Universal and nonuniversal contributions to block-block entanglement in many-fermion systems

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(Received 3 April 2008; published 13 June 2008)

We calculate the entanglement entropy of blocks of size x embedded in a larger system of size L, by means of a combination of analytical and numerical techniques. The complete entanglement entropy in this case is a sum of three terms. One is a universal x- and L-dependent term, first predicted by Calabrese and Cardy, the second is a nonuniversal term arising from the thermodynamic limit, and the third is a finite size correction. We give an explicit expression for the second, nonuniversal, term for the one-dimensional Hubbard model, and numerically assess the importance of all three contributions by comparing to the entropy obtained from fully numerical diagonalization of the many-body Hamiltonian. We find that finite-size corrections are very small. The universal Calabrese-Cardy term is equally small for small blocks, but becomes larger for $x>1$. In all investigated situations, however, the by far dominating contribution is the nonuniversal term stemming from the thermodynamic limit.

DOI: 10.1103/PhysRevA.77.062324 PACS number(s): 03.67.Mn, 71.10.Fd, 03.65.Ud, 71.10.Pm

I. INTRODUCTION

Entanglement is one of the most studied and least intuitive features of quantum mechanics. Many aspects of it are still not fully understood. Part of the difficulty is that in itself entanglement is not an observable quantity. Rather, entanglement is a property of the quantum mechanical state, defined with respect to some set of degrees of freedom. For different degrees of freedom, and different states, entanglement is characterized and quantified in different ways.

For mixed states, described by a density operator, many alternative measures of entanglement are still under study. For pure states in a bipartite system, described by a wave function, on the other hand, a near consensus has emerged that the entanglement entropy is a suitable entanglement measure. Having identified a suitable measure, the task at hand then changes to evaluating it and analyzing its behavior in various physical systems, in order to extract information that can be useful in quantum information processing and computing.

The present paper is concerned with this task in the particular case of strongly interacting electrons in a finite-size chain. Our interest is in separating universal and system-specific contributions to the entanglement entropy, quantifying their relative importance, and investigating their behavior as a function of system parameters. Specifically, we consider a quantum chain of length L divided in a subsystem A of size x, and a subsystem B of size $L-x$, and calculate the entanglement entropy [1]

$$S(x,L) = -\mathrm{Tr}[\rho_A \log_2(\rho_A)], \tag{1}$$

where the reduced density matrix $\rho_A = \mathrm{Tr}_B[\rho]$ is obtained from the density matrix of the full system ρ by tracing over the degrees of freedom of subsystem B. For interacting many-particle systems the full density matrix is almost impossibly difficult to obtain. For suitable model Hamiltonians, and not too many particles, however, fully numerical diagonalization is within reach, and can be used to calculate ρ_A and S. Before embarking on such a numerical calculation for a specific system, however, it is useful to recall general properties of $S(x,L)$ that were uncovered in ground-breaking analytical work of Calabrese and Cardy [2].

These authors find that the entanglement entropy of a subsystem of size x, embedded in a larger gapless system of size $L \gg x$, consists of two distinct terms: a universal term depending only on x and L, and a nonuniversal term that depends on system-specific parameters, but is independent of x and L [2,3]. Analytical expressions for the universal term were obtained by Calabrese and Cardy (CC) [2], found to be in agreement with partial results obtained earlier in Refs. [3–5], and were further analyzed in, e.g., Refs. [6–10].

For periodic boundary conditions and $L \gg x \gg 1$, these authors find

$$S(x,L) = \frac{c}{3}\log_2\left[\frac{L}{\pi}\sin\left(\frac{\pi x}{L}\right)\right] + s_1, \tag{2}$$

where c is the central charge (conformal anomaly) of the system and s_1 is a nonuniversal term whose magnitude and dependence on system parameters remain undetermined in the approach of Refs. [2–5]. If the condition $L \gg x \gg 1$ is not satisfied there may be additional finite-size corrections not contained in the CC analysis. While the identification of universal terms is one of the principal goals of statistical physics, any quantitative application to realistic models or to actual materials and devices depends crucially on information about the nonuniversal terms. With a view on future realizations of quantum computing and quantum information processing in systems of interacting particles, we therefore now embark on the task to extract information about the nonuniversal function s_1 and on possible finite-size corrections for realistic models of such systems.

