Theory of Finite-Entanglement Scaling at One-Dimensional Quantum Critical Points

Frank Pollmann,[1] Subroto Mukerjee,[1,2] Ari M. Turner,[1] and Joel E. Moore[1,2]
[1]*Department of Physics, University of California, Berkeley, California 94720, USA*
[2]*Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
(Received 20 April 2009; revised manuscript received 2 June 2009; published 26 June 2009)

Studies of entanglement in many-particle systems suggest that most quantum critical ground states have infinitely more entanglement than noncritical states. Standard algorithms for one-dimensional systems construct model states with limited entanglement, which are a worse approximation to quantum critical states than to others. We give a quantitative theory of previously observed scaling behavior resulting from finite entanglement at quantum criticality. Finite-entanglement scaling in one-dimensional systems is governed not by the scaling dimension of an operator but by the "central charge" of the critical point. An important ingredient is the universal distribution of density-matrix eigenvalues at a critical point [P. Calabrese and A. Lefevre, Phys. Rev. A **78**, 032329 (2008)]. The parameter-free theory is checked against numerical scaling at several quantum critical points.

DOI: 10.1103/PhysRevLett.102.255701 PACS numbers: 64.70.Tg, 03.67.Mn, 75.10.Pq

A system in its ground state can undergo a second-order (continuous) quantum phase transition as a control parameter is varied through a critical value. As at a thermal phase transition, the critical point has correlations over long length scales. These correlations are described by properties of the critical point that are ''universal,'' i.e., independent of microscopic details. The entanglement entropy is a measure of the quantum-mechanical nature of correlations and in many cases is also universal [1–8]. The entanglement entropy of a pure state of a bipartite system AB is defined as

$$S = -\mathrm{Tr}\rho_A \log\rho_A = -\mathrm{Tr}\rho_B \log\rho_B, \tag{1}$$

where ρ_A (ρ_B) is the reduced density matrix of subsystem $A(B)$.

We would like to understand a consequence of diverging entanglement at quantum criticality: any approach constructing states with a limited amount of entanglement will show universal, systematic errors in describing quantum critical states. It was shown previously by Tagliacozzo *et al.* [9] in a numerical study of two one-dimensional critical models that finite entanglement leads to scaling behavior like that induced by other perturbations of a critical point: it introduces a finite correlation length $\xi \sim \chi^{\kappa}$, where χ (defined below) is related to how much entanglement is retained and κ is the finite-entanglement scaling exponent. That work gave convincing evidence for this behavior in the two models studied but did not attempt to explain its origin or develop a theory predicting κ. As the retained entanglement χ increases, $\xi \to \infty$ and criticality is restored.

The main result of this Letter is a theory for this behavior for conformally invariant critical points in one dimension. The theory predicts that κ, unlike other scaling exponents, is determined by the central charge of the critical point. It leads to a specific formula for this dependence and also explains the observed scaling of entanglement entropy. The iTEBD algorithm [10], which has finite-entanglement errors but not finite-size ones, is then used to study a number of critical points. The numerical results confirm that central charge determines finite-entanglement scaling and show parameter-free agreement with the theoretical predictions.

The best understood quantum critical points are in one spatial dimension, where most translation-invariant systems have critical points with ''conformal invariance,'' an infinite-dimensional group related to conformal maps of the plane. (In higher dimensions the conformal group is finite-dimensional.) The entanglement entropy between two halves of a large one-dimensional system close to the critical point (large correlation length ξ) is [5]

$$S = \frac{c}{6}\log(\xi/a). \tag{2}$$

Here c is the ''central charge'' of the critical point, a number that counts how many degrees of freedom of the system are critical, and a is a short-distance length scale, such as the lattice spacing in a spin chain.

Our goal is to understand how the increased entanglement of a quantum critical state [Eq. (2)] affects classical representation of the state, e.g., in a computer algorithm. A powerful approach to obtain low-energy states of one-dimensional systems is the density-matrix renormalization group algorithm [11]. This algorithm and its descendants [10] construct trial wave functions that are ''matrix product states'' (MPSs) [12]. Consider a system with N sites and periodic boundary conditions, where each site has d orthogonal states. Any pure state of the system is a superposition of the product basis states $|s_1 s_2 \ldots s_N\rangle = |\{s\}\rangle$ where $1 \le s_i \le d$. A MPS for such a system has the form

$$|\psi\rangle = \sum_{s_1,\ldots,s_N=1}^{d} \mathrm{Tr}[A^{[1]}_{s_1}\ldots A^{[N]}_{s_N}]|s_1\rangle\ldots|s_N\rangle. \quad (3)$$

For each site i there are d matrices $A^i_{s_i}$ of a finite dimension $\chi\times\chi$. A product wave function describing an unentangled chain of particles or spins is obtained by multiplying together scalar amplitudes for the particle or spin state at each site. The MPS generates entanglement by using matrices instead of amplitudes, and more information can be stored as the matrix dimension χ increases.

