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Thermodynamic singularities in the entanglement entropy at a 2D quantum critical point

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We study the bipartite entanglement entropy of the two-dimensional (2D) transverse-field Ising model in the thermodynamic limit. Series expansions are developed for the Renyi entropy around both the small-field and large-field limits, allowing the separate calculation of the entanglement associated with lines and corners at the boundary between sub-systems. Series extrapolations are used to extract power laws and logarithmic singularities as the quantum critical point is approached, giving access to new universal quantities. In 1D, we find excellent agreement with exact results as well as quantum Monte Carlo simulations. In 2D, we find compelling evidence that the entanglement at a corner is significantly different from a free boson field theory. These results demonstrate the power of the series expansion method for calculating entanglement entropy in interacting systems, a fact that will be particularly useful in searches for exotic quantum criticality in models with and without the sign problem.

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I. INTRODUCTION

The study of entanglement properties of ground states of one-dimensional (1D) statistical systems and free field theories in arbitrary dimensions is a very mature field.[1–3] Many exact results have been established, and numerical methods such as the Density Matrix Renormalization Group (DMRG) enable studies of relatively large system sizes in 1D.[4] In contrast, the study of entanglement properties for ground states of interacting quantum lattice models in higher dimensions is a subject still in its infancy.[5–8] In particular, although a great potential exists to connect properties of entanglement to universality at quantum critical points (QCPs),[9] the critical scaling behaviors of very few interacting lattice models are known. Ultimately, the study of entanglement entropies may provide unique signatures of novel or deconfined QCPs.[10] Yet, much work is required before this advance is possible; little is quantitatively known about the nature of the singularities and crossovers at a QCP as a function of system size and other thermodynamic parameters.

Recent developments in Quantum Monte Carlo methods offer a promising avenue for calculating entanglement properties of higher dimensional quantum lattice models.[11,12] Another fruitful approach is the study of entanglement in suitably parameterized variational wavefunctions.[13,14] DMRG and Matrix Product State methods provide other powerful variational approaches to study quantum entanglement in higher dimensional systems.[15–17] However, in contrast to these methods that require careful scaling analyses of finite-size lattices, series expansions at $T = 0$ provide a simple yet powerful alternative approach to studying ground state entanglement entropy directly in the thermodynamic limit. Calculations are carried out order-by-order in perturbation theory as a power series in some expansion variable λ, providing a pedagogically transparent introduction to the development of entanglement entropy in many-body systems. These expansions are typically convergent inside a phase, but become singular as a phase boundary is approached. Once the expansions are developed to some order (in practice typically of order 10), series extrapolation methods can be used to approximate the singular behavior in entanglement near a QCP.

Here, we demonstrate the power and utility of series expansions by calculating thermodynamic singularities in the entanglement entropy of the archetypical 2D quantum critical point of the transverse-field Ising model,[18]

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x, \qquad (1)$$

where the first sum runs over the nearest-neighbor bonds of the square-lattice and the second over its sites. Both the limits $h = 0$ and $J = 0$ have very simple ground states, and series expansions can be separately developed in h/J or J/h. At small h one has two ordered ground states and the system has spontaneously broken Z_2 symmetry (called the "ordered" phase). In developing the series expansion in h/J, we pick one of the two ground states of the system to expand around. The state at $h = 0$ is a simple product state with all the spins pointing along the z axis. At large h (the "disordered" phase), one also has a simple product ground state, where every spin points along the x-axis. Thus both at $h = 0$ and at $J = 0$ the ground states have no entanglement between any pair of sites. A quantum critical point intervenes between the ordered and disordered phases, which is known to be in the universality class of the 3D classical Ising model.[18] Using series expansion, we provide accurate calculation of the thermodynamic singularities in the entanglement

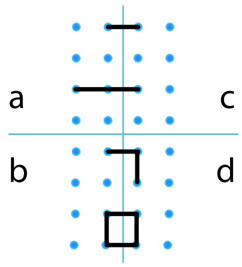

FIG. 1: The infinite square-plane is partitioned into four quadrants a, b, c and d. The region A could be a half-plane such as $a \cup b$ or a quadrant such as b or c, while the rest of the square-lattice forms the region B. For the former partition, several low-order clusters that cross the boundary between A and B are also shown.

entropy for this universality class, demonstrating in particular differences from Gaussian free-field universality.

