Quantum Critical Universality and Degrees of Freedom in the Singular Entanglement Entropy of Bilayer Heisenberg-Ising model

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We consider a bilayer quantum spin model with anisotropic intra-layer exchange couplings. By varying the anisotropy, the quantum critical phenomena changes from XY to Heisenberg to Ising universality class, with two, three and one modes respectively becoming gapless simultaneously. We use series expansion methods to calculate the second and third Renyi entanglement entropies when the system is bipartitioned into two parts. Leading area-law terms and subleading entropies associated with corners are separately calculated. We find clear evidence that the logarithmic singularity associated with the corners is universal in each class. Its coefficient along the Ising critical line is in excellent agreement with those obtained previously for the transverse-field Ising model. Our results provide strong evidence for the idea that the universal terms in the entanglement entropy provide a measure of the number of low energy degrees of freedom in the system.

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In recent years, the studies of ground state phases of strongly interacting quantum many-body systems have been greatly informed and enriched by new ideas from quantum information theory\cite{1, 2}. Locality of ground state entanglement propagation embodied in the ubiquitous ‘area-law’ for entanglement entropy, allows for powerful new variational approaches\cite{5, 6} that have the potential to transform computational materials science. This has naturally led to great interest in understanding and quantifying the amount of quantum entanglement present in the true ground states of many-body systems.

Bipartite entanglement entropy in the ground states of systems with a gap in the excitation spectrum is known to obey the area-law\cite{8}, that is, the leading term scales with the ‘area’ measuring the boundary between the bipartitioned subsystems. In addition, such systems may also contain quantifiable signatures of topological phases in the form of a long-range entanglement entropy that is unrelated to any boundary\cite{8, 9, 10}. Gapless modes can create additional longer-range entanglement and indeed the study of entanglement properties can provide novel ways to decipher goldstone modes associated with spontaneous symmetry breaking\cite{11}. Study different quantum critical universality classes\cite{12, 13}, as well as the geometrical properties of fermi surfaces\cite{15, 16}. However, while the studies of universality in entanglement properties of one-dimensional systems is rather extensive\cite{13, 21}, quantitative studies in higher dimensional lattice models remain few and far between\cite{22, 26}.

Singular pieces in the entanglement entropy also provide deep connections to underlying quantum field theories and the stability of fixed points under renormalization\cite{24, 28}. In one dimensional models, the singularities in the entanglement entropy are known\cite{26} to be related to the conformal anomaly $c$, and thus, naturally provide a connection to Zamalodchikov’s c-theorem\cite{29} that posits that under renormalization systems flow towards smaller $c$-values. There have been many recent efforts to generalize Zamalodchikov’s c-theorem to higher dimensional systems and the entanglement entropy is central to such efforts\cite{30}. In a very general sense, one expects the singularities in the entanglement entropy to provide a measure of low lying fluctuations or a count of degrees of freedom in the underlying continuum theory\cite{27, 28}. Computational approaches are essential to establish such connections in interacting lattice models.

Here, we consider a bilayer consisting of two-planes of square-lattices, with an anisotropic quantum Heisenberg model with Hamiltonian,

\begin{equation}
\mathcal{H} = \sum_{(i,j)} \left( S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) + \alpha \sum_{\langle(i,k)\rangle} \left( S_i^x S_k^x + S_i^y S_k^y + \lambda S_i^z S_k^z \right),
\end{equation}

where the first sum runs over pairs of spins between the two layers, while the second sum runs over the nearest-neighbor spins, within each layer. For $\alpha = 0$, this model is in the singlet phase, where each pair of inter-planar spins form a dimer. When $\alpha$ is large, the system goes from an XY order at small $\lambda$ to Ising order at large $\lambda$. Right at $\lambda = 1$, full Heisenberg symmetry is realized and we have the well studied bilayer quantum Heisenberg model\cite{26, 31, 33}. In the singlet phase there are three single-particle excitations corresponding to $S^z = \pm 1$, 0 and $-1$ respectively. As is evident from the symmetries of the model for $\lambda < 1$, the gap to $S^z = \pm 1$ modes closes first leading to XY order. For $\lambda > 1$, the gap to $S^z = 0$ mode closes first leading to Ising order. At $\lambda = 1$, all three modes remain exactly degenerate and the system has higher symmetry and Heisenberg universality. Thus, this model provides an elegant way to study the quantum-critical behavior and different universality.
classes and their crossovers in a two-dimensional quantum system.