A convenient representation of this state $|\Psi\rangle$ for entanglement purposes is the Schmidt decomposition. Splitting the system into two parts at one bond, the Schmidt decomposition is a basis choice that expresses the original wave function as a sum of product states of wave functions for the two halves of the system:

$$|\Psi\rangle = \sum_{n=1}^{\infty} \lambda_n |\Phi_{nA}\rangle|\Phi_{nB}\rangle. \quad (4)$$

The $|\Phi_{nA}\rangle$ and $|\Phi_{nB}\rangle$ form orthonormal bases for the Hilbert spaces of the subsystems A and B to the left and right of the bond. The Schmidt decomposition contains more than one term for entangled states: measurements on subsystem B put the system in a state Φ_{nB} with probability λ_n^2 and force the left half of the system into the corresponding basis state. This converts the system into a mixed state with entropy

$$S = -\sum_n \lambda_n^2 \log\lambda_n^2. \quad (5)$$

We use the recently developed infinite time-evolving block decimation (iTEBD) algorithm [10] to study several local one-dimensional Hamiltonians with translationally invariant ground states. Exploiting translational invariance, there are only finitely many different matrices $A^i_{s_i}$. The iTEBD algorithm finds an approximation of the ground state by performing an imaginary time evolution of a random initial MPS with fixed dimension χ. Because this method always constructs wave functions for the infinite system, its errors result from finite entanglement rather than finite size; it was similarly used in [9] for the original numerical study of how finite entanglement affects quantum criticality. Here our focus is a theory for how the numerical observations differ fundamentally from conventional finite-size scaling, together with additional iTEBD results. We study cases in which the iTEBD algorithm converges effectively to the matrices of a given dimension that are the best approximation of the ground state [10]. Away from a critical point, the entanglement entropy of the exact wave function is finite, and the approximation by MPSs converges rapidly [13].

At the critical point, finite-dimensional matrices cannot approximate the ground state as well; the maximum entropy for χ Schmidt eigenvalues is $\log\chi$. The numerical eigenvalues for the system at the critical point but with finite χ actually obey a distribution that does not maximize the entropy. Instead, there is a physical interpretation of the observed distribution, which underlies the theoretical analysis. We first note that the observed eigenvalue distribution at finite χ and at the critical point (correlation length $\xi=\infty$) is similar to the infinite-χ distribution away from the critical point (at some finite ξ determined by χ). This is the microscopic origin of the observation [9] that physical quantities computed at infinite ξ and finite χ reproduce those at finite ξ and infinite χ, with an empirical scaling law $\xi\propto\chi^{\kappa}$ in which the exponent κ depends on the specific critical point. More precisely, the eigenvalue distribution of the reduced density matrix of a one-dimensional system with a large correlation length ξ was recently studied [14]: the mean number of eigenvalues larger than a given value λ is

$$n(\lambda, b) = I_0[2\sqrt{b(-b-2\log\lambda)}]. \quad (6)$$

Here I_0 is the zeroth modified Bessel function, and b is a parameter that varies with g, diverging at the critical point; in fact, summing Eq. (5) shows that b is determined by the entanglement entropy: $b=S/2$. We find that this distribution is a good description of the observed eigenvalue distributions, even at criticality, with finite but large χ. We now discuss a theory for the finite-entanglement scaling exponent κ, which also appears in the scaling of entanglement entropy with χ,

