p')} - \sum_r \mathbf{S}_r p q r' q' \left( \theta_{\alpha_r} \right)^{N_f(r)} \left( \theta_{\beta_r} \right)^{N_f(p)} \left( \theta_{\gamma_r} \right)^{N_f(q)} \left( \theta_{\beta_r'} \right)^{N_f(p')} \left( \theta_{\gamma_r'} \right)^{N_f(q')} . \tag{65}
\]

Now it is clear that up to a sign twist, the GSVD cost function is equivalent to the cost function of its complex coefficient tensors:
\[
f_{\text{GSVD}} = ||\delta \mathbf{T}^f|| = ||\delta \mathbf{T}|| = ||\mathbf{T}' - \mathbf{S} \cdot \mathbf{S}'|| \tag{66}
\]

Explicitly the same as in the TERG case, the best approximation for a given \(D_{\text{cut}}\) is nothing but the SVD decomposition for the coefficient tensor \(\mathbf{T}'\). (If we view \(\mathbf{T}'_{pp'q'}\) as a matrix \(\mathbf{M}_r q p q' = \mathbf{T}'_{pp'q'} \cong \sum_{r=1}^{D_{\text{cut}}} \mathbf{S}_r q p q'\)) On the other hand, as already having been discussed in Ref.\(^1\), the constraint Eq. (5) of GTPS implies their double tensors containing even number of Grassmann number. As a result, \(\mathbf{M}\) is block diagonalized and the index \(r\) will have a definite parity \(\mathbf{P}^f(r) = \mathbf{P}^f(p) \mathbf{P}^f(q) = \mathbf{P}^f(p') \mathbf{P}^f(q')\). We notice the novel sign factor \((-)^{N_f(p')}\) here arises from the anti-commuting nature of the Grassmann variables and will encode the fermion statistics. The second RG step remains the same as in GTERG and a similar novel sign factor will also emerge there.

All the above discussion will still be correct if the inner index of the double tensor \(\mathbf{T}'^f\) contain multiple species of Grassmann variables. Indeed, starting from the standard GTPS, the double tensor \(\mathbf{T}'^f\) in the first RG step will contain two species of Grassmann variables. This is because \(\mathbf{T}'^f_{A(B)} = \sum_m \tilde{\mathbf{T}}^m_{A(B)} \otimes \tilde{\mathbf{T}}^m_{A(B)}\) and \(\mathbf{T}'^f_{A(B)} = \mathbf{T}'_{A} \cdot \mathbf{T}'_{B}\). In the second and later RG steps, \(\mathbf{T}'^f_{A(B)}\) will only contain one specie of Grassman variables.

The discussion for the environment effect will be in a similar fashion. Especially, if we use some weighting factor to approximate the environment effect, the coefficient tensors \(\mathbf{S}, \mathbf{S}'\) will take the same form as in usual TPS case. However, an important sign factor should be included when we define the matrix \(\mathbf{M}\). Again, the environment weight for the first step is determined by the time evolution algorithm of GTPS. Same as in the bosonic case, the singular value obtained from the GSVD would perform as the environment weight for next RG step.

In Fig. 14, we implement the above algorithm to the free fermion Hamiltonian Eq.(50) at critical point\((\mu = 0)\). We see an important improvement that the ground state energy decreases when increasing \(D_{\text{cut}}\) and is strictly above the exact energy, unlike the simple GTERG approach, which can overestimate the ground state energy for small \(D_{\text{cut}}\). However, for larger enough \(D_{\text{cut}}\), the two approaches converge to the same values, as expected. We further use the new algorithm to study the critical model with larger inner dimension \(D\). Up to \(D = 6\), we find that the ground state energy from the GTPS approach is almost the same as the exact one(relative error \(\sim 0.1\%).

\[\text{FIG. 14: A comparison of the ground state energy as function of } D_{\text{cut}} \text{ at } \mu = 0. \text{ By introducing the environment weight in the GTERG method, an important improvement is that the ground state energy is always above the exact value, which is very important for variational approach.}\]

\[\text{V. SUMMARY}\]

In this paper, we first derive a standard form of GTPS that only contains one specie of Grassmann variable for each inner index and significantly simplifies the representations in our numerical calculations. Based on the fermion coherent state representation, we further general-
ize the imaginary time evolution algorithms into fermion systems. We study a simple free fermion example on honeycomb lattice, including both off-critical and critical cases to test our new algorithms. Finally, we discuss the importance of the environment effect of the TERG/GTERG method and present a simple improvement by introducing proper environment weights.

Although the simple time evolution algorithm discussed here is not generic enough, it has already allowed us to study many interesting and important models, such as Hubbard/t − J model, whose ground state is believed to be a superconductor. The evidence for the existence of superconductivity in these models based on the GTPS algorithm will be discussed and marked with other methods elsewhere\cite{13}. Of course, the generic algorithm is also very important and desired, especially for those systems with topological order. Actually, the general discussion in section II have already made some progress along this direction, but not efficient and stable enough at this stage.

On the other hand, further improving the efficiency of contacting (Grassmann) tensor net is also very important. Although the GTERG/TERG algorithm provides us promising results in many cases, it is still not efficient enough since the algorithm is not easy to be parallelized. Recently, a novel idea of combination the concept of renormalization and Monte Carlo (MC)\cite{17} has made great success for boson/spin systems, it would be very natural to generalize it into fermion/electron systems based on the Grassmann variable representations.

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