

Witnessing disorder in quantum magnets

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There are no clean samples in nature. Therefore, when we come to discuss the entanglement properties of quantum materials, the effects of disorder must be taken into account. This question is of particular interest for highly entangled phases, such as quantum spin liquids, which lie outside the Landau paradigm for classifying phases of matter. In this work, we explore what experimentally accessible measures, in the form of concurrence, residual tangle, and quantum Fisher information can teach us about the entanglement in the presence of disorder. As a representative example, we consider the Tomonaga-Luttinger liquids (TLL) and disorder-driven random singlet (RS) phases found in antiferromagnetic quantum spin chains. Using quantum Fisher information and residual tangle, we demonstrate that both TLL and RS phases exhibit multipartite entanglement. In the case of the RS phase, we attribute this to entanglement localized below a crossover length scale. We further show that the order of disorder average matters in calculating measures like concurrence and that this can lead to false inferences when interpreting experiments. Nonetheless, correctly interpreted, these witnesses provide useful information about the effects of disorder. We explore how information about the central charge of the TLL can be extracted from the low-temperature behavior of concurrence and conjecture that this analysis can be extended to the effective central charge of the RS phase. Finally, we establish how RS and TLL phases can be distinguished through the growth of multipartite entanglement, as witnessed by the equal-time structure factor. These results establish that, used carefully, experiments based on entanglement witnesses can provide important information about quantum spin systems in the presence of disorder.

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I. INTRODUCTION

How does disorder affect entanglement within quantum materials? Can we quantify such effects experimentally? In nature, all materials possess a certain degree of disorder. Thus, when trying to understand any phase of matter, the role of disorder is an important factor to take into consideration. Disorder or randomness is especially problematic when trying to identify quantum spin liquid (QSL) phases within candidate materials. This question arises in the context of many different materials, including κ - $\text{ET}_2\text{Cu}_2(\text{CN})_3$ [1–8], $\text{Ba}_6\text{Y}_2\text{Rh}_2\text{Ti}_2\text{O}_{17-\delta}$ [9,10], $\text{ZnCu}_3(\text{OD})_6\text{Cl}_2$ (herbertsmithite) [7,11–20], YbMgGaO_4 [21–24], $\text{H}_3\text{LiIr}_2\text{O}_6$ [25–27], etc. Here the challenge lies in being able to distinguish quantum fluctuations from disorder-induced ones. This puts into question whether it is the QSL or some disorder-induced phase realized within these materials?

Entanglement is a valuable resource to identify phases such as QSLs [28]. Intuitively, one expects disorder, which

localizes correlations, to have an effect on entanglement. The key issue, however, is whether this information can be accessed experimentally. Unlike cold atom systems where nonlocal measures like (Rényi) entanglement entropy are accessible [29,30], the same does not extend to condensed-matter systems. Consequently, only limited information about the underlying phase can typically be accessed experimentally. It is thus important to determine if useful information about the entanglement structure can be obtained within experimental constraints. Can we do so by making use of an experimentally accessible entanglement measure [31–61], for instance?

In this study, we explore how measures based on entanglement witnesses can be used to distinguish the different phases which arise in quantum spin systems, with and without disorder. As a representative example, we consider the $S = 1/2$ Heisenberg (XXX) spin chain with and without bond disorder. The competing phases in this case are the Tomonaga-Luttinger liquid (TLL) [62], found in the absence of disorder, and the random singlet (RS) phase realized for arbitrarily weak bond disorder [63–66]. We consider three different measures, namely, concurrence [67,68], tangle [69], and quantum Fisher information (QFI) [42,50], all of which have previously been discussed in the context of experiment [55,57,59,61], and use exact diagonalization to explore how each of these behaves in the TLL and RS phases.

From our analysis, we conclude:

(1) Both the TLL and RS phases are multipartite entangled. In the TLL, multipartite entanglement is present at all length scales. However, in the RS phase, multipartite en-

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tanglement is restricted to clusters smaller than a crossover length-scale, beyond which the effects of disorder become relevant.

(2) Convex roof functions, like concurrence, are sensitive to the order in which disorder averages are calculated. In practice, this means that the distribution of concurrence in real space cannot be used to distinguish TLL from RS in experiments on systems with quenched disorder.

(3) Information about the central charge of the TLL can be extracted from the low-temperature behavior of concurrence. We conjecture that this analysis can be extended to the effective central charge of the RS phase and show how this approach could be used to distinguish TLL from RS in the presence of quenched disorder.

(4) The temperature dependence of multipartite entanglement, as witnessed by QFI, provides a robust means of probing the effect of disorder on quantum spin systems. In the case of quantum spin chains, this provides a clear distinction between the TLL and RS phases, which can be accessed in experiment.

For our investigations, we employed exact diagonalization (ED) and the thermal pure quantum (TPQ) methods [70–73]. Moreover, throughout this article we work in the units where $\hbar = 1$ and $k_B = 1$.

