Geometric entanglement from matrix product state representations

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Abstract. An efficient scheme for computing the geometric entanglement (GE) per lattice site for quantum many-body systems on a periodic finite-size chain is proposed in the context of a tensor network algorithm based on matrix product state representations. It has been systematically tested for three prototypical critical quantum spin chains, which belong to the same Ising universality class. The simulation results lend strong support to the previous claim (Shi et al 2010 New J. Phys. 12 025008; Stéphan et al 2010 Phys. Rev. B 82 180406R) that the leading finite-size correction to the GE per lattice site is universal, with its remarkable connection to the celebrated Affleck–Ludwig boundary entropy corresponding to a conformally invariant boundary condition.

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1. Introduction

In the last decade, significant progress has been made in the investigation of quantum phase transitions from a novel perspective—quantum entanglement (see [1] and references therein). The main idea is to quantify entanglement present in a ground-state wave function for a quantum many-body lattice system in terms of a variety of bipartite entanglement measures, with some anomaly at a critical point. A remarkable result is achieved for the von Neumann entropy that quantifies the bipartite entanglement when a finite-size spin chain is partitioned into two disjoint parts: it scales logarithmically with the subsystem’s size, with a prefactor proportional to the central charge, a fundamental quantity in conformal field theory, as long as the system is at criticality [2–5].

Contrary to bipartite entanglement measures, no consensus has been achieved on multipartite entanglement measures, although much effort has been devoted to characterizing quantum criticality from some multipartite entanglement measures. One promising candidate among them is geometric entanglement (GE) [6, 7]. As a holistic measure of multipartite entanglement, GE quantifies the multipartite entanglement present in a quantum state wave function. For a quantum many-body lattice system, the GE per lattice site is shown to be an alternative way of detecting critical points [7–11].

In addition, an intriguing connection between the GE per site and the Affleck–Ludwig $g$ factor [12] is established for a finite-size spin chain with the periodic boundary conditions at criticality. More precisely, the GE per site, $\mathcal{E}_N$, scales as

$$\mathcal{E}_N \sim \mathcal{E}_\infty + \frac{b}{N} + O\left(\frac{1}{N^2}\right),$$

with $N$ being the lattice size. It was conjectured that the coefficient $b$ in the subleading term is universal [13]. This was confirmed later in [14] for both the transverse Ising and $XXZ$ chains at criticality by relating the coefficient $b$ to the Affleck–Ludwig boundary entropy $s$:

$$b = -\frac{2}{\ln 2} s.$$  \hspace{1cm} (2)

Here, the boundary entropy $s$ is defined through the Affleck–Ludwig $g$ factor: $s = \ln g$ [2–5]. This result is surprising in that the Affleck–Ludwig boundary entropy $s$ appears in the GE per lattice site for a periodic chain. However, it remains unclear whether or not such a connection between the GE per site and the Affleck–Ludwig $g$ factor is universally valid and whether or not there is any criterion to judge which $g$ factor, corresponding to a conformally invariant boundary condition, is chosen for a specific model. Nevertheless, the establishment of the universality of the coefficient $b$ in the subleading term not only unveils a deep and novel connection between boundary conformal field theory and quantum information science, but also offers a practical way of determining the Affleck–Ludwig $g$ factor by performing a finite-size scaling analysis for the GE per lattice site. Therefore, it is necessary to investigate models belonging to the same universality class to see whether the same $g$ factor appears, in order to gain further insights into the connection between the subleading term coefficient $b$ in the GE per lattice site and the Affleck–Ludwig $g$ factor.

One of the main obstacles to addressing these issues is the fact that the computation of the GE per lattice site is a formidable task for a quantum many-body lattice system because it involves optimization over all possible separable states, with some constraints arising possibly from the translational invariance. However, recent progress in the context of the
tensor network algorithms for quantum many-body lattice systems with the periodic boundary conditions [15–19] offers us an efficient method to systematically evaluate the GE per lattice site for quantum many-body lattice systems. In this paper, we first describe how to evaluate the GE per lattice site for a finite-size quantum spin chain from a tensor network algorithm based on the matrix product state representations. Then we present our simulation results for three prototypical spin chains belonging to the Ising universality class.

