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Entanglement scaling in two-dimensional gapless systems

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We numerically determine subleading scaling terms in the ground-state entanglement entropy of several two dimensional (2D) gapless systems, including a Heisenberg model with Néel order, a free Dirac fermion in the π-flux phase, and the nearest-neighbor resonating-valence bond wavefunction. For these models, we show that the entanglement entropy between cylindrical regions of length \( x \) and \( L - x \), extending around a torus of length \( L \), depends upon the dimensionless ratio \( x/L \). This can be well-approximated on finite-size lattices by a function \( \ln(\sin(\pi x/L)) \) akin to the familiar chord-length dependence in one dimension. We provide evidence, however, that the precise form of this bulk-dependent contribution is a more general function in the 2D thermodynamic limit.

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Introduction – The study of quantum condensed matter systems is benefiting from an infusion of ideas related to quantum information and entanglement. The importance of this new resource is strikingly demonstrated in the study of entanglement entropy at one-dimensional (1D) quantum critical points with conformal invariance. Conformal field theory (CFT) provides an important universal number, the central charge \( c \), that appears in an astonishing array of physical quantities.1 A given CFT, and thus any quantum critical points it describes, can be characterized by this number. Its numerical or analytical determination provides an invaluable tool in identifying which, if any, CFT describes the scaling limit of a given Hamiltonian. Computing the entanglement entropy has proven to be a very useful way of finding \( c \) numerically. It can be extracted directly from the ground-state wavefunction by measuring its Renyi entanglement entropy, \( S_n = 1/(1 - n) \ln[\text{Tr} \rho^n] \), where region \( A \) is entangled with its complement, region \( B \). Namely, in a system with total length \( L \), where the region \( A \) has length \( x \), the scaling of the Renyi entropy in 1D critical systems depends on the “chord length” as,2–5

\[
S_n = \frac{c}{6} \left(1 + \frac{1}{n}\right) \ln \left[ \frac{L}{\pi} \sin \left(\frac{\pi x}{L}\right) \right], \tag{1}
\]

with the central charge appearing as the coefficient.

In higher dimensions, the scaling behavior of the entanglement entropy is much less well-understood. Ground states of local Hamiltonians are generally believed to produce an “area-law” (i.e. boundary) scaling,6 the subleading corrections to which may be universal quantities that can be used to identify and characterize quantum phases and phase transitions. A well-established example of such is the topological entanglement entropy7–10 of a gapped state with topological order. In gapless states, the subleading corrections may still potentially harbor universal quantities. It is conceivable that such quantities could be used to define an “effective” central charge in two spatial dimensions, but there are strong constraints on any proposal.11 The best-understood gapless situation in two dimensions is the special case of a conformal quantum critical point, where the ground state itself is written in terms of a two-dimensional (2D) CFT.12–18 In the presence of a spontaneously broken continuous symmetry, Goldstone modes produce a subleading bulk logarithmic correction.19,20 Subleading logarithms from corner contributions with universal coefficients also occur at some critical points,12,21,22

The purpose of this paper is to analyze one type of subleading term in 2D gapless systems, and to study whether this term is universal. Gapless modes typically have long-range correlations, so it is possible for the entanglement entropy to depend on the size and shape of the regions \( A \) and \( B \). Indeed, the 1D result (1) is manifestly size-dependent. We show how similar behavior also occurs in 2D.

We study the finite-size scaling of the second Renyi entropy for the ground states of several two-dimensional gapless systems on the square lattice using quantum Monte Carlo (QMC) simulations. It is possible to vary the size of regions \( A \) and \( B \) without changing the length of the boundary between in a toroidal lattice geometry, where \( A \) and \( B \) are cylinders as in Fig. 1. We examine the Néel ground state of the Heisenberg model, and the nearest-neighbor resonating-valence-bond (RVB) wavefunction, in this geometry. In both cases, we find a size- and shape-dependent scaling function that closely mimics the chord-length contribution in 1D in Eq. (1).

To probe this behavior in a simpler system, we also study free spinless fermions in the π-flux phase and find that the entanglement scaling also has a universal size- and shape-dependent piece. For finite-size systems, this closely mimics the chord length, but in the infinite-size limit we observe it to cross over to a different non-trivial function. Among other consequences, this term will give a non-zero signature in the entanglement quantities9,10
design to look for topological order, which complicates any possible generalization of the topological entanglement entropy to gapless spin-liquid states.