$$S = \frac{c\kappa}{6}\log\chi = \frac{c}{6}\log\xi. \quad (7)$$

We wish to compute the effective correlation length ξ that describes the state obtained by minimization of energy at the critical point and finite χ. Since the true ground state has infinite ξ, a state with a finite ξ carries an energy cost proportional to $1/\xi^2$ [15]. However, this energy cost is balanced because the retention of only the first χ eigenvalues has a more severe effect on a $\xi=\infty$ critical state than a noncritical state. Thus, we have to include another term which accounts for the increase in energy per unit length due to truncating the Schmidt states at a bond. We assume that this increase is proportional to the overlap of the truncated state with excited states, which is given by the residual probability $P_r(b,\chi)=\sum_{n=\chi}^{\infty}\lambda(b,n)^2$ (making the b dependence explicit). The energy scale which multiplies $P_r(b,\chi)$ is proportional to the gap which goes as $1/\xi$ [15]. Thus, the energy per unit length is given by

$$E(\xi) = E_\infty + \frac{A}{\xi^2} + \beta\frac{P_r(b,\chi)}{\xi}. \quad (8)$$

Here E_∞ is the ground-state energy per unit length of the critical system, and β and A are nonuniversal constants that drop out of the asymptotic behavior for large χ [15].

In the asymptotic large-χ limit, the discarded eigenvalues can be assumed to form a continuum and be distributed according to Eq. (6). The residual probability is now an integral with the values of $\lambda(b,n)$ obtained by inverting Eq. (6). For large χ, we find

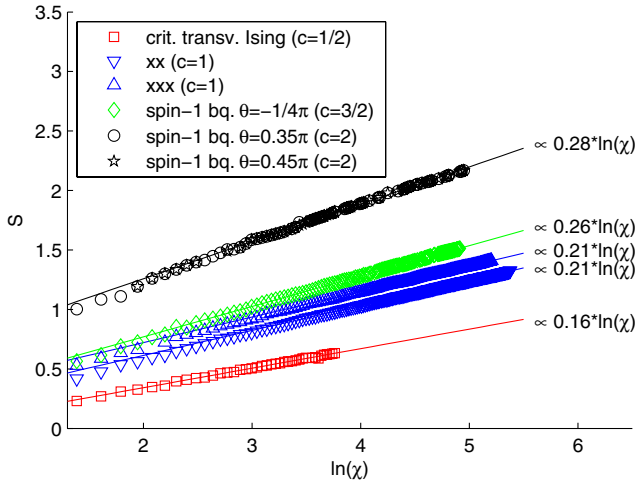

FIG. 1 (color online). Scaling of the entropy with matrix dimension χ. The entropy is calculated numerically using the iTEBD algorithm for several critical points in one dimension: the XX and Heisenberg (XXX) models, the transverse Ising model, and the $s = 1$ biquadratic Heisenberg model. It can be seen that in each case $S \propto \log\chi$. The lines for models with the same central charge c have the same slope, although other density-matrix-renormalization-group-observed properties differ, such as the marginal operator present in the XXX model [24] but not the XX model.

$$P_r(b, \chi) = \frac{2be^{-b}\chi}{\log\chi - 2b} e^{-(\log\chi)^2/4b}. \tag{9}$$

Replacing ξ in favor of b using $\xi = e^{6S/c} = e^{12b/c}$ and using Eq. (9) in Eq. (8) gives the energy per unit length as a function of b and χ. To find the ground state at fixed χ, we minimize the energy with respect to b and find that

$$\kappa = \frac{6}{c(\sqrt{\frac{12}{c}} + 1)} \Rightarrow S = \frac{1}{\sqrt{\frac{12}{c}} + 1} \log\chi, \tag{10}$$

with corrections of order $1/\log\chi$. The relationship between κ and c is a central result of this Letter.

We have performed numerical tests of the scaling prediction in Eq. (10) on several critical points. The specific one-dimensional systems we have studied are the quantum Ising model in a transverse field, the XXZ spin chain for spin-1/2, and the spin-1 generalized Heisenberg model. The quantum Ising model whose Hamiltonian is

$$H = -\sum_i (\sigma_i^x \sigma_{i+1}^x + g\sigma_i^z)$$

is critical at $g = 1$ with central charge $c = 1/2$. The XXZ spin chain is described by the Hamiltonian

$$H = \sum_i (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \gamma\sigma_i^z \sigma_{i+1}^z)$$

and is critical in the entire range $\gamma \in [0, 1]$ with central charge $c = 1$. Critical exponents change continuously with γ [16]. However, κ is the same for different γ as predicted by the theory. The last system we have studied is the $S = 1$

