Probing the conformal Calabrese-Cardy scaling with cold atoms

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(Dated: November 16, 2016)

We demonstrate that current experiments using cold bosonic atoms trapped in one-dimensional optical lattices and designed to measure the second-order Rényi entanglement entropy S_2, can be used to verify detailed predictions of conformal field theory (CFT) and estimate the central charge c. We discuss the adiabatic preparation of the ground state at half-filling where we expect a CFT with $c = 1$. This can be accomplished with a very small hoping parameter J, in contrast to existing studies with density one where a much larger J is needed. We provide two complementary methods to estimate and subtract the classical entropy generated by the experimental preparation and imaging processes. We compare numerical calculations for the classical $O(2)$ model with a chemical potential on a 1+1 dimensional lattice, and the quantum Bose-Hubbard Hamiltonian implemented in the experiments. S_2 is very similar for the two models and follows closely the Calabrese-Cardy scaling, $(c/8)\ln(N_s)$, for N_s sites with open boundary conditions, provided that the large subleading corrections are taken into account.

The concept of universality provides a unified approach to the critical behavior of lattice models studied in condensed matter, lattice gauge theory (LGT) and experimentally accessible systems of cold atoms trapped in optical lattices. Conformal symmetry [1, 2] offers many interesting examples of universal behavior that can be observed for lattice models in two [3–5], three [6], and four [7, 8] dimensions. In these examples, the conformal symmetry is explicitly broken by the lattice regularization and only emerges in the continuum and infinite volume limits. Identifying the underlying conformal symmetry through well-understood symmetry breaking patterns in numerical or experimental simulations involving finite lattices is an important tool to explore new universality classes. The entanglement entropy, which measures the correlations between degrees of freedom in different regions of a system, is an important tool [9] to address this question.

For a conformal field theory (CFT) in one space and one time (1+1) dimension, the ground state entanglement entropy increases logarithmically with the spatial volume of the system and its subsystems [9–14]. Using basic CFT results, Calabrese and Cardy [11] established that the coefficient of proportionality is in general the central charge divided by an integer depending on the boundary conditions (CC scaling). The central charge, denoted c, is of primordial importance in CFT. It plays a crucial role in the construction of the unitary representations of the conformal algebra, characterizes the universality class and is present in a variety of physical observables [2, 11].

In view of the rich collection of interesting CFTs in 1+1 dimensions, it would be highly desirable to study their universality classes using quantum simulations. It has been proposed to use a quantum gas microscope to study the second-order Rényi entropy S_2 of one-dimensional fermionic Hubbard chains [15, 16] at half(quarter)-filling which seem consistent with $c = 1(2)$. Recently, manipulations of small one-dimensional chains of cold bosonic ^{87}Rb atoms trapped in optical lattices have allowed experimental measurements of S_2 [17, 18] using a beam splitter method [19, 20]. In these experiments, the superfluid (SF) phase, where S_2 is significant and we expect a CFT behavior, is reached by increasing the hopping parameter J to large values in a one-dimensional "tube" with one atom per site.

In this Letter, we consider instead the case where the tubes are close to half-filling [21] and where a SF phase with significant values for S_2 can be reached at small J. Using procedures available in existing experimental setups [17, 18], we describe the adiabatic preparation of the ground state. Experimental measurements have been performed for small chains of four [17] and six [18] atoms and only slightly larger sizes are expected to be within experimental reach in the near future [22]. As the CC scaling only dominates for large systems, the subleading corrections are very important. These corrections are restricted by CFT and allow us to estimate the central charge from values of S_2 obtained either from numerical or experimental data.

We focus on the universality class associated with the classical $O(2)$ model where we expect $c = 1$. This is an extension of the Ising model where the spin is allowed to move on a circle, making an angle θ with respect to a direction of reference. This model has important common features with models studied in LGT. Despite being called classical, we can take the time continuum limit and identify a quantum Hamiltonian [23–26] for which

the notion of entanglement is perfectly meaningful [27]. A detailed analysis of numerical results [28], shows that unlike the von Neumann entanglement entropy with periodic boundary conditions (PBC), where the CC scaling is obvious at small volume, S_2 with open boundary conditions (OBC) has large subleading corrections. We discuss methods to eliminate finite temperature effects due to the experimental preparation and manipulation of the tubes which can be compared with results for fermionic systems[15, 16].