II. SERIES EXPANSION METHODS FOR RENYI ENTROPIES

From a computational point of view, the Renyi entropies[19] are particularly convenient measures of bipartite entanglement. If we divide our system into two parts A and B, such that each spin belongs to either A or B, then the ground state of the full system can be written in the local basis as

$$|\Psi_g\rangle = \sum_a \sum_b \psi_{a,b} |a\rangle |b\rangle, \tag{2}$$

where a and b refer to basis states for subsystems A and B respectively. The Renyi entropies are defined as:

$$S_n = \frac{1}{1-n} \ln \left[\mathrm{Tr}(\rho_A^n) \right], \tag{3}$$

where, the trace is over all the states of the subsystem A and the reduced density matrix for the subsystem A is given by the matrix elements

$$\langle a_1 | \rho_A | a_2 \rangle = \sum_b \psi^*_{a1,b} \psi_{a2,b}. \tag{4}$$

In this paper we will focus attention solely on the second Renyi entropy S_2. We will divide the infinite system into two subsystems such that the subsystem A is either a half-plane or a quadrant (See Fig. 1). We begin with the case when A is a half-plane. First non-zero terms in perturbation theory arise when pairs of spins from across the dividing line get entangled. Because the entropy is an extensive measure, each such pair contributes equally to the sum and it leads to an entropy proportional to the length of the boundary. In the next order either a pair of spins from one side can be entangled with one spin from the other side, or a pair of spins from one side can entangle with a pair of spins from the other side. These contributions have a natural graphical interpretation in terms of clusters that go across the boundary separating A and B (See Fig. 1). The linked cluster method[18,20] allows one to separate the entanglement that comes from a pair of spins versus the additional entanglement that comes from a larger cluster of spins. One can find the additional entanglement from a larger cluster (also called the weight of the cluster W) by calculating the full entanglement for that cluster of spins when the perturbations are turned on, and then subtracting from it the weight of all its subclusters,[18]

$$W(c) = S_2(c) - \sum_s W(s), \tag{5}$$

where the sum is over all subclusters of the cluster c. In the thermodynamic limit, one can use the translational symmetry along the length of the boundary to write the entropy per unit length as

$$s_2 = S_2/L = \sum_{c_d} W(c_d). \tag{6}$$

Here the sum is over all translationally distinct clusters $\{c_d\}$. Expanding as a power series in $\lambda = h/J$ or $\lambda = J/h$ one obtains

$$s_2 = \sum_n p_n \lambda^n. \tag{7}$$

To obtain the corner terms, we need to consider the case where A is a quadrant (See Fig. 1). In fact, by considering different choices for the division of the infinite lattice into A and B it is possible to completely cancel out the line contributions.[21] If we calculate the entanglement entropy for (i) when A is the quadrant (b) and (ii) when A is the quadrant (c), then their sum will amount to entanglement from two 90 degree corners plus two infinite lines that cut across the lattice. The line contributions can be subtracted off by subtracting the entanglement entropies for the cases, where A is the half plane formed by (i) $a \cup b$ and (ii) $a \cup c$. This subtraction can be done on a graph by graph basis. Thus series for a corner, in the thermodynamic limit, can be expressed in terms of graphs that lie at the intersection of two lines. This leads to the expansions for the entanglement entropy at a single corner as

$$c_2 = \sum_n q_n \lambda^n. \tag{8}$$

The coefficients p_n and q_n are calculated to order 14 in J/h and order 24 in h/J and provided in supplementary material.[22]

Note that one of the advantages of the series expansion method is that the line and corner contributions are obtained separately. In higher dimensions, entropy associated with each type of manifold, planes, lines, corners can also be calculated separately.

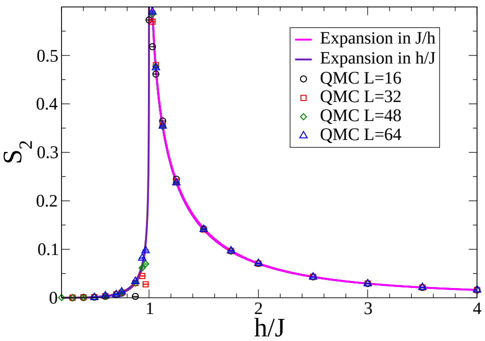

FIG. 2: Entanglement entropy of the transverse-field Ising chain, for two edges, obtained by series expansions. For comparison QMC data on finite systems are also shown. In the ordered phase log 2 has been subtracted from the QMC data to correspond to the fact that series expansions are done around a single ordered ground state.