2. The geometric entanglement (GE) per lattice site

We first introduce the maximum fidelity \( \Lambda_{\text{max}} \) between a quantum pure state \(|\psi\rangle\) and all the possible separable and normalized states \(|\phi\rangle\) of the \( N \) parties:

\[
\Lambda_{\text{max}} = \max_{|\phi\rangle} |\langle \phi | \psi \rangle|.
\]  

(3)

The larger the \( \Lambda_{\text{max}} \), the closer a quantum state wave function is to a separable state. Therefore, a holistic measure of the multipartite entanglement present in a quantum state wave function \(|\psi\rangle\) is defined as

\[
E(|\psi\rangle) = -\log_2 \Lambda_{\text{max}}^2.
\]

(4)

Since the contribution to \( E(\psi) \) from each party is additive, \( E(\psi) \) scales linearly with \( N \) for a multipartite system consisting of \( N \) parties. Therefore, it is convenient to define the GE per party as

\[
E_N(|\psi\rangle) = \frac{1}{N - 1} E(|\psi\rangle).
\]

(5)

For a quantum many-body lattice spin system, each lattice site constitutes a party. Thus, \( E_N \) is the GE per lattice site. Note that it is well defined even in the thermodynamic limit.

3. A matrix product state algorithm

Let us recall the key steps to produce a ground-state wave function from an efficient variational algorithm [17] for a translational-invariant finite-size periodic lattice system. Firstly, choose a random state as an initial state \(|\psi_0\rangle\). Secondly, perform the imaginary time evolution for \(|\psi_0\rangle\). Thus, we get the evolved state \(|\psi_\tau\rangle\) at imaginary time \( \tau \),

\[
|\psi_\tau\rangle = \frac{\exp(-H\tau)|\psi_0\rangle}{\| \exp(-H\tau)|\psi_0\rangle \|}.
\]

(6)

If \( \tau \to \infty \), the ground-state wave function is projected out, as long as the initial state is not orthogonal to the real ground state. Thirdly, exploit the Trotter–Suzuki decomposition and turn the imaginary time evolution operator into a series of two-site gates over a time slice \( \delta \tau \), with \( \tau = M \delta \tau \). Therefore, the problem becomes how to absorb a two-site gate acted on a matrix product state. For a periodic spin chain with \( N \) sites, we assume that the matrix product state representation is translation-invariant under two-site shifts. Thus we only need two three-index tensors, \( A_o \) and \( A_e \) (cf figure 1(i)), to represent a tensor network for the ground-state wave function and two one-index tensors, \( B_o \) and \( B_e \) (cf figure 1(ii)), to represent a separable state, as shown in figures 1(ii) and (iii), respectively. Here, the subscripts o and e represent odd and even sites, respectively. In this setting, a two-site gate is absorbed by performing a singular value decomposition for a matrix contracted from a few tensors involving the two-site gate.
A peculiar feature of the algorithm for a finite-size periodic system is to take into account the \( p \) largest eigenvalues and the corresponding eigenvectors of the transfer matrix \( E_{\langle \phi|\psi \rangle} \) when one evaluates the ground-state energy per site. That is, \( E_{\langle \phi|\psi \rangle}^m = \sum_{i=1}^{D^2} u_i s_i^m v_i \approx \sum_{i=1}^p u_i s_i^m v_i, \) where \( s_i \) is the \( i \)th largest eigenvalue, \( u_i \) and \( v_i \) indicate the left and right eigenvectors, respectively, with \( D \) denoting the bond dimension. When the energy per site converges, the ground-state wave function is generated. Note that the computational cost of the algorithm is \( pD^3 \).

4. The GE per lattice site from matrix product state representations

Now we are ready to compute the GE per lattice site. The crucial step is how to maximize the fidelity \( |\langle \phi|\psi \rangle| \) over all possible separable states \( |\phi \rangle \). In figure 1(iv), we introduce the transfer matrix \( E_{\langle \phi|\psi \rangle} \) to represent the fidelity between \(|\psi \rangle\) and \(|\phi \rangle\), with \( E_{\langle \phi|\psi \rangle} \) constructed from two three-index tensors, \( A_o \) and \( A_e \), and two one-index tensors, \( B_o^* \) and \( B_e^* \). Mathematically, the fidelity between a ground-state wave function \(|\psi \rangle\) and a separable state \(|\phi \rangle\) is expressed as

\[
f = \frac{|\langle \phi|\psi \rangle|}{\sqrt{\langle \psi|\psi \rangle \langle \phi|\phi \rangle}}.
\]