Our effort is directly related to recent attempts [29–31] to develop quantum simulators for models studied in LGT where one needs to connect measurements in cold atom systems described by quantum Hamiltonians evolving in real time to classical theories that are typically studied in LGT. The long-term goal is to study real time evolution and deal with sign problems that are not amenable with conventional classical computation. In LGT, space and Euclidean time are treated on the same footing, a remnant of the Lorentz invariance expected in the continuum limit. For these reasons, we start with the classical $O(2)$ model in 1+1 dimensions described by the action

$$S = -\beta_\tau \sum_{(x,t)} \cos(\theta_{(x,t+1)} - \theta_{(x,t)} - i\mu)$$
$$- \beta_s \sum_{(x,t)} \cos(\theta_{(x+1,t)} - \theta_{(x,t)}) \qquad (1)$$

on a $N_s \times N_\tau$ rectangular space-time lattice with sites labeled (x,t). The time continuum limit can be achieved by increasing β_τ while keeping constant the product $\beta_s \beta_\tau \equiv 2J/U$, and $\mu\beta_\tau \equiv \tilde{\mu}/U$ tuned in order to keep the desired particle density, denoted λ hereafter. With this procedure, Eq. (1) defines a rotor Hamiltonian [23, 24]:

$$\hat{H} = \frac{U}{2} \sum_x \hat{L}_x^2 - \tilde{\mu} \sum_x \hat{L}_x - 2J \sum_{\langle xy \rangle} \cos(\hat{\theta}_x - \hat{\theta}_y) , \quad (2)$$

with $[\hat{L}_x, e^{i\hat{\theta}_y}] = \delta_{xy} e^{i\hat{\theta}_y}$. These commutation relations can be approximated with finite integer spin [27]. In the following, we use the spin-1 approximation when $\lambda < 1$. The only exception is Fig. 1, where we have $\lambda = 1.5$ in the upper part and the spin-2 approximation has been used. Note that at $U \gg J$ and half-filling ($\lambda = 1/2$ and μ sufficiently large, see below), we have approximately a spin-1/2 XX model which is integrable and has a central charge $c = 1$ [9, 10].

For the purposes described above, quantum simulators involving two kinds of bosonic atoms have been proposed for the $O(2)$ model [27, 32]. This doubling is required to take care of the anti-particles (negative Fourier modes in the tensor renormalization group (TRG) formulation [27, 33, 34]). However, if $\tilde{\mu}$ is large enough these negative modes can be omitted and we can rely on simulators with only one kind of boson, which is easier experimentally. In the following, we focus on the region of the

phase diagram where $\tilde{\mu} \simeq U/2 \gg J$ and where there is an approximate connection with the Bose-Hubbard (BH) model with only one type of particle. In this regime, the particle occupancies 0 and 1 dominate for BH (hard core limit) and the correspondence with the XX model approximation mentioned above is clear. Replacing $\hat{L}_x$ by the occupation number n_x and $e^{i\hat{\theta}_x}$ by the creation operator $a_x^\dagger$ in Eq. (2), we obtain the BH Hamiltonian:

$$H = \frac{U}{2} \sum_x n_x(n_x - 1) - J \sum_x (a_x^\dagger a_{x+1} + h.c.). \qquad (3)$$

This approximate correspondence [25, 26] is supported by numerical results discussed below.