In this paper, we focus on the one-dimensional fermionic Hubbard model. For this model, we (i) numerically assess the magnitude of the universal (CC) term and the nonuniver-

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sal s_1 term for realistic values of system parameters, arriving at the unexpected conclusion that the universal term is only a small correction to the much larger nonuniversal term; (ii) obtain an analytical expression for s_1 of the Hubbard model, allowing us to study its dependence on various system parameters; and (iii) compare the analytical expression with numerical results obtained by full diagonalization of the many-body Hamiltonian, finding satisfactory agreement, both for single-site and block-block entanglement, in interacting and noninteracting systems of various sizes and densities.

II. UNIVERSAL CONTRIBUTION TO THE ENTROPY VERSUS EXACT ENTROPY

In this section we numerically calculate the exact entanglement entropy of the one-dimensional finite-size Hubbard model and compare it to the analytical prediction made by keeping only the universal term in the CC formula

$$S^{\text{univ}}(x,L) = \frac{c}{3}\log_2\left[\frac{L}{\pi}\sin\left(\frac{\pi x}{L}\right)\right]. \tag{3}$$

The one-dimensional Hubbard model, one of the most widely used models of strongly interacting particles [11–13], is described by the Hamiltonian

$$\hat{H} = -t\sum_{i,\sigma}(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i+1,\sigma} + \text{H.c.}) + U\sum_{i}\hat{c}^{\dagger}_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^{\dagger}_{i\downarrow}\hat{c}_{i\downarrow}, \tag{4}$$

where t is the hopping between neighboring sites, U is the on-site particle-particle interaction, and $\hat{c}^{\dagger}_{i\sigma}$ and $\hat{c}_{i\sigma}$ are (fermionic) creation and annihilation operators of particles at site i with spin σ. The system described by this Hamiltonian is completely characterized by its size L, interaction U [14], and either the particle number $N \leq 2L$ or the particle density $n=N/L$ [15]. For small L, this Hamiltonian can be diagonalized numerically. Since this involves no approximation other than the use of finite-precision numbers on a computer, we follow common terminology and denote this as exact diagonalization. The resulting eigenfunctions can be used to construct the density matrix, and from this the entanglement entropy can be extracted.

A quantitative comparison between the resulting S^{exact} and S^{univ}, as given by Eq. (3), is presented in Table I for various different choices of system parameters and $x=1$. Interestingly, the universal term makes only a very small negative contribution to the exact single-site entropy. We conclude from this analysis that for the single-site entanglement the universal CC term is hardly relevant quantitatively: when L is large enough for the full CC formula to become asymptotically exact (recall that it was derived for $L \gg x$), the universal term is already a vanishingly small correction to the nonuniversal term.

From Eq. (3) it is clear that the universal term increases as a function of block size x. The interesting question is then by how much it grows relative to the nonuniversal, system-specific, term s_1. In order to investigate this quantitatively, we fix L at 10 sites, and calculate $S(x,L=10)$ as a function of the size x of the subsystem B. Benchmark data for comparison at $x>1$ are extracted from Ref. [16], which deals with block-block entanglement in the extended Hubbard model. By setting the parameter V of that model equal to zero, reference values for $S(x,L=10)$ can be extracted from Fig. 3 of that work. Below we do refer to these data as "exact" because they were also obtained by numerically exact full diagonalization, but we note that we extracted them graphically from Fig. 3 of Ref. [16]. The difference between these "exact" values and S^{univ}, which is the effect we are after, is clearly much larger than any possible error of the benchmark data, which can therefore safely be used for comparison.

TABLE I. Universal contribution to the single-site ($x=1$) entanglement of a chain of size L with periodic boundary conditions, compared to data from numerically exact full diagonalization, at $U=4$. The last column is the deviation, in percent, of the universal contribution from the exact numerical value.

n	L	S^{univ}	S^{exact}	Deviation (%)
0.5	4	−0.101	1.541	106.5
	8	−0.025	1.564	101.6
	12	−0.011	1.576	100.7
1.0	4	−0.050	1.594	103.1
	8	−0.012	1.701	100.7
	12	−0.005	1.718	100.3

The data in Table II show that for larger blocks the universal term makes a more noticeable contribution to the block-block entanglement entropy. While for $x=1$ the deviation of the universal term from the numerical value is very similar to that of Table I, it becomes smaller for $x>1$. However, quantitatively, it is still amounts to less than half of the exact entropy. As an example, even for $x=5$, i.e., a maximal subsystem half the size of the complete system, it is still only about one third of S^{exact}. Part of this difference must be due to s_1.

