Finite-size geometric entanglement from tensor network algorithms

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New Journal of Physics 12 (2010) 025008 (10pp)
Received 20 April 2009
Published 26 February 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/2/025008

Abstract. The global geometric entanglement (GE) is studied in the context of newly developed tensor network algorithms for finite systems. For one-dimensional quantum spin systems it is found that, at criticality, the leading finite-size correction to the global GE per site behaves as \( b/n \), where \( n \) is the size of the system and \( b \) a given coefficient. Our conclusion is based on the computation of the GE per spin for the quantum Ising model in a transverse magnetic field and for the spin-1/2 XXZ model. We also discuss the possibility of coefficient \( b \) being universal.

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1. Introduction

At zero temperature, quantum many-body systems exhibit important collective phenomena. The complex structure of these systems has attracted great attention in recent years. In particular, the role played by quantum correlations (or entanglement) in quantum phase transitions has been the subject of numerous studies (see e.g. [1]). Several results for the ground states of quantum many-body systems in one spatial dimension (one-dimensional (1D)) show that a number of entanglement measures obey universal scaling laws close to or at quantum critical points [2]–[6]. These results are, in part, due to the unique properties of the reduced density matrices of the ground states [6]. Complementarily, the so-called fidelity approach to quantum phase transitions [7]–[10] has proven specially fruitful in determining the existence and nature of possible critical points in quantum many-body systems.

There has also been a growing interest in investigating the distance between the ground state of a quantum many-body system and the closest separable state in the Hilbert space. This idea has been quantified in terms of the so-called geometric entanglement (GE) [11, 12], which is a measure of the global quantum correlations of a quantum many-body system. Remarkably, the study of the GE in 1D many-body systems has proven fruitful because of its connections to both the renormalization group and conformal field Theory [5]. Moreover, the study of the GE allows us to identify separable ground states of quantum many-body systems [13]. As emphasized in [13, 14], the occurrence of such factorized ground states is a typical signature of quantum phases of matter with symmetry-breaking order, as opposed to phases with topological order where the ground state is globally entangled. While these properties show the conceptual significance of the GE, the GE has unfortunately also proven to be very hard to compute both analytically and numerically. In the case of 1D systems, many previous studies of the GE have focused on its properties for infinite size systems, where translational invariance together with the infinite-size limit can be fully exploited to simplify the calculations. Its behavior for finite size 1D systems has only been analyzed in a few special cases [12].

In this paper, we show that the GE can be easily extracted for finite systems with the aid of newly developed tensor network (TN) algorithms to simulate strongly correlated systems. This connection allows us to further extend the study of the GE by obtaining the finite-size corrections to the GE for two important 1D models at criticality: the quantum Ising and XXZ spin-1/2 chains. The calculations consist of two steps: firstly, we compute a matrix product state (MPS) representation of the ground state using TN algorithms. Secondly, we determine the GE from the MPS representations thus obtained. Our numerical observations can be summarized as follows: for a 1D system at criticality, the finite-size corrections to the GE per site \( E_n \) for a system of size \( n \) obey

\[
E_n \sim E_\infty + \frac{b}{n} + O \left( \frac{1}{n^2} \right), \quad n \gg 1,
\]

(1)

with \( b \) a given coefficient. As we shall see, \( E_n \) can also be interpreted as twice the free energy per site of a classical 1D vertex model. The possibility of coefficient \( b \) being universal is also briefly discussed.