For completeness, we note that concurrence at zero temperature has previously been discussed in the context of disordered spin chains [74,75]. An interesting alternative approach distinguishing RS from the TLL phase employing Bell's inequality was discussed in [74].

The remainder of the article is structured as follows. In Sec. II we start out by giving a brief background on how one can access and/or detect entanglement in a limited setting using only one- and two-point spin-correlation functions. In our work, we employ concurrence to characterize the pairwise entanglement, residual tangle (RT) to detect the presence of multipartite entanglement, and the QFI to characterize the depth of multipartite entanglement within the state. The subtleties, where they arise, are explained along the way.

In Sec. III we detail our notation for evaluating averages. Section IV reviews key results related to the two states under investigation: the TLL and RS phases. Section V introduces the model, disorder, and parameters used to investigate the entanglement structure of these phases. Following which, in Sec. VI we present our zero-temperature results for concurrence, RT and QFI. Section VII explores the finite-temperature behavior of concurrence and equal-time structure factor as witnesses. Here we address the subtleties involved with disorder averaging when dealing with convex roof measures like concurrence. We also discuss how to access the central charge for these phases using concurrence and demonstrate the utility of using a multipartite entanglement witness like the equal-time structure factor as a probe for observing disorder effects.

In Sec. VIII we discuss at length the nature of entanglement in the RS phase, explaining the observed multipartite entanglement and its origins. Finally, we conclude our findings in Sec. IX.

II. ACCESSING ENTANGLEMENT IN MANY-BODY QUANTUM SYSTEMS

Entanglement in the modern perspective is thought of as a resource, one that can be used for quantum computation and information processing [76]. To this end, an important goal within quantum information is to quantify how entangled a state is? Unfortunately doing so is quite challenging, and aside from a few special cases, there is no solution as of yet. Even figuring out, given a density matrix, whether a state is separable or entangled, computationally, turns out to be very complex: in fact, it is an *NP-hard* problem [77].

On the other hand, when it comes to quantifying or detecting entanglement in experimental settings, especially in condensed matter, the challenge diverges from computational complexity to practical feasibility. With a large number of particles involved, a complete state reconstruction by techniques like quantum state tomography is not possible. Thus quantifying entanglement using entanglement entropy, Eq. (1),

$$E(|\phi_{AB}\rangle) = S(\rho_A) = -\text{Tr} \rho_A \log(\rho_A), \quad (1)$$

where ρ_A corresponds to a reduced density matrix obtained by tracing out subsystem B ,

$$\rho_A = \text{Tr}_B(|\phi_{AB}\rangle\langle\phi_{AB}|), \quad (2)$$

is not an option.

So how does one quantify or detect entanglement in a way that is experimentally tractable for condensed matter systems? One strategy is to employ *entanglement witnesses* [37,38], which are observables that provide a means to detect entanglement in situations where one possesses limited information about the state. These observables violate certain bounds to indicate the existence of a bipartite or multipartite entanglement.

In what follows we briefly review the concepts and definitions needed to understand this article. We start by introducing the concept of entanglement and then introduce three entanglement witness-based measures: concurrence [67,68], tangle [69], and quantum Fisher information (QFI) [42,50]. The advantage of using these measures is that they can be measured from spin correlations and structure factors which are readily accessible by techniques like inelastic neutron scattering (INS).

A. Entanglement essentials

A bipartite mixed state ρ is said to be separable if it can be expressed as

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B \quad (3)$$

and entangled otherwise. When A and B comprise a single element, we use the term 2-partite for clarity. For example, A and B could correspond to $S = 1/2$ particles on a lattice site. The product state,

$$\rho = \rho^A \otimes \rho^B, \quad (4)$$

is a special case of the separable state.

The classification of multipartite states is slightly more subtle, since there are many inequivalent ways to partition

the system [42,78]. Let us begin by imagining a pure state comprised of N particles which we partition into M blocks. Now, if all the blocks are of size at most k , then the state is termed k -producible, i.e.,

$$|\psi_{k\text{-prod}}\rangle = \otimes_{l=1}^M |\psi_l\rangle \quad \text{such that} \quad N_l \leq k \quad \forall l, \quad (5)$$

where it is understood that

$$\sum_l N_l = N. \quad (6)$$

A state is k -partite entangled if it is k -producible but not $(k-1)$ -producible, which translates to

$$|\psi_{k\text{-ent}}\rangle = \otimes_{l=1}^M |\psi_l\rangle \quad \text{such that} \quad N_l = k \text{ for some } l, \quad (7)$$

i.e., there exists a nonfactorizable state $|\psi_l\rangle$ with exactly $N_l = k$ particles. A mixed state $\rho_{k\text{-prod}}$ is said to be k -producible if it can be written as a convex mixture of k -producible pure states,

$$\rho_{k\text{-prod}} = \sum_r p_r |\psi_{k\text{-prod}}^r\rangle \langle \psi_{k\text{-prod}}^r| \quad (k_l \leq k \quad \forall k), \quad (8)$$

where

$$p_r > 0 \quad \text{and} \quad \sum_r p_r = 1. \quad (9)$$

Having introduced the necessary terminology, we are in a good position to introduce the entanglement measures. We focus our investigation towards those suited for $S = 1/2$ particles. There do exist generalizations of the measures discussed for arbitrary spin quanta, but we do not discuss them here. An exception is the QFI that we discuss in Sec. II D.