The s_1 term can be eliminated by studying not S, but its derivative as a function of block size x. This behavior can be evaluated in various ways. First, we calculate analytically the derivative $\partial S(x,L)/\partial x$ of the CC expression (2), by treating x as a continuous variable. Results for integer values of x are represented by open circles in Fig. 1. Note that since s_1 is taken to be a constant, this derivative samples only the universal term. Second, we calculate the numerical derivative of

TABLE II. Universal contribution to the block-block entanglement of a chain of size $L=10$ with $U=0$ and $n=1$, compared to values for the full entropy extracted for the same system from Ref. [16]. The last column is the deviation, in percent, of the universal contribution from the reference value.

x	S^{univ}	S^{exact}	Deviation (%)
1	−0.016	2.00	100.8
2	0.602	2.69	77.6
3	0.910	3.02	69.9
4	1.065	3.17	66.4
5	1.114	3.22	65.4

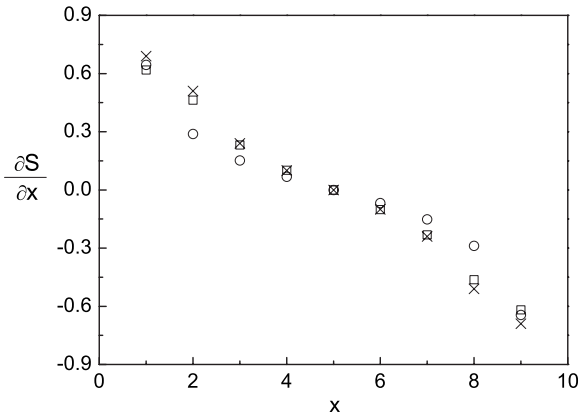

FIG. 1. Derivative of the block-block entanglement entropy with respect to block size, obtained analytically from Eq. (2) (open circles), numerically from five data points obtained from Eq. (2) (open squares), and numerically from the five data points in Table II.

the five data points for $x=1,\ldots,5$ collected in Table II. Results are represented by crosses in Fig. 1. A direct comparison between both sets of data is marred by the intrinsic inaccuracy of a numerical derivative. To minimize this problem, we also obtained the derivative of the CC formula (2) by evaluating that expression numerically at $x=1,\ldots,5$ and taking the numerical derivative of the resulting values. This set of data, represented by open squares, is directly comparable to the numerical derivative of the benchmark data in Table II.

The deviation between the open circles and open squares is thus between analytical and numerical five-point derivatives of the same function. The difference between the open squares and the crosses is between the CC prediction of the trend as a function of x and the numerical results, both obtained from five data points. Evidently, the behavior of the CC expression and of the numerical data is very similar. The small differences remaining between crosses and squares are due to finite-size corrections to the CC expression (more on these below) and the intrinsic error bar of the reference data from Table II.

Since the behavior of the derivative $\partial S/\partial x$ is very closely reproduced by the CC expression, we conclude that the much larger differences observed in Table II for the entropy itself must be almost entirely due to the term s_1. This analysis thus points to the importance of nonuniversal terms, which remain undetermined in the CC approach.

Additionally, it should be noted that the CC formula was derived for large $L \gg x$, while in order to be able to compare to data from full numerical diagonalization we evaluate it for $L<13$. Finite-size corrections to the CC formula are another possible explanation for the large fraction of the exact entropy not recovered by the universal term only. In the next sections we attempt to disentangle and quantify these two distinct effects, by deriving an analytical expression for s_1 of the Hubbard model, and comparing it to the same set of exact data.