III. SERIES ANALYSIS

It is clear from the formalism that the 'area law' is built into the series expansion method, namely that the entanglement entropy scales with the boundary 'area' between subsystems. As long as the perturbation theory converges, the 'area law' continues to hold. This is consistent with general arguments that gapped phases obey the area law.[3] As one approaches a quantum critical point, where the gap goes to zero, the series become singular. One can study whether the area law continues to hold at the critical point and the nature of the critical singularity by analyzing the limiting behavior of the series using extrapolation methods.

Series extrapolations can deal with convergent or divergent power-law singularities by using differential approximants.[23,24] A differential approximant approximates a function $f(\lambda)$ by $f_{[m,n,j]}(\lambda)$, the solution to the differential equation:

$$Q_m(\lambda)\frac{df_{[m,n,j]}(\lambda)}{d\lambda} + P_n(\lambda)f_{[m,n,j]}(\lambda) = U_j(\lambda). \qquad (9)$$

Here $Q_m(\lambda)$, $P_n(\lambda)$ and $U_j(\lambda)$ are polynomials of order m, n and j, which are constructed such that the first $m+n+j+2$ powers in the series expansion in λ for $f_{[m,n,j]}(\lambda)$ agree with those for $f(\lambda)$. A given choice of integers m, n and j uniquely determines the approximant $f_{[m,n,j]}(\lambda)$ and its singularities.[23,24] Different choices of the integers m, n and j lead to different approximants. If the location of the critical point λ_c is known by some other means, one can construct biased approximants, whose singularity arises at λ_c. Note that the inhomogeneous term $U_j(\lambda)$ is essential to allow a non-zero slowly varying background in addition to a power-law singularity.

In the special case of a log singularity, one can approximate $\frac{df(\lambda)}{d\lambda}$ by a ratio of polynomials (also called Padé approximants) $\frac{df}{d\lambda}^{[m,n]}(\lambda) = \frac{P_n(\lambda)}{Q_m(\lambda)}$.

First, we discuss the results for the transverse-field Ising chain for which closed form expressions for the von Neumann entropy and asymptotic expressions for the Renyi entropies are available in the literature.[2] Our goal here is not to study the 1D model per se, but to simply see how well one can estimate the critical properties using series expansions of the same length that can be done in any dimension. In Fig. 2, the results of series extrapolation are shown. As a comparison, we also show finite-size data from Quantum Monte Carlo (QMC) on an L length chain with periodic boundary conditions, where A and B are both of length $L/2$. The QMC was performed using a $T = 0$ projector method,[25] adapted to calculate Renyi entropy via the *Swap* operator[11] on a replicated system.[26] The comparison shows that both the series expansion and QMC results are very accurate, at least until one gets very close to the critical point, where finite size effects become large and the QMC data drops away from the series extrapolation curve.

In 1D, the boundary 'area' between subsystems is just a point or a corner. At the critical point this corner contribution diverges logarithmically leading to a breakdown of the 'area law'. The second Renyi entropy associated with a single boundary is given asymptotically close to the critical point by the expression,[1,2]

$$s_2 = \frac{c}{8}\log\xi, \qquad (10)$$

where the central charge $c = \frac{1}{2}$ for this model and the correlation length ξ diverges as $1/|1-\lambda|$ as λ approaches unity. This means that the coefficient of the logarithmic singularity in $\log|1-\lambda|$ should equal -0.0625. Our extrapolations give different answers from the expansions in h/J and J/h. From one side we estimate the coefficient of the log singularity to be $-0.053(1)$ where as from the other side we obtain $-0.077(2)$. Here the quoted small uncertainty is a measure of internal consistency between different approximants. We also find that using longer series both terms are changing in the right direction but only by about 0.001 and 0.002 respectively in each order. If we make the reasonable assumption that the coefficient must be the same from both sides and thus average the two answers, we obtain $-0.065(12)$, which gives a stringent limit on the uncertainty in the calculations.

We now turn to the 2D transverse-field Ising model. In this case, one expects the corner term to be log divergent as in 1D.[1] However, the singular behavior associated with the line term should be of the form

$$s_2 = s_2^c + A/\xi \sim s_2^c + B(\lambda_c - \lambda)^\nu, \qquad (11)$$

where ν is the exponent charactering the divergence of the correlation length ξ. As ξ diverges, the singular part of s_2 goes to zero. In this sense, it is subdominant to the non-singular non-universal term s_2^c. In order to analyze this singular behavior, we bias the critical point to previously determined value of $h/J = 3.044$.[18,27] The extrapolated line and corner terms for the entanglement entropy of the 2D model are shown in Fig. 3. Several