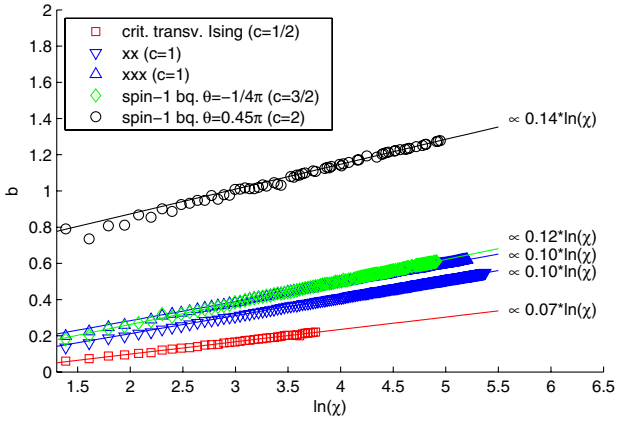

FIG. 2 (color online). Scaling of the parameter b. $b = -\log\lambda_{\max}$ is calculated numerically for different models, where $\lambda_{\max}$ is the largest eigenvalue of the Schmidt decomposition. For all models, $b \propto \log\chi$ for sufficiently large matrix dimension χ. A comparison to Fig. 1 shows that the relationship $S = 2b$ (single-copy entanglement) is approximately satisfied.

Heisenberg chain with biquadratic term,

$$H = \sum_i [\cos\theta(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin\theta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2].$$

This system is known to have two exactly solvable critical points, the $SU(2)_2$ point at $\theta = -\pi/4$ with $c = 3/2$ [17] and the $SU(3)_1$ point at $\theta = \pi/4$ with $c = 2$ [18]. The entire region $\theta \in [\pi/4, \pi/2)$ is critical with $c = 2$ [19], which is consistent with our results. A detailed study of critical $SU(N)$ can be found in Ref. [20].

The prediction that the scaling of the entropy S depends only on c can be checked directly (Fig. 1). The relationship between the entropy and the largest density-matrix eigenvalue, which is used by Calabrese and Lefevre [14], is approximately satisfied (Fig. 2). The model above implies

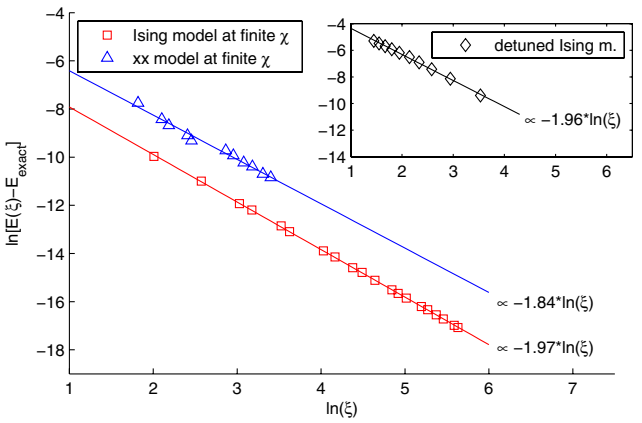

FIG. 3 (color online). Energy vs correlation length. The energy calculated numerically scales as $1/\xi^2$ with correlation length ξ. The same scaling also appears (inset) when the state in question is obtained as the ground state of a slightly off-critical Hamiltonian. The correlation length in a matrix product state can be obtained from the transfer operator [25].

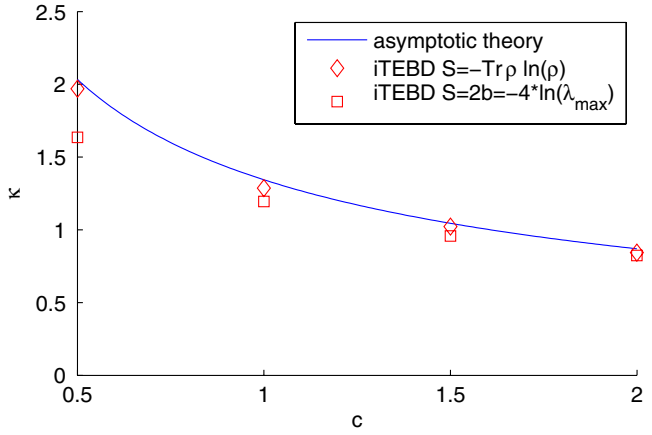

FIG. 4 (color online). κ for different values of the central charge. κ is calculated numerically using different definitions of the entropy [definitions from Eqs. (2) and (5) nearly agree, while the single-copy entanglement $S = 2b$ gives different values as shown], and according to the parameter-free asymptotic theoretical result in Eq. (10). The values of κ are, within the numerical accuracy, identical for different models with the same central charge c.

that the energy in the critical Hamiltonian for a state with finite value of ξ should go as $E = E_0 + B/\xi^2$, where E_0 is the actual ground-state energy and B a nonuniversal constant. This connection between the actual correlation length ξ and the energy was tested (Fig. 3) for ground states on and off criticality.