III. ANALYTICAL EXPRESSION FOR THE BLOCK-ENTANGLEMENT ENTROPY

In the thermodynamic limit, $L\to\infty$, the CC expression (2) reduces to

$$S(x,L\to\infty)=\frac{c}{3}\log_2(x)+s_1, \tag{5}$$

from which the function s_1 of the model under study can be determined once the entanglement entropy of this model is known in the thermodynamic limit. Since s_1 does not depend on x, we are free to evaluate it for any convenient value of x. In the special case of single-site entanglement ($x=1$), the logarithm on the right-hand side vanishes, and

$$s_1=S(x=1,L\to\infty), \tag{6}$$

which implies

$$\frac{S(x,L\to\infty)}{S(1,L\to\infty)}=1+\frac{c}{3}\frac{\log_2(x)}{s_1}, \tag{7}$$

This identification neglects possible finite-size corrections arising from the fact that the CC expression was derived only for $L\gg x\gg 1$. The difference between numerical data and predictions of the preceding equation allows one to estimate the size of such corrections.

Next, we apply this procedure to the Hubbard chain. Recent research has resulted in a complete physical picture of and explicit expressions for $S(x=1,L\to\infty)$ [17–19]. Specifically, the single-site entanglement entropy for the Hubbard model in the absence of external electric or magnetic fields is given by [17–19]

$$\begin{aligned}S(x=1,L\to\infty;n,U)=&-2\left(\frac{n}{2}-\frac{\partial e}{\partial U}\right)\log_2\left[\frac{n}{2}-\frac{\partial e}{\partial U}\right]\\&-\left(1-n+\frac{\partial e}{\partial U}\right)\log_2\left[1-n+\frac{\partial e}{\partial U}\right]\\&-\frac{\partial e}{\partial U}\log_2\left[\frac{\partial e}{\partial U}\right],\end{aligned} \tag{8}$$

where the ground-state energy per site $e=E_0(n,U)/L$ can be obtained from the Bethe-Ansatz integral equations [11–13,20].

By combining this Bethe-ansatz-based expression for $S(x=1,L\to\infty)$ with the CC formula, based on conformal field theory, we obtain

$$\begin{aligned}S(x,L;n,U)=&\frac{c}{3}\log_2\left[\frac{L}{\pi}\sin\left(\frac{\pi x}{L}\right)\right]\\&-2\left(\frac{n}{2}-\frac{\partial e}{\partial U}\right)\log_2\left[\frac{n}{2}-\frac{\partial e}{\partial U}\right]-\frac{\partial e}{\partial U}\log_2\left[\frac{\partial e}{\partial U}\right]\\&-\left(1-n+\frac{\partial e}{\partial U}\right)\log_2\left[1-n+\frac{\partial e}{\partial U}\right],\end{aligned} \tag{9}$$

which is the sum of a universal term, depending only on geometry (x and L), and a term depending on specific system parameters (n and U). This explicit expression allows us to investigate the actual size of each of these terms under real-

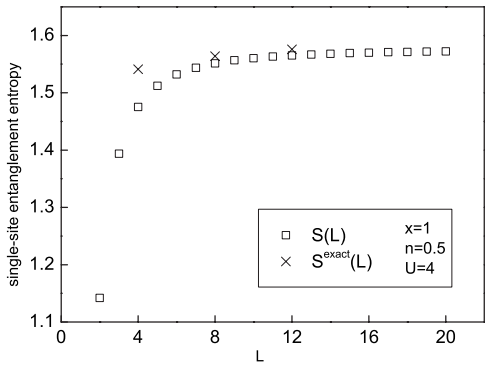

FIG. 2. Single-site entanglement entropy as a function of system size L for the Hubbard model. Open squares, analytical results from our Eq. (9). Crosses, numerical data obtained by diagonalizing the many-body Hamiltonian.

istic circumstances, by obtaining $e(n,U)$ numerically from the Bethe-ansatz integral equations, and evaluating Eq. (9) as a function of x, L, n, and U.

IV. FULL ENTROPY VERSUS EXACT ENTROPY

Figure 2 contains a comparison of our numerical data for $x=1$ with our analytical expression (9) for the specific case of a Hubbard chain with $U=4$ and $n=0.5$. Exact data are given only for $L=4,8,12$, because odd particle numbers N would result in a finite magnetization [which is not included in Eq. (8)] and $L\geq 13$ is already too large for full exact diagonalization on our computing equipment. The available data, however, are clearly sufficient to conclude that trend and magnitude are the same for both analytical and numerical data.