B. Concurrence

Concurrence quantifies the pairwise entanglement between two $S = 1/2$ particles by quantifying the “entanglement of formation” [79], required to construct a given state. This could be in a system of only two or many $S = 1/2$ particles. For a mixed state ρ_{ij} shared between them where i and j are the indices pointing to the particles in question, it was shown [67,68] to have the following relationship:

$$C_{ij} \equiv C(\rho_{ij}) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}. \quad (10)$$

Here, λ 's correspond to the square root of the eigenvalues of a non-Hermitian matrix

$$\rho_{ij} \tilde{\rho}_{ij} |v_\lambda\rangle = \lambda^2 |v_\lambda\rangle, \quad (11)$$

arranged in descending order, with

$$\tilde{\rho}_{ij} = (\sigma^y \otimes \sigma^y) \rho_{ij}^* (\sigma^y \otimes \sigma^y) \quad (12)$$

being a spin-flipped state and $*$ denoting the complex conjugation operation performed in the computational basis.

Following this definition, concurrence ranges from 0 corresponding to a separable state to 1, a maximally entangled Bell state. It quantifies the degree of 2-partite entanglement regardless of whether the state is pure or mixed. Thus, it remains a good measure of entanglement even at finite temperature. The practical advantage of using concurrence is that it is related to spin correlations [80,81] and is thus a very useful tool to access the 2-partite entanglement in the system. For instance,

a SU(2) symmetric system, a $S = 1/2$ spin chain Eq. (38), for example, is given by [81]

$$C_{ij} = 2 \max \left\{ 0, 2|g_{ij}^{zz}| - \left| \frac{1}{4} + g_{ij}^{zz} \right| \right\}, \quad (13)$$

where

$$g_{ij}^{zz} = \langle S_i^z S_j^z \rangle. \quad (14)$$

In a system with more than two particles, one should note that vanishing concurrence does not imply absence of higher partite entanglement. Often, one also uses the *two-tangle* [69,82,83],

$$\tau_{2,i} = \sum_{j \neq i} C_{ij}^2, \quad (15)$$

as a measure of pairwise entanglement, which characterizes all possible pairwise entanglements within a many-partite system.

As a parting comment, we note that in the case where a pair of spins exist in a pure state, the definition of concurrence reduces to a simpler form [67]. However when considering states with multipartite entanglement, it is necessary to use the more general definition, Eq. (10), since the reduced density matrix for a pair of spins will not, in general, be a pure state. This point is addressed in greater detail in Appendix.

C. Residual tangle

Residual tangle (RT) [61,69,83] is a measure that accesses entanglement beyond the pairwise setting, in other words, a multipartite measure. It is defined as the difference between one-tangle and the sum of pairwise entanglement measured via the two-tangle,

$$\tau_{3,i} = \tau_{1,i} - \tau_{2,i}, \quad (16)$$

where

$$\tau_{1,i} = 1 - 4 \sum_{\alpha=\{x,y,z\}} \langle S_i^\alpha \rangle^2 \quad (17)$$

is the one-tangle [61,69,83].

Strictly, $\tau_{3,i}$ is only well defined for pure states [61]. Consequently, the interpretation of RT as an entanglement measure becomes inapplicable at finite temperatures. Moreover, although a nonzero RT suggests the presence of multipartite entanglement, a zero RT does not necessarily indicate its absence.

D. Quantum Fisher information

The measures discussed previously are very useful; however, they come with the limitations of being unable to access multipartite entanglement or become invalid as measures at finite temperatures. A measure that does take care of both these issues is the quantum Fisher information (QFI). For a mixed state described using the spectral decomposition

$$\rho = \sum_k p_k |k\rangle \langle k|, \quad (18)$$

such that $p_k > 0$ and $\sum_k p_k = 1$, the QFI is specified, with respect to some operator $\hat{O}$, as

$$F_Q[\rho, \hat{O}] = 2 \sum_{k,k'} \frac{(p_k - p_{k'})^2}{p_k + p_{k'}} | \langle k | \hat{O} | k' \rangle |^2, \quad (19)$$

which for pure states simplifies to

$$F_Q[|\psi\rangle, \hat{O}] = 4(\Delta\hat{O})^2 = 4(\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2). \quad (20)$$

Thus, for pure states it simplifies to the variance of $\hat{O}$ up to proportionality. At finite temperature, for a system in thermodynamic equilibrium, the probability p_k Eq. (18) corresponds to the occupation probability as ascribed by the canonical ensemble

$$p_k = \exp(-E_k\beta)/Z, \quad (21)$$

where Z corresponds to the partition function and β is the inverse temperature. For this case, the QFI density,

$$f_Q = F_Q/N, \quad (22)$$

can be accessed,

$$f_Q(\beta) = \frac{4}{\pi} \int_0^\infty d\omega \tanh\left(\frac{\omega\beta}{2}\right) \chi''(\beta, \omega), \quad (23)$$

from $\chi''(\beta, \omega)$, the imaginary, dissipative part of dynamic susceptibility [50], $\chi(\beta, \omega)$, defined as

$$\chi(\beta, \omega) = \frac{i}{N} \int_0^\infty dt e^{i\omega t} \text{tr}(\rho[\hat{O}(t), \hat{O}]), \quad (24)$$

with β being the inverse temperature.