To carry out our series expansions, we consider one value of the anisotropy \( \lambda \) at a time. We expand around the dimerized phase at \( \alpha = 0 \). To determine the critical coupling \( \alpha_c \) at each \( \lambda \), we calculate series for the staggered susceptibility and excitation gap. For \( \lambda < 1 \), we consider the staggered susceptibility to a field in the \( x \)-direction, and the \( S^2 = +1 \) excitation gap. For \( \lambda \geq 1 \), we instead consider the staggered susceptibility to a field in the \( z \)-direction, and the \( S^2 = 0 \) excitation gap.

We then calculate series expansions for the ‘area-law’ term for the 2nd and 3rd Renyi entanglement entropies at various values of \( \lambda \). To do this, we consider a bipartition of the infinite system by a straight line into two subsystems \( A \) and \( B \). The \( n \)th Renyi entropy is defined as

\[
S_n(A) = \frac{1}{1-n} \ln \text{Tr} (\rho_A^n),
\]

where \( \rho_A = \text{Tr}_B |\Psi\rangle \langle \Psi| \) is the reduced density matrix for subsystem \( A \). The entropy per unit boundary-length, defined as,

\[
s_n = S_n/L,
\]

can then be calculated by a linked cluster method[24, 34, 35].

The entropy due to the presence of a 90\(^\circ\) corner in the boundary, for the \( n \)th Renyi entropy \( c_n \), can be isolated in our series expansions[24, 26]. This is done by considering the entanglement entropy due to the four possible bipartitionings of the system by two perpendicular lines. The straight line contributions from the linear boundaries can be subtracted out, leaving only the corner term[24].

All series coefficients are calculated up to \( \alpha^1 \). A single calculation of this order can be completed within a day on a moderately powerful personal computer.

The series are analyzed using Padé and differential approximants[24, 33]. First we analyze the series for the susceptibility and gap series. These lead to the determination of the phase-boundary shown in Figure 1. The critical couplings \( \alpha_c \) obtained from the susceptibility and gap series are consistent with each other. The critical exponents \( \gamma \) for the susceptibility divergence and \( \nu \) for the gap closing (taking \( z = 1 \)) are calculated and shown in Figure 2. Here, and throughout this paper, the error bars shown represent a spread in the different approximants and are not true statistical uncertainties. On the Ising side the exponents are within 1-2 percent of accepted values for the 3-dimensional Ising universality class, while on the XY side they are within 2-3 percent of accepted values for the 3-dimensional O(2) universality class[32]. Only at the Heisenberg point (\( \lambda = 1 \)), the deviations are larger (approximately 6-7 percent for the susceptibility exponent \( \gamma \)). These are largely correlated with uncertainties in \( \alpha_c \), which varies sharply near the Heisenberg point. For example, the susceptibility series leads to estimates of \( \alpha_c = 0.3982 \pm 0.0008 \), with \( \gamma = 1.51 \pm 0.02 \). If we bias approximants to much more accurate values of the critical point from Quantum Monte Carlo simulations[31] \( \alpha_c = 0.39651 \), it leads to estimates for exponent of \( \gamma = 1.43 \pm 0.02 \), which are much closer to accepted values for the 3-dimensional classical O(3) universality class.

The area-law entanglement entropy is known to have a weak singularity at the critical coupling. We simply used biased differential approximants, with the critical points \( \alpha_c \) estimated from the susceptibility series, to obtain their values up to the critical coupling. The plots for \( s_2 \) and \( s_3 \) are shown in Figures 3 and 4 respectively. Our results should be highly accurate except possibly when one is within a few percent of the critical coupling. Two different approximants are plotted for \( s_2 \) for \( \lambda = 1 \) to show the expected deviations. The difference is barely visible in the plots. For the second Renyi entropy a comparison with recent Quantum Monte Carlo study[33] is also made. The overall agreement is very good. Results from series expansion should be much more accurate away from the critical point.