Note that in experimental situations, the number of particles is fixed and there is no chemical potential to be tuned. On the other hand, in numerical calculations, it is possible to determine the value of $\tilde{\mu}$ for which the 0-particle ground state in the Mott phase crosses the 1-particle ground state. At small J, a first order calculation shows that this occurs for $\tilde{\mu}/U = 1/2 - 2J/U$. Replacing particles by holes, the same calculation shows that the transition from the SF phase to the particle density $\lambda = 1$ Mott phase occurs at $\tilde{\mu}/U = 1/2 + 2J/U$. These two lines are visible near the tip of the SF phase in Fig. 1 for small J/U. For larger J/U, our results agree with Refs. [35, 36] for BH.
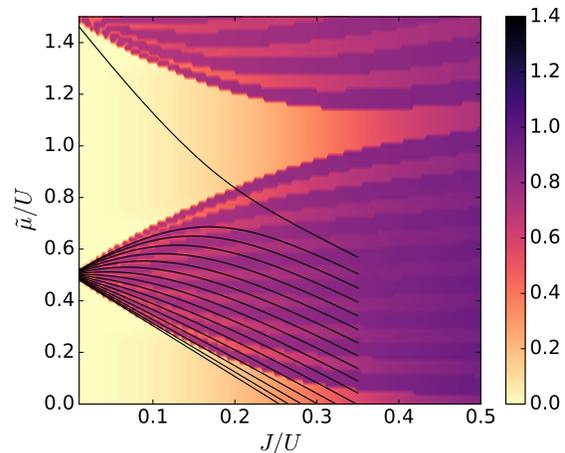
FIG. 1. S_2 for $O(2)$ with $N_s = 16$ and OBC. Laid over top are the BH boundaries between particle number sectors.

We now discuss in parallel the calculation of the entanglement entropy for the $O(2)$ model in the time continuum limit and the BH model. In order to connect with recent cold atom experiments [17, 18], we focus the discussion on the second-order Rényi entropy for the subsystem $\mathcal{A}$

$$S_2(\mathcal{A}) \equiv -\ln(\text{Tr}(\rho_\mathcal{A}^2)) , \qquad (4)$$

with OBC. The reduced density matrix $\hat{\rho}_{\mathcal{A}}$ is obtained by tracing over the complement of $\mathcal{A}$. CFT provides severe restrictions on the dependence of S_2 on the size of the system and the subsystem [11–14, 37]. A detailed study [28] of fits of accurate numerical results with various subsets of the available subsystems shows that using subsystems of size $N_s/2$ allows to obtain estimates of c very close to the expected value 1, while, for $N_s \leq 16$, using larger subsets increase the difference between numerical results and CFT predictions.

In the following, we restrict ourselves to systems with an even number of sites and a subsystem $\mathcal{A}$ of size $N_s/2$. Fig. 1 displays S_2 for $N_s = 16$ as a function of J/U and the chemical potential. The lower (upper) light part is the Mott phase with density $\lambda = 0$ (1), and the 15 plateaus corresponding to the particle number sectors 1, 2, ..., $N_s - 1$ in the SF phase in between are visible. In the following, we focus on the half-filling region which is more or less horizontal in the SF region and can be reached numerically at arbitrarily small J/U.

Since existing experiments only allow a very limited number of sites, it is crucial to take into account subleading corrections. Using existing results [11–14, 37] for subsystems of size $N_s/2$, we get

$$S_2(N_s) = K + A \ln(N_s) + \frac{B \cos\left(\frac{\pi N_s}{2}\right)}{(N_s)^p} + \frac{D}{\ln^2(N_s)}, \quad (5)$$

where K, A, p, B, and D are fitting parameters. For OBC, the CC scaling gives $A = c/8$. In order to verify this prediction, we have calculated S_2 at half-filling for $J/U = 0.1$ for the two models considered using the Density Matrix Renormalization Group (DMRG) method [38, 39] using the ITensor C++ library [40]. For the $O(2)$ model, the results were cross-checked [28] with TRG methods [27, 33, 34].

If we use the numerical data for N_s up to 64, we obtain $A = 0.1263$ for $O(2)$ and 0.1278 for BH which is close to the CC prediction 0.125 for $c = 1$. The difference between the two models can be reduced significantly by decreasing J/U, which also brings A closer to 0.125 [28]. In order to test the predictive ability of the fit for smaller spatial sizes we have reduced the maximal value N_s^{max} of N_s from 64 to smaller values, down to 12. The results for S_2 and A are shown in Fig. 2 which suggests that the estimates converge slowly to the CFT value as N_s^{max} increases.