The connection between QFI and multipartite entanglement holds [42] for local operators $\hat{O}$ with a bounded spectrum. For instance, consider a scenario where $\hat{O}$ is composed of a sum of one-body operators $\hat{o}_j$,

$$\hat{O} = \sum_{j=1}^N \hat{o}_j, \quad (25)$$

with an associated spectral width

$$\Delta_o = o_{\max} - o_{\min}, \quad (26)$$

where $o_{\min}$ and $o_{\max}$ correspond to minimum and maximum eigenvalues of $\hat{o}$. Then the operator, $\hat{O}$ is said to have a bounded spectrum if the spectral width Δ_o is finite. For such operators, the QFI is bounded from above for k -producible states,

$$F_Q[\rho_{k\text{-prod}}, \hat{O}] \leq \left\{ \left\lfloor \frac{N}{k} \right\rfloor k^2 + \left(N - \left\lfloor \frac{N}{k} \right\rfloor k \right)^2 \right\} \Delta_o^2. \quad (27)$$

In the special case when k is a divisor of N , this condition simplifies to

$$f_Q \leq k \Delta_o^2. \quad (28)$$

An assumption is made in situations when N is very large, i.e., in the thermodynamic limit then every k is treated as a divisor of N . Thus, in the event the QFI density violates the bound above, we can say that underlying state has at least $(k+1)$ -partite entanglement, i.e., has a minimum entanglement depth of $(k+1)$:

$$f_Q > k \Delta_o^2 \Rightarrow \rho \text{ is at least } (k+1)\text{-partite entangled.} \quad (29)$$

In preparation for what is coming, we will work the following operator:

$$\hat{O}(q) = \sum_r e^{iqr} \hat{S}^z(r), \quad (30)$$

where r is a discrete lattice site index and q is the discrete momentum. By using the fluctuation-dissipation theorem (FDT), the dissipative part of the dynamical susceptibility χ'' can be related to the dynamic structure factor $S^{zz}(q, \omega)$ [84],

$$\chi''(q, \beta, \omega) = \pi(1 - e^{-\beta\omega}) S^{zz}(q, \omega, \beta), \quad (31)$$

a quantity accessible in INS.

For temperatures below some threshold value $T < T_Q$, it was shown [85] that the equal-time structure factor, using its connection to the QFI, can also be used as multipartite entanglement witness,

$$4S^{zz}(q, \beta) > k \Rightarrow \rho \text{ is at least } k\text{-partite entangled,} \quad (32)$$

where $S^{zz}(q, \beta)$ is the equal-time structure factor

$$S^{zz}(q, \beta) = \int_{-\infty}^{\infty} d\omega S^{zz}(q, \omega, \beta). \quad (33)$$

Note that at zero temperature, for a pure state, the equal-time structure factor is proportional to the QFI density,

$$f_Q(q) = 4S^{zz}(q). \quad (34)$$

III. NOTATION

With many averages and sums being taken, we would like to bear out the notation here for ease of reading the plots. To evaluate the disorder average over M random realizations within an ensemble we consider

$$\bar{\Gamma} = \frac{1}{M} \sum_{m=0}^{M-1} \Gamma^{(m)}, \quad (35)$$

where Γ can correspond to some observable

$$\Gamma^{(m)} \equiv \langle \Gamma \rangle_m, \quad (36)$$

or an entanglement measure discussed in Sec. II. For measures with explicit site dependence, we also perform an average over sites,

$$\bar{\Gamma}_n = \frac{1}{MN} \sum_{i=0}^{N-1} \sum_{m=0}^{M-1} \Gamma_{ii+n}^{(m)}, \quad (37)$$

representing the disorder-averaged observable for the n th neighbor of the N -site spin chain. For example, Γ_{ij} can be thought to depict the two-point spin correlation or the pairwise concurrence.

IV. OVERVIEW OF HEISENBERG SPIN CHAINS

In this section we will briefly summarize the necessary background pertaining to the Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phase in $d = 1$. In this article, by TLL we refer to the long-length-scale theory of the Heisenberg (i.e., XXX) spin chain characterized by the Luttinger parameter, $K = 1/2$ [86]. On the other hand, we interpret the

strong disorder renormalization group (SDRG) [65] as the long-length-scale theory of the RS phase.

