Scaling of entanglement entropy at quantum critical points in random spin chains

Prashant Kumar 1,2 and R. N. Bhatt³

¹Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

²Kadanoff Center for Theoretical Physics, University of Chicago, Chicago, Illinois 60637, USA

³Department of Electrical and Computer Engineering, Princeton University, Princeton, New Jersey 08544, USA



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We study the scaling properties of entanglement entropy (EE) near the quantum critical points in interacting random antiferromagnetic (AFM) spin chains. Using density-matrix renormalization group, we compute the half-chain EE near the topological phase transition between the Haldane and random singlet phases in a disordered spin-1 chain. It is found to diverge logarithmically in system size with an effective central charge $c_{\rm eff}=1.17(4)$ at the quantum critical point (QCP). Moreover, a scaling analysis of EE yields the correlation length exponent $\nu=2.28(5)$. Our unbiased calculation establishes that the QCP is in the universality class of the infinite-randomness fixed point predicted by previous studies based on the strong disorder renormalization group technique. However, in the disordered spin-1/2 Majumdar-Ghosh chain, where a valence bond solid phase is unstable to disorder, the crossover length exponent obtained from a scaling analysis of EE disagrees with the expectation based on the Imry-Ma argument. We provide a possible explanation.

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Introduction. Entanglement entropy (EE) measures gross quantum mechanical correlations between different parts of a system and incorporates experimentally observable quantities in an agnostic manner. It has recently been a subject of extensive investigation as a paradigm for understanding and classifying a wide range of quantum phases and phase transitions (QPTs) [1–15]. The list includes topological phenomena where it has been especially useful [16-25], in addition to conventional symmetry breaking, impurity-driven phases, [6,8,26], etc. Particularly appealing aspects of EE are it being a diagnostic for QPTs, a tool for extracting universal scaling behavior, and new characterizations such as the (effective) central charge [6,8,18,27,28] and topological entanglement entropy [16,17,29]. The extent to which it can be practically useful, in extracting quantitative properties essential to classifying the QPTs, continues to be an exciting area of research.

One-dimensional spin chains with randomness have been of interest for several decades [30-39]. A frequent theme in these systems is the emergence of infinite-randomness fixed points (IRFPs). Pioneering works [6] and subsequent studies [8,26,40-48] have established that different IRFPs can be distinguished from each other using the properties of EE, in particular via the "effective" central charge that controls the scaling of EE with the logarithm of size of a subsystem [49]. The exact results have been primarily obtained using the archetypal strong disorder renormalization group (SDRG) that becomes exact as the width of disorder distribution approaches infinity. However, several impurity-driven transitions occur at zero and finite disorder strengths where SDRG is not applicable, at least on the lattice scale. Hence alternate methods, that can provide independent and unbiased perspectives, are vital to exploring the properties of EE at these critical points.

In this Letter, we utilize the density-matrix renormalization group (DMRG) that is a powerful technique for solving interacting low-dimensional systems and that has recently been improved for applications in problems involving randomness [50-55] (details of our DMRG approach can be found in the Supplemental Material [56]). We investigate the behavior of EE at the topological phase transition between the Haldane [57–59] and random singlet phases in a spin-1 chain. The former is a symmetry-protected topological phase that is known to be stable up to a finite disorder strength owing to its gapped nature. It transitions into a random singlet phase (RSP) upon increasing disorder beyond a critical value [36,37,60,61]. The quantum critical point is proposed to be an IRFP in Refs. [8,37,39]. EE was studied in Ref. [8] using the SDRG technique applied to a domain wall picture and they found that it diverges with system size L logarithmically, i.e., $S = \frac{c_{\text{eff}}}{6} \log L + \cdots$, with $c_{\text{eff}} = 1.232$. Here, L is the number of spins in an open chain and we take S to be the midchain EE. Additionally, the correlation length critical exponent ν was predicted to be approximately 2.30 in Ref. [37].

Since this fixed point exists at an intermediate disorder strength, SDRG is not applicable for the initial steps. One may ask therefore if the critical point could be in a different universality class than the aforementioned IRFP. We investigate this question using DMRG that, as we show, can solve weak to intermediate disordered Hamiltonians if used carefully, exactly where SDRG is not trustworthy. Rather than the Heisenberg model, we study the Affleck-Kennedy-Lieb-Tasaki (AKLT) model [57] which has a short coherence length and is exactly solvable. We add randomness such that it becomes and flows to the same RSP as the Heisenberg model at large disorder. By studying EE scaling with the system size at the critical point, we obtain $c_{\text{eff}} = 1.17(4)$ and a correlation length exponent $\nu = 2.28(5)$ that agree with the SDRG-based predictions of Refs. [8,37], respectively. This confirms that the Haldane phase to RSP transition is indeed in the same universality class as the IRFP studied in these works.