The quantity of primary interest in our study is the corner entropy and its singular behavior. On approach to the critical coupling, we expect the corner entropy to behave as

\[
c_n = a_n \ln \xi = -\nu a_n \ln (\alpha_c - \alpha).
\]
FIG. 2: Critical exponents $\gamma$ and $\nu$ for different values of the anisotropy parameter $\lambda$. Our results are consistent with constant values for the exponents in the XY and Ising regimes, with a larger exponent at the special Heisenberg symmetry case.

FIG. 3: Plots of the ‘Area-law’ or entanglement entropy per unit boundary length for the second Renyi entropy $S_2$. Quantum Monte Carlo data from Helmes et al are shown by filled circles.

Here $a_n$ should be a universal coefficient equal to the coefficient $a_n \ln L$ in the logarithmic size dependence when the system is right at the critical coupling [14, 26].

To analyze the corner entropy, we first take a derivative of the series, which converts a logarithmic singularity into a simple pole. We then study this by a simple Pade approximant biasing the critical point to that obtained from the analysis of the susceptibility series. The estimated $a_n$ values are shown in Figure 5. In the Ising limit, our results are in excellent agreement with previous series expansions [24] and Numerical Linked Cluster (NLC) calculations [25] for the transverse-field Ising model. Very near the Heisenberg point, one expects greater uncertainty in the values due to crossover effects. Hence, we consider the values at $\lambda = 2$ and $\lambda = 10$. At $\lambda = 2$ we estimate $a_2 = -0.0055 \pm 0.0003$ while at $\lambda = 10$ we estimate $a_2 = -0.0059 \pm 0.0005$. These values agree well with the transverse field Ising model values of $-0.0055 \pm 0.0005$ from series expansions [24, 37] and $-0.0053$ from the NLC calculations [25]. Quantum Monte Carlo estimates so far have [38] much larger error bars $-0.0075 \pm 0.0025$, but are also consistent with these estimates. For the third Renyi entropy, we estimate $a_3 = -0.0040 \pm 0.0003$ at $\lambda = 2$ and $a_3 = -0.0042 \pm 0.0004$ at $\lambda = 10$. These values are also in excellent agreement with the transverse-field Ising model values calculated by NLC. These results point strongly towards the universality of these coefficients in the Ising phase of this model and also between this model and the transverse-field Ising model.

We are not aware of any previous calculations of log singularities for the XY universality class. Our results lead to estimates of $a_2 = -0.0125 \pm 0.0006$ at $\lambda = 0.2$ and $a_2 = -0.0127 \pm 0.0013$ at $\lambda = 0.5$. Similar results for the third Renyi entropy are $a_3 = -0.0089 \pm 0.0006$ at $\lambda = 0.2$ and $a_3 = -0.0091 \pm 0.0020$ at $\lambda = 0.5$. These results clearly point towards a universal value for this universality class also.

At the Heisenberg point ($\lambda = 1$) our results have greater uncertainty. As the critical point varies more sharply near this limit, we can minimize systematic errors...
by taking the location of the critical point from the Quantum Monte Carlo simulations. These lead to estimates of \( a_2 = -0.016 \pm 0.003 \) and \( a_3 = -0.011 \pm 0.003 \). Corner entanglement entropy of this model has been studied before using NLC\(^{26}\) and QMC\(^{33}\). The NLC values were found to be very close to 3 times the transverse-field Ising model values for all Renyi indices. Also, the QMC fits gave \( a_2 = -0.016 \pm 0.001 \). These are in very good agreement with our findings here. Overall, it is clear that the results imply a rough proportionality between the singular coefficients and the number of soft modes in the system that become gapless at the critical point.

In conclusion, in this paper we have studied a bilayer XXZ model that allows us to tune between Ising, Heisenberg and XY universality classes. We have calculated the ‘area-law’ and corner entanglement Renyi entropies using series expansion. We presented strong evidence that the corner entanglement has a logarithmic singularity, which takes universal values in different universality classes. Furthermore, this universal coefficient is roughly proportional to the number of soft or gapless modes in the system. Within these models, it changes monotonically from more stable to less stable fixed points. However, the question of whether it is truly monotonic under renormalization and can serve the purpose of organizing stability of higher dimensional fixed points of quantum statistical models, analogous to the central charge \( c \) in one-dimensional models, deserves further attention.

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