We now proceed to explain the proposed experimental setup. We consider an optical lattice experiment with single-particle resolved readout and local manipulation of the optical potential, similar to the recent experiments in Ref. [17]. In the experiment, two copies of the one-dimensional many-body state of interest are prepared in adjacent rows of an optical lattice, and global and local Rényi entropies can be measured by a beamsplitter operation implemented via a controlled tunneling operation between the two copies (Fig. 3a). The parity of
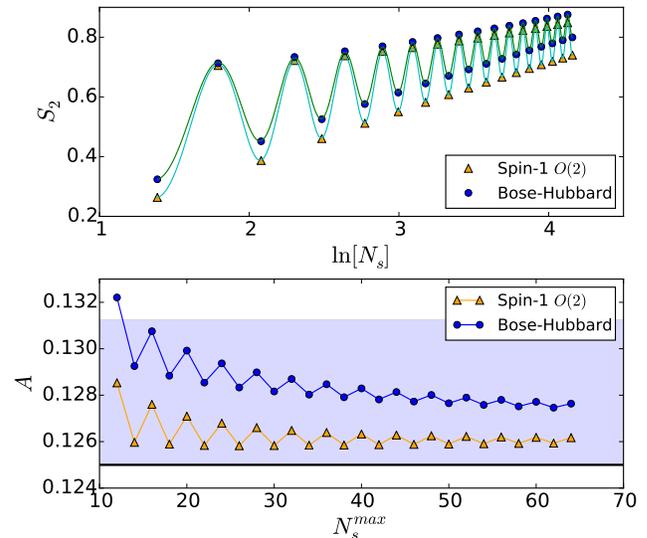
FIG. 2. (top) S_2 at half-filling with OBC for $O(2)$ and BH with $J/U = 0.1$. The solid lines are the fits for Bose-Hubbard and $O(2)$. (bottom) Values of A as a function of the maximal value of N_s used in the fit, the band represents a positive departure of 5 percent from the expected value 0.125.

the atom number in one copy after the beamsplitter operation gives access to the quantum mechanical purity [20].

Bose-Hubbard systems with tunable parameters U and J and well-defined particle number are realized in current experiments with one particle per site. Fig. 3b shows a proposed scheme to achieve half-filling at $J/U \approx 0.1$: N_p bosons are initialized in the Mott regime $J \ll U$, as in current experiments. A superimposed harmonic confinement as well as two sharp, confining walls separated by N_s sites ensure that the system remains in its ground state as the optical lattice depth is adiabatically reduced to achieve the desired J/U. The harmonic confinement is then removed to realize a homogeneous system with hard wall boundary conditions at half-filling. For system sizes considered here, this scheme should allow adiabatic preparation of the ground state with available experimental tools. Alternatively, techniques based on optical superlattices may be able to prepare lattice ground states at half-filling[41].

Assuming that we can prepare twin tubes with half-filling in their ground state, the measurement of S_2 proceeds exactly as in Ref. [17]. After the beamsplitter operation, we select one copy of the twin tubes and measure the number of particles modulo 2 at each site x of this copy, denoted n_x^{copy}, and then use the result [20]:

$$\exp(-S_2) = \text{Tr}(\rho_{\mathcal{A}}^2) = \langle (-1)^{\sum_{x \in \mathcal{A}} n_x^{copy}} \rangle. \quad (6)$$