2. Global GE per party

Let us now introduce the measure of entanglement that we shall use in this paper. Consider a pure quantum state of \( n \) parties \( |\psi\rangle \in \mathcal{H} = \bigotimes_{i=1}^{n} \mathcal{H}^{[i]} \), where \( \mathcal{H}^{[i]} \) is the local Hilbert space...
of party $i$. The global multipartite entanglement of $|\psi\rangle$ can be quantified by considering the maximum fidelity $\Lambda_{max}$ between the quantum state $|\psi\rangle$ and all the possible separable and normalized states $|\phi\rangle$ of the $n$ parties

$$\Lambda_{max} = \max_{|\phi\rangle} |\langle \psi | \phi \rangle|.$$

(2)

A well-defined global measure of entanglement is obtained by taking the base-2 logarithm of $\Lambda_{max}^2$,

$$E(\psi) = -\log_2 \Lambda_{max}^2.$$

(3)

Here, we will be interested in the above quantity per party, which is given by

$$E_n = n^{-1} E(\psi).$$

(4)

The above quantity constitutes what we call the global GE per party, and has been investigated in different contexts [5, 11, 12, 16]. Here, we study the finite-size properties of $E_n$ as the size $n$ of the system changes. Finally, we choose each party to be a single spin, and therefore $E_n$ corresponds to the GE per spin.

3. GE from TN algorithms for 1D systems

For 1D quantum many-body systems, several methods have been developed to compute their ground state properties based on MPS representations of their wavefunctions. Here, we use two of these algorithms to compute ground states of 1D quantum many-body systems under periodic boundary conditions (PBCs). These algorithms are based on the variational optimization of the expectation value of the energy using (i) a direct variational method [17] and (ii) a variational Monte Carlo method [18]. We also show how to numerically extract the GE once the MPS representation of the ground state wavefunction has been obtained. In all our derivations, we assume that the Hamiltonian for $n$ sites is made of nearest-neighbor interactions, $H = \sum_{i=1}^{n} h_{[i,i+1]}$, with $n + 1 \equiv 1$ under PBCs and $h_{[i,i+1]}$ a nearest-neighbor two-body Hamiltonian.

Let us first recall some of the key ingredients of the direct variational algorithm from [17] to find ground states of 1D many-body systems with PBCs. We start from an initial guess state $|\psi_0\rangle$, expressed in terms of an MPS as

$$|\psi_0\rangle = \sum_{s_1,\ldots,s_n} \text{Tr} \left[ A^{[1]}(s_1) A^{[2]}(s_2), \ldots, A^{[n]}(s_n) \right] |s_1,\ldots,s_n\rangle,$$

(5)

where $s_i = 1, \ldots, d$ for $i = 1, \ldots, n$, and $A^{[i]}(s_i)$ are $D \times D$ matrices, with $d$ denoting the dimension of the Hilbert space at every site $i$ and $D$ denoting the so-called bond dimension. The variational optimization algorithm finds an MPS approximation of the ground state wavefunction using (i) a direct variational method [17] and (ii) a variational Monte Carlo method [18]. We also show how to numerically extract the GE once the MPS representation of the ground state wavefunction has been obtained. In all our derivations, we assume that the Hamiltonian for $n$ sites is made of nearest-neighbor interactions, $H = \sum_{i=1}^{n} h_{[i,i+1]}$, with $n + 1 \equiv 1$ under PBCs and $h_{[i,i+1]}$ a nearest-neighbor two-body Hamiltonian.

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for \( i \neq m \). The update of the \( d \) matrices \( A^{[m]}(s_m) \) at site \( m \) follows from minimizing equation (6) with respect to \( A^{[m]} \). This amounts to solving the generalized eigenvalue problem

\[
H^m_{\text{eff}} A^{[m]} = v N^m_{\text{eff}} A^{[m]},
\]

with \( v \) the expectation value of the energy. By updating the MPS matrices site by site, the approximate ground state is obtained as the energy \( E \) monotonically decreases.