Numerical calculations can estimate the entropy scaling using the definition of the entropy in Eq. (2) as well as the relations [Eq. (5)] and the single-copy entanglement $S = 2b$ [21], and compare the results to the parameter-free theoretical prediction [Eq. (10)]. The results are shown in Fig. 4. The agreement of the numerical values among themselves and with Eq. (10) is at worst about 20%; even for small χ the error in the asymptotic theoretical prediction is comparable to the discrepancies between definitions of the entropy. A stringent test of the nonlinear c dependence of Eq. (10) is that systems of decoupled copies are also found numerically to obey this scaling prediction (not shown).

These results suggest that the effect of finite entanglement in any MPS description near a quantum critical point in one dimension results from universal properties of the quantum critical point, specifically its central charge rather than a scaling dimension as in finite-size scaling. There are several potential extensions of this approach. In addition to studying other types of quantum critical points, there are recently developed MPS-type algorithms for time-dependent problems [22] and higher dimensions [23] that may also show universal scaling of errors near quantum criticality.

The authors thank DARPA OLE and the Max Planck Foundation (F. P.), DOE (S. M.), and NSF DMR-0804413 (J. E. M.) for support.

[1] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
[2] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. **B424**, 443 (1994).
[3] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).
[4] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[5] P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.
[6] G. Refael and J. E. Moore, Phys. Rev. Lett. **93**, 260602 (2004).
[7] S. Ryu and T. Takayanagi, Phys. Rev. Lett. **96**, 181602 (2006).
[8] E. Fradkin and J. E. Moore, Phys. Rev. Lett. **97**, 050404 (2006).
[9] L. Tagliacozzo, T. R. de Oliveira, S. Iblisdir, and J. I. Latorre, Phys. Rev. B **78**, 024410 (2008).
[10] G. Vidal, Phys. Rev. Lett. **98**, 070201 (2007).
[11] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[12] S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).
[13] J. Eisert, M. Cramer, and M. B. Plenio, arXiv:0808.3773 [Rev. Mod. Phys. (to be published)].
[14] P. Calabrese and A. Lefevre, Phys. Rev. A **78**, 032329 (2008).
[15] See EPAPS Document No. E-PRLTAO-103-073928 for additional details of the theoretical derivations in the main manuscript, including the asymptotic formula for the finite-entanglement scaling exponent. For more information on EPAPS, see http://www.aip.org/pubservs/epaps.html.
[16] R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, New York, 1982).
[17] F. C. Alcaraz and M. J. Martins, J. Phys. A **21**, L381 (1988).
[18] C. Itoi and M.-H. Kato, Phys. Rev. B **55**, 8295 (1997).
[19] A. Läuchli, G. Schmid, and S. Trebst, Phys. Rev. B **74**, 144426 (2006).
[20] M. Führinger, S. Rachel, R. Thomale, M. Greiter, and P. Schmitteckert, Ann. Phys. (Berlin) **17**, 922 (2008)
[21] J. Eisert and M. Cramer, Phys. Rev. A **72**, 042112 (2005); I. Peschel and J. Zhao, J. Stat. Mech. (2005) P11002; R. Orus *et al.*, Phys. Rev. A **73**, 060303 (2006).
[22] U. Schollwöck and S. R. White, in *Effective Models for Low-Dimensional Strongly Correlated Systems*, edited by G. G. G. Batrouni and D. Poilblanc (AIP, Melville, New York, 2006).
[23] J. Jordan, R. Orus, G. Vidal, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **101**, 250602 (2008).
[24] S.-W. Tsai and J. B. Marston, Phys. Rev. B **62**, 5546 (2000).
[25] M. W. Wolf *et al.*, Phys. Rev. Lett. **97**, 110403 (2006).