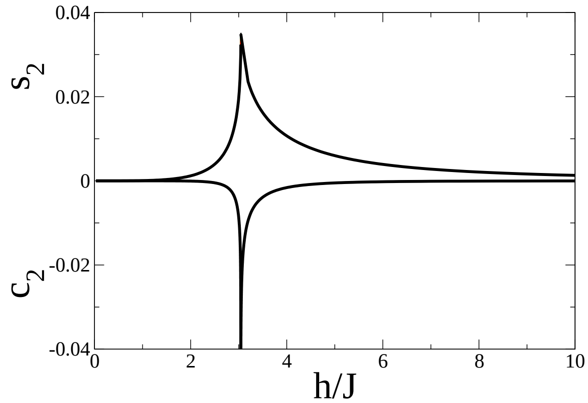

FIG. 3: 'Area law' term s_2 and corner term c_2 of the entanglement entropy of the 2D transverse-field Ising model obtained by series expansions in the variables h/J and J/h. In each case several approximants with critical point biased at $h/J = 3.044$ are shown.

approximants are plotted in each case. They can hardly be distinguished on the scale of the plot, showing the level of internal consistency in the series extrapolations. We estimate $\nu = 0.60(2)$ and entropy per unit length at the critical point of $s_2^c = 0.0324(3)$ from one side and $\nu = 0.66(3)$ and $s_2^c = 0.0350(3)$ from the other side. Averaging these we get, $\nu = 0.63(3)$ and $s_2^c = 0.337(13)$. These values are clearly consistent with the known value of $\nu = 0.629(2)$ for the 3D Ising universality class[28] and recent QMC estimate of $s_2^c = 0.0332(4)$.[29]

The corner term is analyzed for a log singularity. We estimate the coefficient of the logarithm to be 0.0059(3) from one side and 0.0077(1) from the other side. Averaging the two, we get 0.0068(9). One can convert the logarithm in the variable $|\lambda_c - \lambda|$ into $log(\xi)$ by dividing by $-\nu$. Thus, we obtain

$$c_2 = (-0.011 \pm 0.001) log(\xi). \tag{12}$$

These results are clearly distinct from the free field theory result of Casini and Huerta who obtain $c_2 = -0.0062$.[30] The QMC in Ref. 29 quotes a value of $4c_2 = -0.03 \pm 0.01$, with large uncertainties that can not be distinguished from free field theory.

IV. DISCUSSION

We have shown that series expansions can be used to obtain new universal quantities related to entanglement at quantum critical points (QCPs). Specifically, we have calculated thermodynamic singularities in the Renyi entropies with about 10 percent accuracy. We have provided compelling evidence that the entanglement entropy produced at a corner in the boundary between subregions in the 2D transverse field Ising model QCP is different from that of a free boson field theory.[30] Indeed, the transverse field Ising model QCP is in the classical 3D Ising universality class, which is distinct from the free (Gaussian) universality class. Currently there are no theory results for the corner log in the transverse field Ising model; we hope that in the future field theory calculations will be done, in order to compare to our series predictions here.

Through our calculations of c_2 (and our accurate estimate of the exponent ν), we have demonstrated that series expansions already suffice to distinguish between different universality classes.[30,31] It would be useful to study a range of models on different lattices to further consolidate the notion of universality. Given that the numerical values of critical parameters are largely unknown, comparison between series expansions and QMC data, where available, would be most useful. Series expansions can also be developed in higher than two dimensions and also for other Renyi indices n. These can help address questions related to upper critical dimensionality, boundary correlation functions and possible singularities as a function of the Renyi index n.[7]

A weakness of the series method, as presented here, is the inability to study topological entanglement entropy. The calculations discussed here are all related to the boundary between subsystems and in finite orders of perturbation theory only the degrees of freedom at finite distance from the boundary get entangled. This can not address topological entanglement, which is inherently long-ranged. It would be interesting to explore the possibility of addressing this through an approach involving degenerate perturbation theory.[32]

From a computational point of view, series expansion methods may be particularly useful in studying interacting Fermion models and frustrated spin models. Quantum critical points are, in principle, accessible to high temperature series expansions, which might provide a useful route to studying $t - J$ and Hubbard models. At $T = 0$, one should be able to look for exotic critical points at the boundary of magnetically ordered phases, or at the boundary between ordered phases and gapped spin liquids.[10,33] Indeed, several recent works[15,16] have argued that a spin liquid state may arise in the frustrated $J_1 - J_2$ square-lattice Heisenberg model. Investigations of the entanglement scaling at critical points contained in this model will be pursued in future.

V. ACKNOWLEDGMENTS

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