Next, we review the basics of the variational quantum Monte Carlo optimization algorithm (VQMC) from [18]. This algorithm takes advantage of translational invariance as well as of other symmetries in the system to accelerate convergence. More specifically, for a translationally invariant (TI) system, the MPS of its ground state is described by just a single site-independent set of \( d \) matrices, that is, \( A^{[i]}(s_i) \equiv A(s) \forall i \). Furthermore, for systems invariant under reflection symmetry, the condition \( A^T \equiv A \) is imposed. The algorithm starts by giving random values to the components of matrices \( A(s) \). Then, these components are changed in order to minimize the ground state energy. The changes in the components \( A(s)_{\alpha\beta} \) at step \( k \) in the algorithm follow the rule: \( A(s)_{\alpha\beta} \rightarrow A(s)_{\alpha\beta} - \delta(k) r(s)_{\alpha\beta} \text{sign}(\partial E/\partial A(s)_{\alpha\beta}) \), where \( r(s)_{\alpha\beta} \) is some random number between 0 and 1, and \( \delta(k) \) is the maximum allowed variation at step \( k \) (which is set to monotonically decrease with \( k \)). Thus, each component \( A(s)_{\alpha\beta} \) is modified independently by a random and well-bounded variation, and the acceptance or rejection of this variation follows a usual Monte Carlo rule. Also, as the expectation value of the energy decreases and converges, more sampling is required to avoid undesirable noise effects. If the different parameters of the algorithm are chosen properly, then the expectation value of the energy decreases stably during the updating process. Note that the particular value of the parameters used in the procedure also affect the speed and precision of the convergence. Let us also mention that the VQMC algorithm has a more favorable scaling with the MPS parameters than the direct variational algorithm.

Once the MPS for the ground state is obtained using any of the above two methods, the GE can be computed according to its definition. For a system of \( n \) spins 1/2, we maximize equation (2) with respect to the separable states \( |\phi\rangle \) of \( n \) spins, \( |\phi\rangle = \bigotimes_{i=1}^n (\cos(\xi_i)|0\rangle + \sin(\xi_i)|1\rangle) \), where \( |0\rangle \) and \( |1\rangle \) are the eigenstates of the \( S_z \) spin operator with eigenvalue \( \pm 1/2 \), respectively. For the TI Hamiltonians that we consider in this work, we assume that the maximization of equation (2) can be done with respect to the set of separable states that are also TI, that is, we assume that \( \xi_i \equiv \xi \forall i \). Let us further justify this assumption: the Hamiltonians that we consider in this paper favor a ferromagnetic alignment of the spins in the quantum system, that is, spins tend to be parallel to each other. This simplifies the calculation of the GE in that it is possible to optimize over the family of TI product states with a period of one site. Note that if the Hamiltonians were such that the spins would tend to align antiferromagnetically, then the GE should be obtained by optimizing over a broader family of states (most probably over those product states that are TI with a period of two sites). As we shall see, this is not the case in our work. In fact, for systems of small size, and for the Hamiltonians that we will consider here, we have numerically checked that the GE obtained by optimizing over the family of TI product states with period of one site is equal to that obtained by optimizing over the family of TI product states with period of two sites (see the appendix), which corroborates the validity of our assumption.

One may argue that there should be two parameters in the TI factorized states instead of one parameter \( \xi \), with an extra parameter as a relative phase between \( |0\rangle \) and \( |1\rangle \). However, such an ansatz yields the same conclusion.
As such, the fidelity $\Lambda(\xi)$ between the separable state $|\phi\rangle$ and the MPS approximation to the ground state $|\psi_g\rangle$ takes the form

$$\Lambda(\xi) = \left| \langle \psi_g | \phi \rangle = \left| \text{Tr} \left( T^{[1]} T^{[2]} \ldots T^{[n]} \right) \right|, \tag{8}$$

where $T^{[i]} = \sum_{s_i} A^{[i]}(s_i) \otimes B(s_i)$ are zero-dimensional transfer matrices $\forall i$ of some 1D classical vertex model, with $B(0) = \cos(\xi)$, $B(1) = \sin(\xi)$, and $A^{[i]}(s_i)$ the matrices at site $i$ in the MPS representation of the ground state wavefunction $|\psi_g\rangle$. Equation (8) can be further simplified if the matrices $A^{[i]}(s_i)$ are site-independent. In this case, we have that $T^{[i]} = T \forall i$ and therefore the fidelity can be expressed as $\Lambda(\xi) = |\text{Tr}(T^n)| = |\sum_{\lambda} (\lambda^n)|$, where $\lambda$ are the eigenvalues of transfer matrix $T$. Finally, the maximization of the fidelity $\Lambda(\xi)$ with respect to the angle $\xi$ can be achieved by means of standard numerical optimization algorithms, and from here the GE per spin $\mathcal{E}_n$ readily follows from equations (3) and (4). Importantly, $\mathcal{E}_n$ can be understood as twice the free energy per site of the 1D classical vertex model with partition function $\Lambda(\xi_{\text{max}})$, where $\xi_{\text{max}}$ is the maximizing angle.