We consider the Heisenberg Hamiltonian with antiferromagnetic (AF) interactions,

$$H = \sum_{i=0}^{N-1} J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad (38)$$

where J_i corresponds to the coupling strength between nearest neighbors, and $\mathbf{S}_i$ are the usual $S = 1/2$ vector operators at site i .

The isotropic case corresponds to the scenario when all the couplings are equal, i.e.,

$$J_i = J (> 0) \quad \forall i. \quad (39)$$

In this case, the model realizes a $SU(2)$ symmetric ground state, whose long-wavelength behavior provides an example of a TLL phase, with correlation function [87,88]

$$\lim_{|i-j| \rightarrow \infty} g_{ij}^{zz} \sim \frac{(-1)^{|i-j|} \sqrt{\log(|i-j|)}}{2\pi^{3/2} |i-j|^{\eta_{\text{TLL}}}}, \quad (40)$$

showcasing a power-law decay with exponent

$$\eta_{\text{TLL}} = 1, \quad (41)$$

specific to $K = 1/2$. We note that the logarithmic corrections in Eq. (40) arise due to the irrelevant operators that become marginal for the isotropic Hamiltonian [87,88].

We now turn to the case where the couplings J_i in Eq. (38) are positive and randomly drawn from some probability distribution $P(J)$. In this case one realizes a RS phase whose long wavelength is well characterized by the SDRG framework [65]. Disorder-averaged correlation functions decay algebraically,

$$\lim_{|i-j| \rightarrow \infty} \bar{g}_{ij}^{zz} \sim \frac{(-1)^{|i-j|}}{|i-j|^{\eta_{\text{RS}}}}, \quad (42)$$

with exponent

$$\eta_{\text{RS}} = 2, \quad (43)$$

independent of the choice of $P(J)$. We note that logarithmic corrections to power-law decay, Eq. (42), have been reported [89]. However, their validity has been questioned in subsequent studies [90,91].

V. SETTING UP THE PROBLEM

In this section we make concrete our problem. Our goal here is to analyze what the previously introduced measures inform about the nature of entanglement of the TLL and RS phases, respectively, and whether one can use them in a meaningful way to distinguish between the two phases. We investigate the antiferromagnetically interacting Heisenberg Hamiltonian in Eq. (38), with interactions drawn from a box distribution,

$$P(J) = \begin{cases} \frac{1}{2\Delta}, & \text{if } J \in (1 - \Delta, 1 + \Delta) \\ 0, & \text{otherwise,} \end{cases} \quad (44)$$

where Δ parametrizes the strength of disorder. For our investigations we set

$$\Delta = 1 \text{ [disordered]}, \quad \Delta = 0 \text{ [clean]}. \quad (45)$$

We make use of exact diagonalization for our analysis and use the quantum typicality method for finite-temperature investigations [72,73]. Throughout our analysis we restrict ourselves to spin chains of even length with periodic boundary conditions. For $T = 0$ investigations we focused on $M = 1001$ disorder realizations for N ranging from 16 to 30. For $T \neq 0$, we consider $M = 200$ disorder realizations for $N = 16$ and 24. For $N = 20$, we consider $M = 100$ disorder realizations. In addition, we have taken into account 100 thermal pure quantum (TPQ) state samples for all three system sizes.

VI. ZERO-TEMPERATURE RESULTS

In what follows we will discuss the entanglement structure of TLL and RS phases as characterized by concurrence, RT, and QFI at zero temperature.

A. Nearest neighbor and beyond

We start by looking at the distribution of pairwise entanglement in the two phases. In Fig. 1 we explore how the concurrence is distributed on the spin chain. For the RS phase, we calculate the disorder-averaged concurrence, i.e., we evaluate the g_{ij}^{zz} correlation function for each realization and then from it obtain the corresponding concurrence using Eq. (13). Thereafter we average over the concurrence per disorder realization as per Eq. (37). For the TLL, we evaluate the sum in Eq. (37) without the disorder average.

As evident in Fig. 1, the TLL only has nearest-neighbor pairwise entanglement [92,93], while the RS also has a finite contribution coming from further neighbors, as can be seen in Fig. 2 for chosen disorder realizations. The concurrence of the RS phase vanishes at even distance, $n = \{2, 4, 6, \dots\}$, while showing a slow decay at odd distance $n = \{1, 3, 5, \dots\}$, consistent with earlier calculations for disordered XY spin chains [74]. This echoes the patterns found in spin correlations at long distances where the decay is controlled by rare, strong singlet bonds [65,94]. Nonetheless, it would be a mistake to identify the concurrence of the RS singlet phase identically with its correlations, a point addressed in Appendix.

We note that, relative to the contribution from the nearest neighbors, the concurrence observed at longer length scales is quite small, and in fact, from the point of view of INS probes, is not observable. We explain this later in Sec. VII A.

B. TLL and RS are multipartite entangled

To further understand the entanglement structure of these phases, next we employ the multipartite measures, i.e., RT and QFI. We find that both the TLL and RS phase show a finite multipartite entanglement, as seen through the RT Fig. 3 and QFI Fig. 4.