The quantitative deviation observed in Fig. 2 between analytical and numerical results for small L is due to the fact that the CC formula was derived for large L, whereas data from full numerical diagonalization are only available for $L<13$. For small L, there may be additional L-dependent

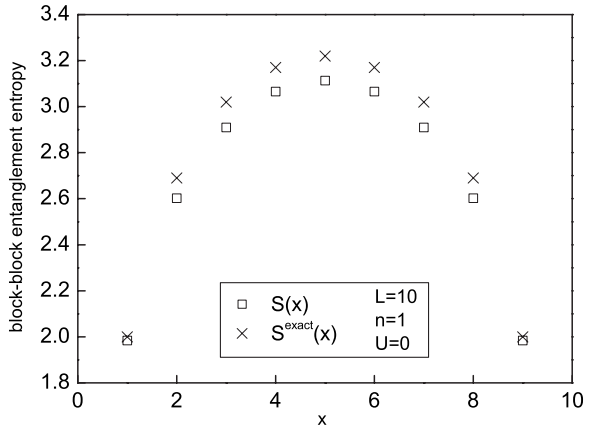

FIG. 3. Block-block entanglement entropy as a function of the block size x for the noninteracting Hubbard model ($L=10$, $U=0$, and $n=1$). For $x>L/2$ we obtained S from the symmetry relation $S(x,L)=S(L-x,L)$, and for $x<L/2$ it is calculated from Eq. (9). Benchmark data have been extracted from Ref. [16].

TABLE III. Same as Table I, but with $S^{\mathrm{univ}}(x,L)$ replaced by our expression (9), comprising $S^{\mathrm{univ}}(x,L)$ and expression (8) for $s_1(n,U)$.

n	L	$S(x=1,L)$	Exact	Deviation (%)
0.5	4	1.475	1.541	4.3
	8	1.551	1.564	0.8
	12	1.565	1.576	0.7
1.0	4	1.678	1.594	5.3
	8	1.716	1.701	0.9
	12	1.723	1.718	0.3

terms in the full expression for the entropy, which go to zero as L increases. These are the finite-size effects referred to above. The data in Fig. 2 show that already for L as small as 12, such possible small-L corrections are negligible.

Figure 3 extends this analysis to larger block sizes, by evaluating Eq. (9) as a function of x, and comparing to the same set of reference data at $x>1$ and $U=0$, used in Sec. II. The overall agreement between expression (9) and the benchmark data is rather satisfactory. The remaining deviations now have two distinct sources. One is, as above, the use of the CC expression at rather small L. The other is the imprecision in the extraction of the benchmark data from the figure presented in Ref. [16]. Still, there can hardly be any doubts that the dependence on block size x is reproduced correctly. Clearly, in Eq. (9) this dependence comes exclusively from the universal term, which makes a much more pronounced contribution for $x>1$ than it made for $x=1$.

Tables III and IV compare expression (9) to benchmark data at $x=1$ and $x>1$. The last column of Tables III and IV shows that expression (9) practically exhausts the exact entropy, both for single-site entanglement and for block-block entanglement. As before, we attribute the remaining small differences, of order $\sim 1\%$, to finite-size corrections, contained in the numerical data for small L but not in the CC expression derived for large L. Since for some values of n the full expression (9) predicts more than 100% of the exact entropy, these finite-size corrections must alternate their sign as a function of n.

As a second test, we have also fitted the exact data for $L=10$ and $x\leq 5$ in Tables II and IV with expression (2), treating c and s_1 as fitting parameters. The result is $c=2.17\pm 0.02$ and $s_1=2.02\pm 0.007$. Since in the situation of these tables the exact values are known to be $s_1=c=2$, this fit

TABLE IV. Same as Table II, but with $S^{\mathrm{univ}}(x,L)$ replaced by our expression (9), comprising $S^{\mathrm{univ}}(x,L)$ and expression (8) for $s_1(n,U)$.

x	$S(x,L)$	Exact	Deviation (%)
1	1.984	2.00	0.8
2	2.602	2.69	3.3
3	2.910	3.02	3.6
4	3.065	3.17	3.3
5	3.114	3.22	3.3

again illustrates the smallness of finite-size corrections to the CC formula (2) for x and L outside the range $L \gg x \gg 1$, where it becomes exact.