For our purpose, we consider \( F = f^2 \) instead of \( f \) itself. To maximize \( F \), we compute its logarithmic gradient with respect to a one-index tensor \( B^* \),

\[
\frac{\partial \ln F}{\partial B^*} = \frac{1}{\langle \phi|\psi \rangle} \frac{\partial \langle \phi|\psi \rangle}{\partial B^*} - \frac{1}{\langle \phi|\phi \rangle} \frac{\partial \langle \phi|\phi \rangle}{\partial B^*}.
\]

Here, \( B^* \) is either \( B_o^* \) or \( B_e^* \). We take \( B_o^* \) as an example to explain the updating procedure. The pictorial representation for the derivative of \( \ln F \) with respect to \( B_o^* \) is shown in figure 2.

In figure 2(i), \( E_{\langle \phi|\psi \rangle} \) is approximated by the first \( p \) largest eigenvalues and the corresponding
The transfer matrix $E_{\langle \phi | \psi \rangle}$ may be approximated by the $p$ largest eigenvalues $\Lambda$ and the corresponding left and right eigenvectors, $U$ and $V$, of the transfer matrix $E_{\langle \phi | \psi \rangle}$. (ii) Pictorial representation of the derivative of $\langle \phi | \psi \rangle$ with respect to $B^*_o$. (iii) Pictorial representation of the derivative of $\langle \phi | \phi \rangle$ with respect to $B^*_o$.

eigenvectors of $E_{\langle \phi | \psi \rangle}$. That implies that $E^m_{\langle \phi | \psi \rangle} \simeq \sum_{k=1}^p U_k \Lambda^m_{k,k} V_k$, with $p$ specifically depending on $m$: the larger the $m$, the lower the $p$. In figure 2(ii), the derivative of $\langle \phi | \psi \rangle$ with respect to $B^*_o$ is shown. In figure 2(iii), we represent the derivative of $\langle \phi | \phi \rangle$ with respect to $B^*_o$. Once the fidelity gradient is determined, the real and imaginary parts of $B^*_o$ may be updated as follows:

$$\Re B^*_o = \Re B^*_o + \delta \Re \left( \frac{\partial F}{\partial B^*_o} \right)$$  (9a)

and

$$\Im B^*_o = \Im B^*_o + \delta \Im \left( \frac{\partial F}{\partial B^*_o} \right),$$  (9b)

where $\delta$ is the step size in the parameter space, which is tuned to be decreasing during the updating procedure. Here, we have normalized the tensors $B^*_o$, $\Re(\partial F/\partial B^*_o)$ and $\Im(\partial F/\partial B^*_o)$ by setting their respective largest entries to be unity. In exactly the same way, we may update the other tensor $B^*_e$. Repeating the procedure until the fidelity per lattice site converges, we achieve the closest separable state $|\phi\rangle$ that ensures its maximum fidelity with the ground-state wave function $|\psi\rangle$. Thus, the GE per lattice site follows, as desired.

5. The models

We test our scheme by considering three prototypical critical quantum spin chains with the periodic boundary conditions. Note that the models belong to the same Ising universality class. The first model is the quantum Ising model in a transverse magnetic field on a finite-size ring. The Hamiltonian takes the form

$$H = - \sum_{i=1}^{N} \left( \sigma^{[i]}_x \sigma^{[i+1]}_x + \lambda \sigma^{[i]}_z \right),$$  (10)

where $\sigma^{[i]}_\alpha (\alpha = x, z)$ are the Pauli spin operators at site $i$ and $\lambda$ is a transverse magnetic field. The model is critical at $\lambda_c = 1$. 