4. Models

We focus on the quantum Ising spin chain with transverse magnetic field, and on the XXZ quantum spin chain. The Hamiltonian that accommodates both models as two limiting cases takes the form

$$H = -\sum_i^n \left( \frac{1 + \gamma}{2} S^{\alpha}_i S^{\alpha}_{i+1} + \frac{1 - \gamma}{2} S^y_i S^y_{i+1} + \frac{\Delta}{2} S^z_i S^z_{i+1} + \lambda S^z_i \right), \tag{9}$$

where $S^{\alpha}_i$ ($\alpha = x, y, z$) are the spin operators of the $i$th spin-1/2, and parameters $\Delta$, $\gamma$ and $\lambda$ characterize different aspects of the model (anisotropies and magnetic field). The Hamiltonian from equation (9) exhibits very rich physics. Here, we consider the following two cases:

1. For $\gamma = 1$ and $\Delta = 0$, the model corresponds to the 1D quantum Ising model in a transverse magnetic field, with a critical point at $\lambda = \pm 1$ in the universality class of a free Majorana fermionic field theory. Without loss of generality, here we consider the case $\lambda = 1$.
2. For $\gamma = 0$, $\lambda = 0$ and $\Delta$ generic, the model is the anisotropic XXZ model, which is critical for $\Delta \in [-1, 1]$ and in the universality class of a free compactified bosonic field theory. The system exhibits ferromagnetic and antiferromagnetic orders, respectively, for $\Delta > 1$ and $\Delta < -1$. In this work we focus on the critical regime $\Delta \in [-1, 1]$.

5. Simulation results

As a first test, we have compared results for the GE obtained using both the direct variational algorithm and the VQMC algorithm. In practice, we observe that the direct variational algorithm seems more stable but breaks translational invariance, while the VQMC algorithm imposes translational invariance from the beginning but needs more effort to become stabilized. In order to check both methods quantitatively, we have computed the GE for the periodic quantum Ising

Note that the presence of a minus sign in front of the Hamiltonian (9) makes our notation different from the conventional one. As a result, the antiferromagnetic XXZ model corresponds to $\Delta = -1$. 

New Journal of Physics 12 (2010) 025008 (http://www.njp.org/)
Table 1. The GE per spin $\mathcal{E}_n$ is calculated by means of both the direct optimization and the VQMC algorithms for the quantum Ising chain in a transverse magnetic field, at critical magnetic field $\lambda = 1$ and system sizes $n$ from 20 to 28. Fixing the precision of the ground state energy at $10^{-6}$, the results obtained from both algorithms for $\mathcal{E}_n$ are comparable, with relative differences smaller than $2 \times 10^{-5}$.

| Size $n$ | 20      | 22      | 24      | 26      | 28      |
|----------|---------|---------|---------|---------|---------|
| Direct $\mathcal{E}_n \times 10^2$ | 7.7469  | 7.3564  | 7.0259  | 6.7441  | 6.4878  |
| VQMC $\mathcal{E}_n \times 10^2$ | 7.7464  | 7.3563  | 7.0263  | 6.7436  | 6.4884  |

Figure 1. Main: relation between the GE per spin $\mathcal{E}_n$ and the chain size $n$ for the 1D quantum transverse Ising model with PBCs. For sizes $n$ from 8 to 120, the data are fitted to $\mathcal{E}_n = a + b/n + f/n^2$. Inset: the relative fitting errors $|\mathcal{E}_n^{\text{fit}} - \mathcal{E}_n^{\text{MPS}}|/\mathcal{E}_n^{\text{MPS}}$ are always smaller than $2.5 \times 10^{-3}$, where $\mathcal{E}_n^{\text{fit}}$ is the value extracted from the fit and $\mathcal{E}_n^{\text{MPS}}$ is the value extracted from the MPS algorithm for each $n$.