V. CONCLUSIONS AND OUTLOOK

We can summarize our combined analytical-numerical analysis in the statement that the block-block entanglement entropy for any system size L and block size x is given by

$$S(x,L;n,U) = S^{\mathrm{univ}}(x,L) + S(x=1,L\to\infty;n,U) + \Delta S(x,L;n,U), \tag{10}$$

where the first term is the universal CC term of Eq. (3), depending on x and L only, and the second is the system-specific term s_1, depending on n and U, which we extract from the thermodynamic limit (6). The third by definition comprises all possible finite-size corrections not resulting from the CC analysis or contained in the infinite-size limit leading to the identification $s_1(n,U)=S(x=1,L\to\infty;n,U)$.

By comparing this full expression to the data in Tables I–IV, and the trends visible in Figs. 1–3, we conclude that the nonuniversal term $s_1=S(x=1,L\to\infty;n,U)$ quantitatively dominates the physics of the entanglement entropy of the Hubbard model in all investigated situations. For $x=1$, the universal term and the finite-size corrections are of comparable magnitude, $O(1\%)$, and essentially negligible relative to the nonuniversal term, even for rather small L. For $x>1$, the universal term is of order $O(10\%)$ of the full entropy, while finite-size corrections remain $O(1\%)$. The trend as a function of x, on the other hand, is not at all affected by s_1, but dominated by the universal term, receiving only small $(\sim 1-10\%)$ finite-size corrections from $\Delta S(x,L;n,U)$. While all of this highlights the intellectual achievement of CC in having identified the universal contribution to the entanglement entropy, it also shows that if one wants to quantify the entropy in an actual material or device—a need that arises as soon as one considers using entanglement as a resource for quantum computing in real systems—a detailed description of system-specific features is unavoidable.

One way to obtain an approximate system-specific description also in systems with inequivalent sites is the local-density approximation (LDA) to density-functional theory (DFT), which locally applies results obtained in a spatially homogeneous system (with constant density n) in order to simulate the corresponding inhomogeneous system (with spatially varying density n_i). This approximation is commonly applied in *ab initio* calculations of the electronic structure of atoms, molecules, and solids [21–24], where the local approximation (or one of its refinements) is made for the exchange-correlation energy. In earlier work we proposed to apply the same strategy also to the Hubbard model [25], and suggested a simple local-density approximation for the single-site entanglement entropy [26]. (For related applications of DFT concepts to the study of entanglement, see Refs. [27,28].)

That approximation was constructed specifically for $x=1$. The present Eq. (10), valid for all x, suggests two ways to extend the validity of the local-density approximation to block-block entanglement. One, is to simply add to the LDA of Ref. [26] the term $MS^{\mathrm{univ}}(x,L)$, which the original entropy LDA did not contain. Here $M=L/x$ is the number of blocks in the system. The other is to take Eq. (10) as entropy of the homogeneous reference system on which the local approximation is based. This leads to

$$S^{\mathrm{LDA}}[x,L;n_i,U] = MS^{\mathrm{univ}}(x,L\to\infty) + \frac{1}{x}S^{\mathrm{LDA}}[x=1,L;n_i,U], \tag{11}$$

which differs from the *ad hoc* correction in the L dependence of the first term and the x dependence of the second. Future work directed at block-block entanglement in spatially inhomogeneous systems is expected to identify which of these two extensions is more reliable. Interesting inhomogeneities in this context include impurities, defects, spatial modulations of the system parameters, confining potentials, etc.

A combination of the methodologies employed in Ref. [26] and in the present paper thus allows one to analyze and quantify the entanglement entropy in a wide variety of spatially inhomogeneous many-body systems. Such analysis, and an extension of these investigations to spin-polarized systems, is the subject of future work.

ACKNOWLEDGMENTS

We thank M. Sarandy, D. Larsson and P. Calabrese for useful communication. This work was supported by FAPESP, CNPq, and CAPES. We thank Vivaldo L. Campo, Jr. for providing us with his efficient LANCZOS subroutine.

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