The probability for parity $(-1)^{n_x} = \pm 1$ is $(1 \pm \exp(-S_2))/2$. It is clear that as S_2 increases, more cancellations occur and one needs on the order of $\exp(2S_2)$
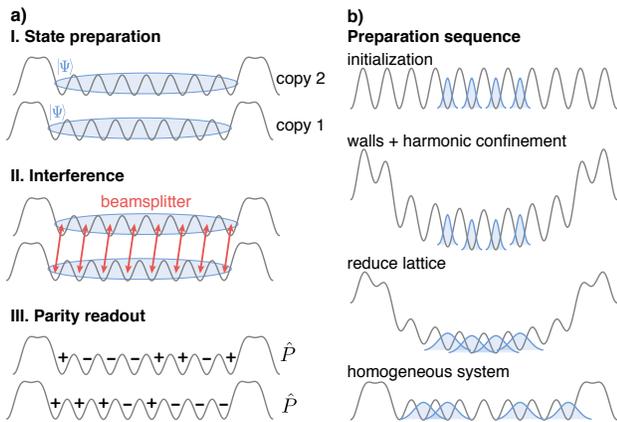
FIG. 3. Measuring entanglement entropy in optical lattices. a) Two copies of a quantum state $|\Psi\rangle$ interfere under a beam-splitter operation, and site-resolved number measurements reveal the local parity $\hat{P}$ and entanglement entropy. b) Proposed state preparation for Bose-Hubbard systems at half-filling, here for 4 atoms on 8 sites. Particles indicated by wavefunctions (blue online) are initialized in a deep optical lattice, where the local environment can be shaped via harmonic confinement and sharp features projected with a spatial light modulator. As the lattice depth is reduced, the particles delocalize but are confined by repulsive walls.

measurements to overcome the fluctuations. From Fig. 2, and assuming N_s to be less than 16 (i. e., less than 8 particles at half-filling), the maximal measured S_2 is less than 1.1. For $\mathcal{N}$ independent measurements, we find that the statistical error is

$$\sigma_{S_2} = \sqrt{(e^{2S_2} - 1)/\mathcal{N}} \ . \tag{7}$$

For the maximal value $S_2 = 1.1$, it takes about 800 measurements to reach $\sigma_{S_2} \simeq 0.1$. Due to the logarithmic growth of S_2, the number of measurements only needs to increase like $N_s^{1/4}$ to maintain a desired accuracy, which is not a prohibitive growth.

In addition to the statistical errors, one needs to take into account that finite temperature as well as preparation and manipulation errors contribute a classical entropy $S^{class.}$. Assuming that this classical entropy is linear in the number of particles in the system, it can be removed by making use of an approximate particle-hole symmetry: near half-filling, $S_2(N_s)$ of the ground state is in good approximation symmetric in the particle number about $N_p = N_s/2$. By measuring $S_2^{exp.}(N_s)$ for a range of particle numbers in the vicinity of $N_s/2$, the excess classical entropy per particle in the experiment can be determined. Subtracting this estimate of the classical entropy from the experimentally measured $S_2^{exp.}$ gives a corrected estimate of the ground state entanglement entropy $S_2^{corr.}$, which we compare to CFT via Eq. (5). For the system sizes considered here, deviations from an exact particle-hole symmetry are small and exhibit a regular behavior at zero and finite temperature [42]. Understanding and

fitting these effects is important to get estimates of $S_2^{corr.}$ with errors less than 0.02 [43].

In order to give an idea of possible experimental outcomes, we have numerically studied the sensitivity of the fit results of Eq. (5) to statistical errors in the measured values of S_2. By repeatedly fitting synthetically generated data (SGD) with Gaussian noise on S_2 of magnitude σ_{S_2} as illustrated in Fig. 4 (left), we find that it translates into errors of the fit approximately as $\sigma_A = 3.2\sigma_{S_2}$ for a global fit of the central charge involving data up to $N_s = 16$. To reach a statistical uncertainty in A comparable to systematic errors of the order 0.02, the statistical error on σ_{S_2} has to be on the order of 0.005.