As a check, we have also derived the thermodynamic limit of $\mathcal{E}_n$ from the exact solution of the transverse Ising model in 1D\(^5\), and obtained that at the critical point $\lambda = 1$ it takes the value $\mathcal{E}_\infty = -\frac{2}{\pi^2} \max_{\mu} \int_0^{1/2} d\mu \ln[\cos \theta(\mu) \cos^2 \frac{\xi}{2} + \sin \theta(\mu) \sin^2 (\xi/2) \cot \pi \mu], \quad \text{where} \quad \tan 2\theta(\mu) = \sin 2\mu/(1 - \cos 2\pi \mu)$.

However, the results for finite size systems turn out to be different, since the Jordan–Wigner transformation is used to solve the model. This transformation changes the boundary conditions, therefore affecting the GE per spin for finite size systems, but not in the thermodynamic limit.

\(^5\) Using the results in [12], the thermodynamic limit of the GE per spin is $\mathcal{E}_\infty = -\frac{2}{\pi^2} \max_{\mu} \int_0^{1/2} d\mu \ln[\cos \theta(\mu) \cos^2 \frac{\xi}{2} + \sin \theta(\mu) \sin^2 (\xi/2) \cot \pi \mu], \quad \text{where} \quad \tan 2\theta(\mu) = \sin 2\mu/(1 - \cos 2\pi \mu)$.

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\[ E_n = a + \frac{b}{n} + \frac{f}{n^2} \]

This is comparable with the value obtained from the extrapolation \( n \to \infty \) of our fit for \( E_n \), which is \( a = 0.03096 \). Notably, the relative error between the exact value \( E_\infty \) and our fitted value \( a \) is of the order of \( 10^{-3} \).

A remark is now in order regarding potential sources of error in our fits. Firstly, as \( n \) becomes larger, it is clear that the fits should be better, therefore large system sizes are required in order to get accurate results. Secondly, the effects of our numerical approximation to the ground state based on MPSs are also important. Namely, at criticality (as is the case) the introduction of a finite bond dimension in the MPS introduces an artificial correlation length for large system sizes (see the analysis in [19]). This, in turn, moves the ground state of the system slightly away from the true critical ground state, which implies that our results about critical properties of 1D systems can only be approximate even if we were able to get the thermodynamic limit. The fact that critical systems can only be approximately reproduced is a well-known property of all numerical algorithms based on MPSs. Our calculations use a bond dimension of the MPS which is sufficiently large to assure the correctness of the GE.

We have also computed \( E_n \) for the XXZ model with PBCs. In the critical regime \( \Delta \in [-1, 1] \), we choose nine different values \( \geq 0 \) of the anisotropy \( \Delta \) to investigate the finite size behavior of the GE per spin. For sizes \( n \) ranging from 10 to 94 spins, \( E_n \) is again well fitted numerically by \( E_n = a + \frac{b}{n} + \frac{f}{n^2} \) as seen in figure 2. In this case, we obtain different fitting coefficients as a function of \( \Delta \), and the relative fitting errors are always smaller than \( 10^{-3} \). The specific fitting coefficients for each \( \Delta \) are given in table 2.