For the TLL in Fig. 3 we observe the RT approaching

$$\bar{\tau}_3 = 0.701553, \quad (46)$$

its value in the thermodynamic limit, calculated using Bethe ansatz [93,95]. On the other hand, for the RS phase, the RT is fairly constant, evidencing the existence of multipartite entanglement. The multipartite nature of the TLL [85] and RS is also predicted by the QFI. At the $q = \pi$, we observe that the TLL is at least 6-partite entangled and that the RS

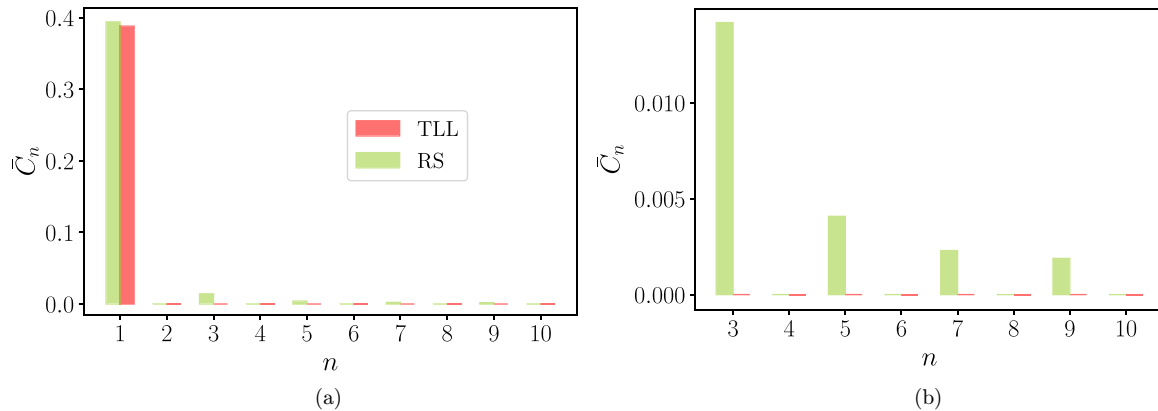


FIG. 1. Comparison of distribution of concurrence as a function of separation of spins within the Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phases. (a) Distribution of concurrence C_{ij} on n th neighbor bonds, for $n = 1 \dots 10$. Within the TLL (orange bars), concurrence vanishes identically for all bonds with $n > 1$. In contrast, within the RS phase (green bars), concurrence takes on a finite value for all odd values of n . (b) Detail of C_{ij} for $n > 2$, showing slow decay of concurrence within the RS phase. All results shown are taken from exact diagonalization of an $N = 30$ spin chain, with C_{ij} defined through Eq. (13), and disorder averages calculated for $M = 1001$ instances, using Eq. (37), with $\Gamma = C_{ij}$. For ease of viewing, error bars have been suppressed.

phase is at least 4-partite entangled for the largest spin chain size ($N = 30$) we access. From Fig. 4 one can also see an increasing entanglement depth with system size both in the TLL and RS phase at the $q = \pi$ point. This growth, however, is more pronounced in the TLL as compared to the RS phase.

The implication of such a result is that if one observes a multipartite entanglement using QFI in an experiment, then one cannot simply rule out the RS phase, as one might have prematurely inferred from its schematic picture. This is not in contradiction with the SDRG method. The fixed point of the SDRG method, the infinite randomness fixed point (IRFP), is a description of dominant physics at long length scales, whereas the multipartite entanglement observed here pertains to short length scales (discussed further in Sec. VIII). The specific characteristics of this multipartite entanglement will generally depend on the disorder distribution. Nevertheless, this multipartite information is encoded within the ground state of the disordered spin chain and has consequences when trying to rule out the RS phase experimentally. Whether there are further corrections to the structure of the RS state [75] at longer length scales is something we cannot answer from the system sizes we investigate.

In the thermodynamic limit, one expects the QFI for the TLL to diverge logarithmically [96]. On the other hand, for the RS phase, a complete suppression of QFI to a constant value is expected [89,94].

As a historical footnote, we remark that the presence of multipartite entanglement in the RS state could have been anticipated from the arguments of Fisher, who envisaged random singlets forming between effective spin-1/2 objects of “finite extent” [65]. However at the time the SDRG method was introduced, ideas of entanglement had yet to permeate beyond the quantum information community.

VII. FINITE-TEMPERATURE RESULTS

Having discussed the zero-temperature entanglement structure of the two phases, we move to explore the effects

of finite temperature on this structure. For the task at hand, we employ concurrence and the equal-time structure factor as entanglement-witness-based measures. In Sec. VII A we discuss the importance of realizing what is being experimentally accessed and how it affects the way one performs the disorder average in their analysis. In particular, we highlight the importance of knowing how to perform the disorder average, keeping in mind the observables accessible in an experiment. We point out that this is especially crucial when one is trying to rule out disorder-induced phases by using certain entanglement measures, following which, in Sec. VII C we find that the low-temperature growth of an entanglement-witness-based measure turns out to be very useful to characterize these phases.