Fermions with \( \pi \)-flux—We begin by considering free spinless fermions on a square lattice, with \( \pi \)-flux through each plaquette. We consider a torus of size \( L_x \times L_y \), and measure the entanglement using a cornerless cylindrical region \( A \) (Fig. 1) with a constant boundary length \( \ell = 2L_y \). We denote the width of region \( A \) by \( x \). This system has Dirac points near momentum \( k_y = 0 \) and \( k_y = \pi \). We take anti-periodic boundary conditions in the \( x \)-direction so that there will be no exact zero mode. We use exact numerical diagonalization of the single-particle Hamiltonian to compute the entropy. The entanglement entropy of 2+1-dimensional conformally invariant systems such as this has been argued to be of the form,\(^{23,24}\)

\[
S_n \sim \text{const.} \times \ell / a + \gamma (x / L_x, L_y / L_x),
\]

(2)

where \( \gamma \) is a universal scaling function of the dimensionless ratios. The area-law term proportional to the boundary length \( \ell \) depends on the lattice constant \( a \), and so the constant is non-universal. A crucial difference from the result in 1D, Eq. (1), is that \( a \) only appears in the area law term. In contrast, the one-dimensional result can be written as a sum of two terms as \( S_n = C \ln \left[ \sin \left( \frac{\pi x}{L} \right) \right] + C' \ln \left[ \frac{1}{n} \right] \), where \( C = c / (1 + 1/n) \). The first term is a universal function of the dimensionless ratio \( x / L \), akin to the function \( \gamma \) above, while the second term involves the lattice scale, as it diverges with \( L \).

To illustrate the absence of such an “additive logarithm” (a logarithmic divergence depending on \( L / a \)) in 2D, we treat this free system as a collection of independent systems in 1D labeled by the momenta \( k_y \). The \( k_y = 0 \) mode contributes an additive logarithm \( C \ln(L_x) \) to the entropy, while the modes with small \( k_y \neq 0 \) contribute additive logarithms \( C \ln(k_y^{-1}) \).\(^{2,4,5}\) Summing over \( k_y = 2\pi j / L_y \), this gives an entropy \( C \left[ \ln(L_x) + 2 \sum_{j=-L_y}^{L_y} \ln(L_y / 2\pi j) \right] = C \ln(L_x) + 2C \ln[(L_y / 2\pi)^{L_y / L_y}] \), where the factor of 2 arises from summing over positive and negative \( m \neq 0 \). Using Stirling’s formula for \( L_y! \), one finds that the additive logarithm terms add to \( C \ln(L_x) - \ln(L_y) = C \ln(L_x / L_y) \).

This can be absorbed into the scaling function \( \gamma \), so that there is no additive logarithm. A more precise calculation would include the effect of finite \( L_x \), but we ignore this since it does not affect the cancellation of additive logarithms. A similar calculation near \( k_y = \pi \) leads to a cancellation of the additive logarithm there.

The entropy of a given \( k_y \) mode contains, in addition to the additive logarithmic divergence in \( k_y \), a universal scaling function \( G(x / L_x, k_y x) \). At \( k_y = 0 \), we see the chord-length scaling \( C \ln \left[ \sin \left( \frac{\pi x}{L} \right) \right] \) (Fig. 2), but for \( k_y \neq 0 \) and for \( k_y x \) large, the chord-length scaling disappears and the entropy becomes roughly flat as a function of \( x / L \). In fact, for \( L_y = L_x = L \), the lowest \( k_y \) mode has a mass \( 2k_y = 4\pi / L \). This factor of \( 4\pi \approx 13 \) means this mass is rather large, and so the entropy of this mode is flat for a large range of \( x / L \). As a result, for \( L_y = L_x = L \), the entropy of the 2D system appears to display 1D chord length scaling over a wide range of \( x / L_x \).

Quantum Monte Carlo—Using QMC techniques we simulate both the Heisenberg ground state and the RVB wavefunction in 2D. The Heisenberg ground state is projected from a trial state by applying a high power of the Hamiltonian, \( H = \sum_{\langle ij \rangle} S_i \cdot S_j \), via a QMC method operating in the valence bond (VB) basis.\(^{25}\) The RVB wavefunction is an equal-amplitude superposition \( |\Psi\rangle = \sum_{\alpha} |V_\alpha\rangle \) of all nearest-neighbor valence-bond states,

\[
|V_\alpha\rangle = \frac{1}{2^{N/4}} \prod_{i=1}^{N/2} \left( |\uparrow_i \downarrow_{i+j} \rangle - |\downarrow_i \uparrow_{i+j} \rangle \right),
\]

(3)

defined by requiring that each spin \( i \) on one sublattice be in a singlet with one of its nearest neighbors \( j_\alpha \).\(^{26,27}\) The
functions, we fit the data with the scaling ansatz, dependence as with the Heisenberg case. We next examine the scaling of the Renyi entropy in the RVB wavefunction. As seen in Fig. 3, a striking two-branch structure exists, depending on whether the distance $x$ is even or odd. The presence of the two branches presumably is related to the fact that correlators in the RVB state have a pronounced even-odd depen-

The second Renyi entropy therefore displays at the very least an effective chord-length dependence over a large range of $x$ for the square torus. It is possible that the apparent chord-length scaling of this 2D system is not perfectly obeyed in the thermodynamic limit, and that this fact is manifest in slight deviations from straight-line behavior in Fig. 4(a). This would be a similar scenario to the deviation from chord-length scaling observed for $\pi$-flux fermions in Fig. 2. However, it is difficult to draw a firm conclusion regarding the statistical significance of any deviation from Eq. (4) scaling in our present data, due to limited system sizes and stochastic error.