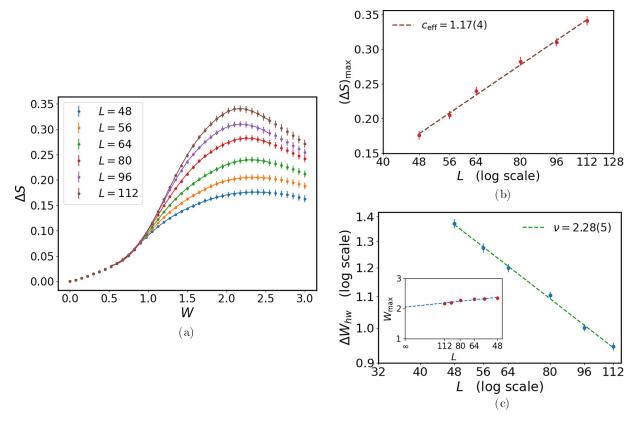


FIG. 1. (a) Excess half-chain entanglement entropy $\Delta S = S - 2\log 2$ vs disorder strength W for various chain lengths L in a random spin-1 chain [Eq. (1)]. It is averaged over $N_D = 16\,000$ disorder realizations except for L = 112 where $N_D = 12\,540$. The solid lines are fits to independent interpolating functions at each L. (b) A least-squares error fit of maxima of ΔS against $\log L$ gives an effective central charge $c_{\rm eff} = 1.17(4)$. (c) Power-law scaling analysis of half width at half maximum on the left side of ΔS , i.e., $\Delta W_{\rm hw} \sim L^{-\frac{1}{\nu}}$. Peak positions $W_{\rm max}$ are nearly independent of L (inset).

As a second example of disorder-induced quantum criticality, we add randomness to the Majumdar-Ghosh model [62,63] such that the second-nearest-neighbor antiferromagnetic exchange term is suppressed at large disorder and the ground state is in the same universality class as spin-1/2 RSP. Without disorder, it breaks translational invariance spontaneously by forming a dimerized state that was found to be unstable to an arbitrarily small amount of disorder in favor of an RSP phase [64]. Here, we compute the midchain EE in its weak disorder regime and observe critical scaling, confirming this expectation. Further, we obtain the crossover length scale exponent $\nu = 1.16(5)$ via a scaling analysis of EE. Surprisingly, this is different than the expectation of $\nu = 2$ based on an Imry-Ma [65] type argument presented in Ref. [64].

Random biquadratic coupling AFM spin-1 model. We consider the following random biquadratic coupling model for the spin-1 chain,

$$H = \sum_{i=1}^{L-1} [J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + D_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \tag{1}$$

where S_i correspond to the spin operators of a spin-1 at the ith site. In the absence of impurities, we take $J_i = 3D_i = J$ so that one obtains the AKLT model where the ground state is in the universality class of the Haldane phase. This state can be understood as a dimerized phase of a spin-1/2 chain of length 2L where each spin-1 is split into two spin-1/2's. The

spin-1/2's at the edges of an open chain are unpaired and the ground state manifold consists of four states with an energy splitting decreasing exponentially in size. Let us introduce disorder using a power-law distribution of J_i 's:

$$P(J) = \frac{1}{W\Omega_0} \left(\frac{J}{\Omega_0}\right)^{\frac{1}{W}-1} \Theta[J(\Omega_0 - J)], \tag{2}$$

$$D_i = \frac{J_i^2}{3\Omega_0}. (3)$$

We have $\langle \log J \rangle = \log \Omega_0 - W$ and the standard deviation $\sigma_{\log J} = W$, hence W corresponds to the strength of disorder. Since Ω_0 is an unimportant energy scale for EE calculation, we choose it by setting $\sum_i \log J_i = 0$. Importantly, Eq. (3) ensures that in the $W \to 0$ limit, one recovers the AKLT model. Moreover, in the $W \to \infty$ limit, $D_i \ll J_i/3$ and are irrelevant perturbations to the RSP fixed point in the spin-1 Heisenberg model as shown in the Supplemental Material [56].

Critical scaling at Haldane-RSP QCP. In Fig. 1, we plot the midchain von Neumann EE versus disorder strength for various chain lengths of the model in Eq. (1). It is defined as follows,

$$S = -\text{Tr}[\rho_A \log \rho_A],\tag{4}$$

where ρ_A is the density matrix of the left half chain. We assume that the ground state is an SU(2) singlet, hence EE at W = 0 is a constant equal to $2 \log 2$ that we subtract from

all data points. The excess EE, ΔS , shows a clear maximum at a critical disorder strength $W=W_c$ where W_c is nearly independent of size. Further, the maximum increases with L, and is consistent with a logarithmic divergence in L. Consequently, we interpret W_c as the critical point between the Haldane phase and RSP.