Alternatively, we can try to fit $S^{class.}$. For this purpose, we have considered the finite temperature (T) effects for $T = 0.2J$ and $0.4J$ in Fig. 4 (left). Remarkably, these effects can be fitted by adding only one term linear in N_s. If $S^{class.}$ generated during the experiment follows this linear behavior, it may be used to determine some effective temperature.
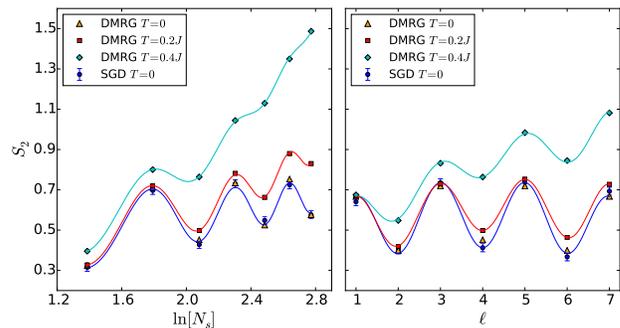
FIG. 4. S_2 at half-filling for BH with $J/U = 0.1$ (triangles, orange online) and SGD with random Gaussian fluctuations with $\sigma_{S_2} = 0.02$ (circles, blue online). (left): vs. $\ln(N_s)$ for a subsystem of size $N_s/2$ with the solid line corresponding to a fit of the SGD from Eq. (5). (right): vs. the subsystem size ℓ for $N_s = 8$; the solid line corresponds to a fit of the SGD using the formulas of Ref. [44]. Same quantities for $T = 0.2J$ (squares, red online) and $T = 0.4J$ (diamonds, cyan online).

So far we have only used the values of S_2 corresponding to a subsystem of size $N_s/2$. CFT also provides prediction for arbitrary subsystem sizes ℓ with $1 \leq \ell \leq N_s - 1$. Typically, one needs to replace $\ell = N_s/2$ by the chord distance. Precise formulas are given in Ref . [44]. The large oscillations when ℓ is changed for $N_s = 8$ are shown in Fig. 4 (right). Importantly, the experimental measurements of the parities at each site shown in Eq. (6) allow us to calculate S_2 for *all* possible subsystems without extra measurements. The possibility of using these additional (but statistically correlated) results to reduce the overall statistical error of the estimates is under study. We can either subtract $S^{class.}$ from $S_2^{exp.}$ as discussed above or instead, use a fit with a term linear in ℓ as in Fig. S2 of Ref. [18]. Fig. 4 (right) shows that finite-T

effects can be fitted with a single additional term linear in ℓ. Estimates of c from fixed N_s fits in other models have up to 20 percent errors [28, 45]. Knowing S_2 for all the subsystems also allows us to calculate the mutual information [15, 17], where the $S^{class.}$ contributions cancel.

In conclusion, we have shown that the simple BH model which is implemented in current experimental measurements of S_2 can be used as a quantum simulator for the classical $O(2)$ model with a chemical potential. We showed that the region of the phase diagram near half-filling and small J/U offers rich possibilities that complement the existing experiments at unity-filling and larger J/U [17, 18]. The changes in S_2 due to the size of the system or the subsystem show strong periodic oscillations which are of the same order of magnitude as the average S_2 for $N_s \leq 16$. We provided complementary methods to estimate and subtract $S^{class.}$ from $S_2^{exp.}$. Existing experiments could immediately confirm the periodic patterns found in the numerical calculations and fits. Accurate determination of c would require larger statistics or a suitable use of the complete information about the subsystems.

New directions should be pursued. Half-filling initial states can also be obtained by a sudden expansion. The presence of additional approximate conserved charges makes the thermalization non-trivial and interesting [46–49]. The possibility of revivals in the time-dependent $S_2(t)$ for time scales of the order of 200 ms for $J/U = 0.1$, a duration about 10 times longer than current experiments [18], is under study. The techniques discussed here for the bosonic case can also be applied to Fermi-Hubbard systems [15], for which optical lattice experiments with single-site resolution are rapidly becoming available [50–53]. It would be desirable to develop specific procedures to study models with other values of c (Ising, Z_N clock, Potts) or with $O(3)$ symmetry with a chemical potential, which have a similar phase diagram [54], and could be quantum simulated [55]. More insight on conformal symmetry could be gained by studying particle number fluctuations [56–58]. The entanglement entropy can also be calculated in 3+1 dimensional pure gauge theories using standard Monte Carlo methods [59]. The rich finite size scaling obtained here for $O(2)$, a model often used to describe the conformal transition [60], suggests to explore multiflavor models [7, 8] with similar methods.

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