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The second model is a spin-1/2 Ising chain with antisymmetric anisotropic and alternative bond interactions. It is described by the Hamiltonian

$$H = \sum_{i=1}^{N} ((1 - (-1)^{r})\sigma_{\alpha}^{(i)}\sigma_{\alpha}^{(i+1)} + D_{\alpha} (\sigma_{\alpha}^{(i)}\sigma_{\alpha}^{(i+1)} - \sigma_{\alpha}^{(i)}\sigma_{\alpha}^{(i+1)})�, \tag{11}$$

where $\sigma_{\alpha}^{(i)} (\alpha = x, y, z)$ are the Pauli spin-1/2 operators at site $i$. The alternative bond interaction is characterized by the relative strength $r$ of the exchange coupling, and $D_{\alpha}$ is the $z$-direction component of the Dzyaloshinskii–Moriya interaction arising from the spin–orbit interaction. The model is critical at $D_{\alpha} \sim 0.263$ if $r$ is chosen to be 0.5 [20].

The third model is the quantum the $XYX$ model in an external magnetic field described by the Hamiltonian

$$H = \sum_{i=1}^{N} (\sigma_{x}^{(i)}\sigma_{x}^{(i+1)} + \Delta_{y}\sigma_{y}^{(i)}\sigma_{y}^{(i+1)} + \sigma_{z}^{(i)}\sigma_{z}^{(i+1)} + h\sigma_{z}^{(i)})�, \tag{12}$$

where $\sigma_{\alpha}^{(i)} (\alpha = x, y, z)$ are the Pauli operators at site $i$, $\Delta_{y}$ is a parameter describing the rotational anisotropy and $h$ is an external magnetic field. For $\Delta_{y} = 0.25$, the critical magnetic field is $h_{c} = 3.206$ [21–23].

6. Simulation results

For the transverse Ising model, we have evaluated the GE per lattice site, as shown in figure 3(a), with $b = 1.016076$, consistent with our previous result in [13]. This yields the Affleck–Ludwig $g$ factor $g = 0.7032$. Compared to the exact value $g_{\text{fixed}} = 1/\sqrt{2}$ [12], the relative error is $|(g - g_{\text{fixed}})|/g_{\text{fixed}} = 1.3 \times 10^{-4}$. We emphasize that, for this model, we have chosen the separable states to be translation-invariant under one-site shifts, although there is no a priori reason to argue that the GE per lattice site does not depend on the unit cell of the separable states under translational shifts. However, the same $g$ factor is yielded even if the separable states are translation-invariant under two-site shifts. In fact, we have evaluated the GE per site without any translation-invariant assumption and the same $g$ factor was achieved. Thus, we conclude that only the smaller $g$ factor, corresponding to the stable conformally invariant boundary condition [24], i.e. the fixed boundary condition, is involved.

In figure 3(b), we plot the GE per lattice site, $E_{N}$, as a function of the number of lattice sites, $N$, for the spin-1/2 Ising chain with the coupling parameters $r = 0.5$ and $D_{z} = 0.263$. The finite-size scaling for the GE per lattice site follows $E_{N} = a + b/N + f/N²$, where the coefficients are $a = 0.083320$, $b = 0.966353$ and $f = -1.398155$. It yields the Affleck–Ludwig $g$ factor $g = 0.715330$. Compared with the exact value $g_{\text{fixed}} = 1/\sqrt{2}$ [12] for the conformally invariant fixed boundary condition, the relative fitting error is $|(g - g_{\text{fixed}})|/g_{\text{fixed}} = 1.1 \times 10^{-2}$. For this model, we have chosen the separable states to be translation-invariant under two-site shifts, given the alternative bond interaction. However, we have evaluated the GE per site without any translation-invariant assumption and the same $g$ factor was achieved. Thus, we conclude that only the smaller $g$ factor, corresponding to the stable conformally invariant boundary condition [24], i.e. the fixed boundary condition, is involved.