An interesting issue raised by the above results is the possible universality of coefficient \( b \) in equation (1). For the quantum Ising model, a comparison of our results with those that can be extracted from [12] indicates that, indeed, \( b \) may actually be equal to 1 for this system. For the XXZ model, the fact that different values of \( \Delta \) correspond to different fitting coefficients could be an indication that the finite size corrections to the GE per site at criticality depend only on the Luttinger liquid parameter \( K \) of the corresponding effective field theory at low energies,
Table 2. Fitting coefficients of the GE per spin, $E_n$, for nine different values of the anisotropy $\Delta \geq 0$ in the XXZ model.

| $\Delta$ | $a$   | $b$   | $f$   |
|---------|-------|-------|-------|
| 0.0     | 0.15930 | 0.9806 | -0.61511 |
| 0.1     | 0.14922 | 1.0308 | -0.68507 |
| 0.2     | 0.13902 | 1.0842 | -0.78287 |
| 0.3     | 0.12858 | 1.1397 | -0.86608 |
| 0.4     | 0.11763 | 1.2061 | -0.9994 |
| 0.5     | 0.10612 | 1.2821 | -1.1607 |
| 0.6     | 0.09383 | 1.3706 | -1.3544 |
| 0.7     | 0.08027 | 1.4827 | -1.6288 |
| 0.8     | 0.06469 | 1.6379 | -2.0860 |

which in turn labels the corresponding universality class. Interestingly, if $b$ were universal then the finite-size behavior of the GE would be in sharp contrast to that of other quantities such as the ground state energy per site, where the universal finite-size scaling correction appears at order $O(1/n^2)$ instead of $O(1/n)$ [15]. Note also that other entanglement measures such as the von Neumann entropy [3], the single copy entanglement [4] and the GE per region for a partition into regions of a macroscopic size [5] already display universal behaviors. Despite its inherent interest, the findings of this paper are not conclusive about the (potential) universality of coefficient $b$. This problem will be specifically addressed in a separate publication [20].

6. Conclusions and discussion

In this paper, we have numerically investigated the finite-size GE for 1D quantum spin lattice systems with PBCs in the context of newly developed TN algorithms. In particular, we have shown how to compute the GE using these techniques. We have also shown that the leading term in the finite-size correction to the GE per spin at criticality behaves as $b/n$, as evidenced by our calculations for the quantum Ising spin chain in a transverse magnetic field and for the XXZ spin chain. The possibility of this leading finite-size scaling being universal has also been discussed.

Although we have restricted ourselves in this work to the study of finite size quantum lattice systems in 1D, it is possible to abandon this restriction in several ways. Specifically, one may directly compute the GE per site for finite and infinite quantum lattice systems both in 1D and 2D by using TN algorithms [21]–[24]. This will be the subject of future works.

Acknowledgments

We acknowledge very insightful comments by the referees and the editors assigned to this paper. This work was supported in part by the National Natural Science Foundation of China (grant nos 10774197 and 10874252), the Natural Science Foundation of Chongqing (grant no. CSTC, 2008BC2023) and the Australian Research Council.
Table A.1. GE for the XXZ model with $n = 10$ sites. The results are for 1-site TI product states, and 2-site TI product states. The ground state has been obtained by an exact diagonalization of the Hamiltonian.

| $\Delta$ | GE 1-site TI | GE 2-site TI |
|---------|--------------|--------------|
| 0.0     | 2.51221      | 2.51221      |
| 0.1     | 2.45308      | 2.45308      |
| 0.2     | 2.39471      | 2.39509      |
| 0.3     | 2.33639      | 2.33639      |
| 0.4     | 2.28193      | 2.28184      |
| 0.5     | 2.22632      | 2.22632      |
| 0.6     | 2.16945      | 2.16945      |
| 0.7     | 2.11964      | 2.12233      |
| 0.8     | 2.07288      | 2.07288      |

Appendix

In this appendix, we show a numerical calculation that gives evidence that the GE obtained by optimizing over the family of TI product states with period of one site is equal to that obtained by optimizing over the family of TI product states with period of two sites. More specifically, for the XXZ model that we consider in this paper with $n = 10$ sites a simple exact diagonalization of the Hamiltonian gives us the results from table A.1.

Remarkably, in table A.1 we can see that in both cases (1-site TI and 2-site TI) we obtain very similar results for the GE. This is an indication that the closest product state can be chosen to be TI with period of one site, in turn being consistent with our qualitative arguments in the main body of the paper. Note that the above numbers also match the results in figure 2 for $n = 10$ using MPSs.

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