Our strategy for extracting W_c and other critical properties is as follows. We fit the data points at each size near the critical point to an independent interpolating function chosen to be a Gaussian envelope times a fourth-order polynomial in W. This function is then used for further analysis as opposed to the raw data. We fit the maximum EE, $\Delta S_{\max}(L)$, to the following expression:

$$\Delta S_{\text{max}}(L) = \frac{c_{\text{eff}}}{6} \log L + \Delta S_0.$$
 (5)

We obtain $c_{\text{eff}} = 1.17(4)$. This is within two standard deviations of $c_{\text{eff}} = 1.232$ predicted in Ref. [8].

We assume that the excess EE follows critical scaling in the thermodynamic limit of the form $\Delta S(W, L) \equiv$ $\Delta S_{\rm max}(L) f[(W-W_c)L^{1/\nu}]$. This predicts that the half width at half maximum to the left side, ΔW_{hw} , scales as $L^{-1/\nu}$. The resulting best-fit value, $\nu = 2.28(5)$, is very close to the SDRG prediction, $\nu = 2.3$, made in Ref. [38]. We note that ν depends somewhat on the precise feature of the EE fitted. We believe this is because higher moments of the curves may not have reached the scaling limit and may require data from larger sizes. Moreover, we use only the left side of maximum. On the right side, we expect a RSP with $c_{\rm eff} = \log 3 \approx$ 1.099 [8]. At large sizes, EE is not expected to reduce by more than 11% from its critical value to the one in RSP. Moreover, DMRG simulations tend to be less reliable at large W due to the wide disorder distribution at both lattice and renormalized scales.

Random second-nearest-neighbor Majumdar-Ghosh spin-1/2 model. We next consider the Majumdar-Ghosh AFM spin-1/2 chain with nearest-neighbor coupling J and next-nearestneighbor coupling K = J/2. We introduce disorder in both Jand K, so our Hamiltonian reads

$$H = \sum_{i=1}^{L-1} J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sum_{i=1}^{L-2} K_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}.$$
 (6)

In the absence of disorder, $J_i = 2K_i = J$. We take L to be an even number so that the ground state is unique and corresponds to singlets at bonds labeled by 2n - 1/2 where $n = 1, \ldots, L/2$. The disorder distribution for J_i 's is the same as in Eq. (2). As in the previous case, K_i 's are chosen such that one obtains the random Heisenberg model at $W \to \infty$. In particular, we choose

$$K_i = \frac{J_i J_{i+1}}{2\Omega_0}. (7)$$

We refer the reader to Refs. [56,66] for a discussion of SDRG equations and the irrelevance of K_i at the RSP in the spin-1/2 Heisenberg model.

Scaling near the valence bond solid (VBS) state in a spin-1/2 chain. There are a few subtleties in the quantitative interpretation of the scaling behavior in the spin-1/2 model. First, the RSP has power-law spin-spin correlations, hence, the correlation length is infinite. We expect the transition to

involve a diverging crossover length scale $\xi_{\rm cross}$ above which the VBS state disappears. Second, as we confirm below, the transition takes place at W=0. Therefore, any positive power of the disorder strength W can serve the role of a tuning parameter making the exact value of the critical exponent ν parametrization dependent. In analogy with a temperature-induced ferromagnet-to-paramagnet transition in a one-dimensional pure quantum Ising model, we choose the tuning parameter to be an energy scale. The standard deviation of J, that has dimensions of energy, is $\approx W \Omega_0$ at $W \ll 1$. Thus we define ν via the scaling relation $W \xi_{\rm cross}^{1/\nu} = {\rm const.}$ More precisely, ν determines the scaling dimension of the relevant parameter W at the VBS fixed point.

In Fig. 2, we present and analyze the data for the random spin-1/2 chain of Eq. (6). At W=0, midchain EE is zero at the bond indexed by (L+1)/2. It increases monotonically with W and saturates to a size-dependent value. We fit our data for EE to the following functional form,

$$S(W, L) = S_{\infty}(L) \frac{\text{erf}[\alpha(L)W + \beta(L)W^{2} + \gamma(L)W^{3}] + 1}{2},$$
(8)

where $S_{\infty}(L)$ is EE extrapolated to the infinite disorder limit and $\alpha(L)$, $\beta(L)$, $\gamma(L)$ are fitting parameters for each size L. $S_{\infty}(L)$ is found to diverge logarithmically with L as in Eq. (5) with $c_{\rm eff}=0.66(2)$. Reference [6] predicts $c_{\rm eff}=\log 2\approx 0.693$ in the RSP of a spin-1/2 chain, within two standard deviations of our numerically computed value. This agreement implies that our spin-1/2 model transitions from the VBS to RSP phase as disorder is introduced. Importantly, we do not observe other features in the EE suggesting that the transition is a direct one.