A. The order of disorder-average matters for concurrence

If one goes by our previous results for concurrence, then one expects to see beyond nearest-neighbor 2-partite entanglement in the RS phase. Does this imply that if experimentally we do not observe further nearest-neighbor concurrence we can rule out the presence of a disorder-induced phase? On the practical side, can the further nearest-neighbor entanglement even be observed in INS? Unfortunately, the answer to both these questions turns out to be negative. Typically, in experimental situations such as in INS, we access disorder-averaged spin correlations. What this means is that when characterizing entanglement from spin correlation, for example, one does not access the entanglement per disorder realization. While this distinction might feel academic, for measures like concurrence, the order of how one performs to disorder-average becomes important if one is comparing a theoretical model against the experimental predictions.

To begin with, let us look at the finite-temperature behavior of concurrence with the way we have been evaluating it as explained in Sec. VI A. In Fig. 5 we find that up to some threshold temperatures the RS phase has finite pairwise entanglement from further neighbors, whereas the TLL phase has

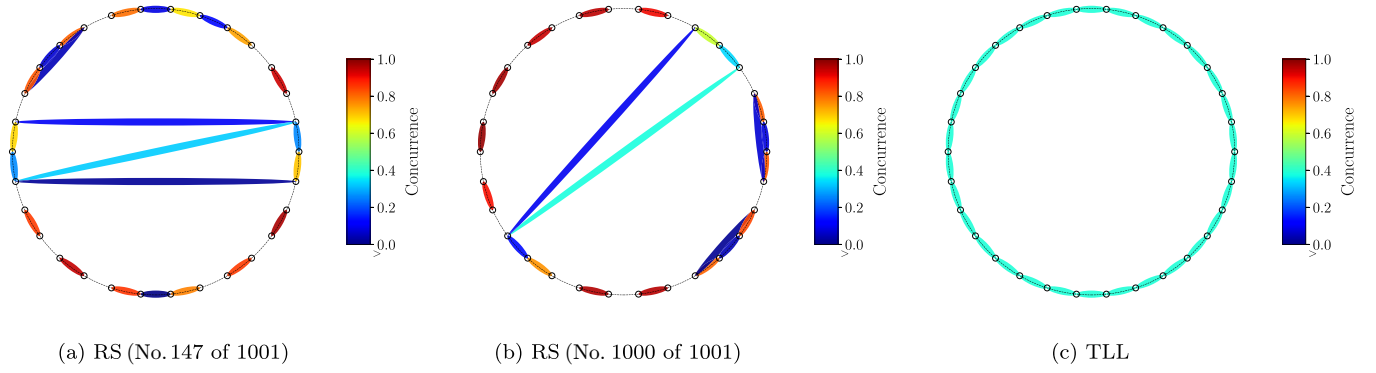


FIG. 2. Visually demonstrating the difference in the concurrence distribution between the random singlet (RS) and Tomonaga-Luttinger liquid (TLL) phase, respectively. (a) Concurrence distribution of the 147th disorder realization. (b) Concurrence distribution of the 1000th disorder realization. (c) Concurrence distribution of the TLL. While TLL only has nearest-neighbor concurrence, the RS phase has a nonzero concurrence for odd neighbors at all length scales. The plots here were obtained for a $N = 30$ spin chain.

only nearest-neighbor pairwise contribution, consistent with what we saw before.

On the other hand, we can also evaluate the disorder average of the spin correlations first and then evaluate the concurrence as below:

$$C_{ij} = 2 \max \left\{ 0, 2|\bar{g}_{ij}^{zz}| - \left| \frac{1}{4} + \bar{g}_{ij}^{zz} \right| \right\}, \quad (47)$$

where $\bar{g}_{ij}^{zz}$ is the disorder-averaged spin-correlation function evaluated as per Eq. (35). From the experimental perspective, it is this concurrence that would be accessed. In Fig. 5 we perform this and find that RS has only nearest-neighbor 2-partite entanglement just like the TLL. We do not observe any finite beyond-nearest-neighbor concurrence as one might have expected. What this means is that experimentally one would not be able to observe beyond-nearest-neighbor pairwise entanglement if they access disorder-averaged spin correlations. Thus, ruling out the RS phase by looking at the 2-tangle or concurrence and observing no beyond-nearest-neighbor 2-partite entanglement is incorrect. We also observe in Fig. 5(b) that the nearest-neighbor concurrence vanishes at the same temperature for both the TLL and RS phase.