In figure 3(c), we plot the GE per lattice site, $E_{N}$, as a function of the number of lattice sites, $N$, for the quantum $XYX$ model in an external field, with $\Delta_{y} = 0.25$, where the size $N$ is chosen...
Figure 3. The scaling relation between the GE per lattice site $\mathcal{E}_N$ and the chain size $N$, for the quantum Ising model (a), with size $N$ ranging from 8 to 120, for the quantum Ising model with antisymmetric anisotropic and alternative bond interactions (b), with size $N$ ranging from 8 to 150, and for the quantum the $XYX$ model (c), with size $N$ ranging from 10 to 100. The data are fitted to $\mathcal{E}_N = a + b/N + f/N^2$, with $a = 0.030960$, $b = 1.016076$ and $f = -1.712521$ in (a) and $a = 0.083320$, $b = 0.966353$ and $f = -1.398155$ in (b). In (c), we have $a = 0.056892$, $b = 0.001581$ and $f = -0.879631$, and $a = 0.010193$, $b = 1.009600$ and $f = -5.005750$, for the upper and lower branches, respectively. Here, the upper (lower) branch is for the separable states that are translation-invariant under one-site (two-site) shifts if the chain size is larger than a threshold. Indeed, the GE per site is the same for two cases, if the chain size is less than the threshold. In addition, the exact diagonalization results for the GE per lattice site are displayed as five-pointed stars, up to chain size 24. The data match very well. Inset: the relative fitting error $\varepsilon_{\text{err}} = (\mathcal{E}^\text{data}_N - \mathcal{E}^\text{fit}_N)/\mathcal{E}^\text{fit}_N$ is less than $2.1 \times 10^{-3}$ in (a), less than $1.8 \times 10^{-2}$ in (b) is less than $1.5 \times 10^{-3}$ in (c), where $\mathcal{E}^\text{fit}_N$ is the value extracted from the fit and $\mathcal{E}^\text{data}_N$ is our simulation value for each $N$. 

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from 10 to 100. Remarkably, it splits into two branches for a large enough chain size: one is for the separable states that are translation-invariant under one-site shifts and the other is for the separable states that are translation-invariant under two-site shifts. The exact diagonalization for small-size chains up to 24 is also performed to evaluate the GE per site without any translation-invariant assumption. However, it only reproduces the second branch, as seen in figure 3(c). A proper explanation of this unexpected result is that, for this model, the translational invariance under one-site shifts constitutes a true constraint to separable states. That is, the closest separable state with the one-site unit cell is different from the closest separable state with the two-site unit cell. Thus the maximum fidelity $\Lambda_{\text{max}}$ is larger for the latter, implying that the GE per lattice site is smaller, as long as the chain size is large enough. This explains the presence of a threshold in the chain size: the GE per site is the same for both the one-site and two-site unit cells if the size is less than the threshold. Two sets of the data are separately fitted into the scaling function $E_N = a + b/N + f/N^2$, with the coefficients $a = 0.056892$, $b = 0.001581$ and $f = -0.879631$, and $a = 0.010193$, $b = 1.009600$ and $f = -5.005750$ yielding $g_{\text{XYX}} = 0.9994$ and $g_{\text{XYX}} = 0.7048$, respectively. They are consistent with the exact values $g_{\text{free}} = 1$ and $g_{\text{fixed}} = 1/\sqrt{2}$ [12] for conformally invariant free and fixed boundary conditions in the Ising universality class.

7. Summary

In this paper, we have developed a scheme for efficiently computing the GE per lattice site for quantum many-body spin systems on a periodic finite-size chain in the context of a tensor network algorithm based on matrix product state representations. The computational cost does not depend on the chain size. A systematic test is performed for three prototypical critical quantum spin chains belonging to the same Ising universality class. The simulation results lend strong support to the previous claim that the leading finite-size correction to the GE per lattice site is universal [13], with its remarkable connection to the celebrated Affleck–Ludwig boundary entropy corresponding to a conformally invariant boundary condition [14]. For all the models tested, the simulated $g$ is compared to the exact $g$ factor from conformal field theory, with relative error less than $1.1 \times 10^{-2}$. It appears that the boundary entropy corresponding to the smallest $g$ factor is always involved. This is somewhat as expected, since this $g$ factor characterizes a stable fixed point along a boundary renormalization group flow, according to the Affleck–Ludwig $g$ theorem [12]. Remarkably, for the quantum XYX model in an external field, either the conformally invariant free or fixed boundary condition appears, depending on the one- or two-site unit cell of the translation-invariant separable states. The fact that only two different values of the Affleck–Ludwig $g$ factor appear in three models belonging to the same Ising universality class is as anticipated given the universality of the subleading term coefficient $b$, with its connection to the $g$ factor. This follows from the well-known result that, for the Ising universality class, there are two and only two conformally invariant boundary conditions [12].

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