Based on the expectation that the VBS phase is unstable to disorder, we consider the scaling ansatz $S(W,L) = f(WL^{1/\nu})$ near W=0 and in the thermodynamic limit. In order to extract the crossover length exponent ν , we find it useful to reparameterize the data using $x=\log W$ and transforming the scaling ansatz to the following:

$$S(x, L) = F\left(x + \frac{\log L}{v}\right). \tag{9}$$

Further, the derivative of S(x,L) with respect to x displays a peak that is a clear feature of the transition and is reliable for a finite-size scaling analysis. Its position, i.e., $x = x_{\text{peak}}$ is determined purely by the function F(y) through the relation F''(y) = 0. Hence the scaling ansatz predicts $x_{\text{peak}} = x_0 - \frac{\log L}{\nu}$ using which we obtain $\nu = 1.16(5)$. A consequence of our scaling assumption is that the width of the dS/dx curve must become independent of size in the thermodynamic limit. In the inset of Fig. 2(c), we plot the full width at half maximum Δx_{fw} vs 1/L. While a significant irrelevant correction is present, it nevertheless approaches a constant in the thermodynamic limit.

Our crossover length exponent is significantly different than the prediction of Ref. [64] who used an argument analogous to Imry-Ma [65] based on the domain wall picture. Since the EE measures quantum entanglement, a quantum mechanical property, whereas the Imry-Ma argument is essentially a classical argument for the domain size, the apparent

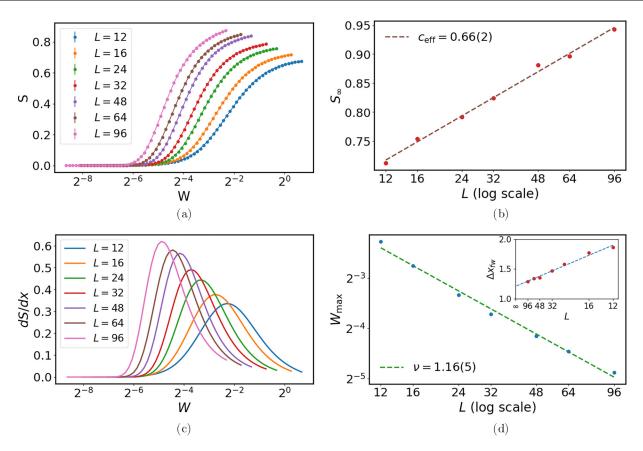


FIG. 2. (a) S vs W for various chain lengths L in the random spin-1/2 model [Eq. (6)]. (b) S extrapolates to $S_{\infty}(L)$ in the $W \to \infty$ limit from which we extract c_{eff} . (c) dS/dx obtained from the fitting functions where $x \equiv \log W$. (d) Power-law scaling analysis of peak positions $W_{\text{max}} = e^{x_{\text{max}}}$. In the inset, full widths at half maxima Δx_{fw} of dS/dx curves are plotted vs L.

discrepancy could be argued away by positing that EE measures a quantum subleading length, not the domain size. We speculate this might be related to the quantum wandering of domain walls. Other possibilities include a complete modification of the domain wall picture due to quantum fluctuations, or strong finite-size effects for sizes studied here.

Discussion. We have shown that ground state entanglement entropy (EE) can not only detect quantum phases and phase transitions (QPTs) in random spin chains but is also useful for characterizing their critical scaling behaviors. EE computed using DMRG in our work has provided important independent perspectives to the strong disorder renormalization group (SDRG) technique. This is especially needed because SDRG may not be valid when the quantum critical point (QCP) occurs at zero or finite disorder strength. Our study suggests that the DMRG technique could be used to study other one-dimensional models with disorder as a complement to other approaches such as SDRG.

At the Haldane phase to random singlet phase (RSP) transition in a spin-1 chain, the effective central charge and

correlation length exponent extracted from the behavior of EE are consistent with previous studies. This provides an independent and unbiased confirmation that the QCP is in the same universality class as the infinite-randomness fixed point proposed by studies based on SDRG. On the other hand, the crossover length scale exponent computed using EE in the disordered Majumdar-Ghosh model differs significantly from prior theoretical predictions [64,65] and we discussed possible causes above. However, we leave a detailed study of this issue to future work.

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