We can however further examine the deviation from conformal-style scaling by extracting the $L$-dependence of the coefficient $c(L)$ in Eq. (4). In order for this shape-dependent term to be universal in 2D, $c(L)$ should approach a constant in the limit $L \to \infty$ for fixed $x/L$. As illustrated in Fig. 4(b), the coefficient does not approach a constant for the system sizes that we have studied, but rather has some functional dependence on $L$. This functional dependence is apparently sub-linear – possibly behaving like $c(L) \sim L^p$ with $p \leq 1$. That scenario could be supported by the QMC data if convergence were assumed to be very slow. Indeed, in the quantum dimer model, the corresponding term can be computed exactly in finite size, and the convergence is very slow. A definitive determination of this limit (and therefore the strict adherence of $\gamma$ to universality in this system) is impossible with our current data; significantly larger system sizes must be studied.

We note however that the second Renyi entropy in the RVB wavefunction displays even-odd dependence over a large range of $x$ for the square torus. It is possible that the apparent chord-length scaling of this 2D system is not perfectly obeyed in the thermodynamic limit, and that this fact is manifest in slight deviations from straight-line behavior in Fig. 4(a). This would be a similar scenario to the deviation from chord-length scaling observed for $\pi$-flux fermions in Fig. 2. However, it is difficult to draw a firm conclusion regarding the statistical significance of any deviation from Eq. (4) scaling in our present data, due to limited system sizes and stochastic error.

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Chord-length scaling at fixed well. This again suggests that, although the fit to a entropy in the ground state of three gapless systems on come into play in the 2D thermodynamic limit. accuracy of our data, subtle corrections to this form may contain a subleading scaling term which depends on the subregion and the lattice linear dimensions. Note that while numerical measurement of topological entanglement entropy\(^9,10\) has been used to probe topological properties of gapped phases,\(^31\) the subleading term considered here means that a measurement of topological entanglement entropy in a gapless phase could give either a zero or non-zero result, even without any topological aspects of the phase (though measurements in the \(U(1)\) superfluid phase yielded a vanishing number\(^31\)). Interestingly, just as strong sub-additivity constrains the sign of the Levin-Wen entropy,\(^10\) it also implies, for fixed \(L_x, L_y\), that \(\gamma\) for the von Neumann entropy is a concave-down function of \(x\).

Our quantum Monte Carlo simulations of the Heisenberg Néel ground state and the short-range RVB wavefunction with \(L_x = L_y = L\) show an almost-perfect logarithmic dependence of \(\gamma\) on the chord length \(\sin(\pi x/L)\). It appears that the coefficient of this term is not a universal constant, however, which might suggest either that care must be taken in the order of limits with which the thermodynamic limit is approached, or that a size-dependence remains in this limit, rendering this term non-universal. A study of the crossover from one to two dimensions might illuminate this issue further. Further evidence that the true 2D scaling function might not be exactly the chord-length form is given by the scaling of gapless Dirac fermions in the \(\pi\)-flux phase. Here we have argued that such scaling is superseded by a sum over transverse modes, leading to a different (unknown) functional form in 2D. Furthermore, spontaneous symmetry breaking in the Heisenberg model may complicate measurement of the entanglement entropy. The fact that a complete characterization of the scaling behavior in the Néel and RVB states remains a challenge, despite the large lattice sizes studied to date, underlines the absolute necessity for using large-scale QMC simulations for the study of entanglement entropy.

Regardless of the precise functional form of the shape-dependent subleading term \(\gamma\), its general existence in gapless wavefunctions in 2D would have some profound consequences. Besides the immediate complications in attempting to use entanglement as a probe to detect gapless spin liquids mentioned above, the similarity of the scaling function to a chord-length (present in 1D conformally invariant systems) raises the tantalizing possibility that our results will prove useful in characterizing higher-dimensional critical points. Indeed, since the search for a \(c\)-theorem\(^32\) valid in higher dimensions is of intense interest across several disparate field of physics,\(^23,33–35\) we hope our results will inspire a broader examination of this scaling term in 2D gapless states.

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