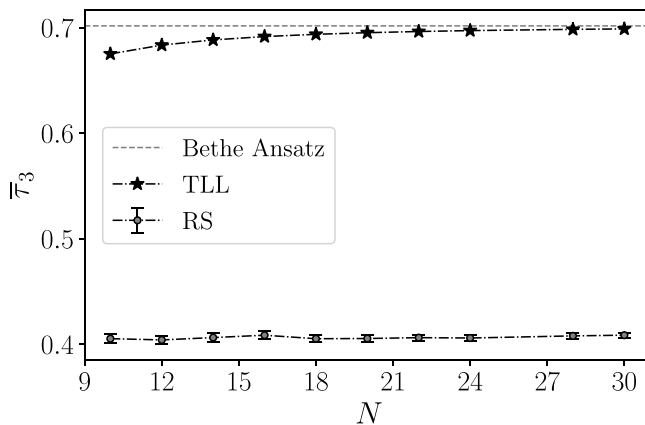


FIG. 3. Finite residual tangle (RT) indicating the existence of multipartite entanglement in the Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phase. RT of TLL is approaching close to its Bethe ansatz value as N increases. For the RS, RT remains fairly constant.

B. The low-temperature behavior of concurrence contains central charge

The low-energy behavior of TLL can be described by a conformal field theory with a central charge, $c_{\text{TLL}} = 1$ [96]. By noting that the nearest-neighbor concurrence for a TLL can be related to internal energy, one can easily obtain the central charge as follows. The key is to realize that the nearest-neighbor concurrence can be related to the internal energy as follows:

$$C_1 = \max\{0, 2|u(T)| - 0.5\}, \quad (48)$$

where

$$u(T) = u(0) + cT^2 \left(\frac{1}{3} + \frac{3 + \log(\pi/T)}{8 \log(\pi/T)^4} \right) \quad (49)$$

is the low-temperature behavior of the internal energy [97] and c is the central charge.

We put this to test in Fig. 6 and find a good agreement with the our fit:

$$u(0) \approx -0.445, \quad c_{\text{TLL}} \approx 1.01. \quad (50)$$

On the other hand, it has been shown that the RS phase is characterized by an effective central charge [75,94,98,99]:

$$c_{\text{RS}} = c_{\text{TLL}} \ln 2. \quad (51)$$

We conjecture that it is possible to access this information from the concurrence of the RS phase where we employ the disorder average that is experimentally relevant. We find the following ansatz fits very well with the observed low-temperature behavior for the RS phase:

$$u(T) = u(0) + \frac{c_{\text{eff}} T^d}{3}, \quad (52)$$

where d is a fit parameter and

$$c_{\text{eff}} = c \log(2) \quad (53)$$

is what we interpret as the effective central charge. In Fig. 6 we obtain

$$u(0) \approx -0.403, \quad c_{\text{eff}} \approx 0.71, \quad d \approx 1.39, \quad (54)$$

where the parameter $u(0)$ is size dependent, and we find c to be very close to c_{TLL} .

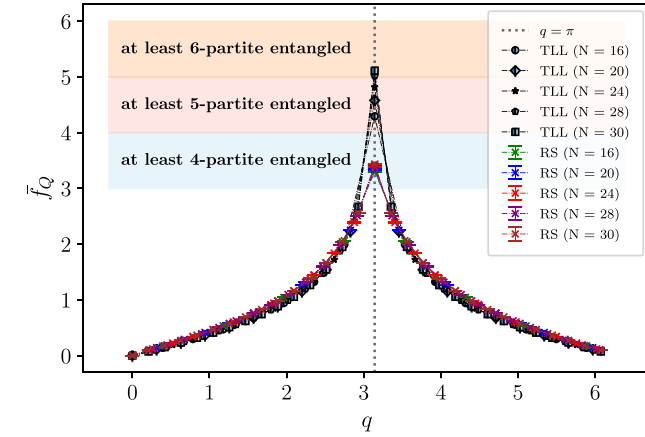
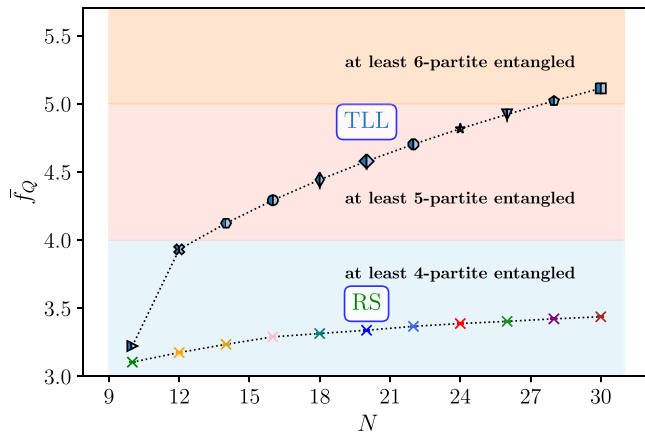
(a) QFI density vs q (b) Scaling of QFI density at $q = \pi$

FIG. 4. Observing the growth of entanglement depth at the $q = \pi$ point in Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phase. (a) Quantum Fisher Information (QFI) density for TLL and RS phase plotted as function of q for $N = 16, 20, 24, 28, 30$. (b) QFI density plotted as function of N at $q = \pi$ point for TLL and RS phase. The rate of growth of entanglement depth is suppressed in the RS phase. Here we observe the TLL phase to be at least 6-partite entangled, while the RS is at least 4-partite entangled.

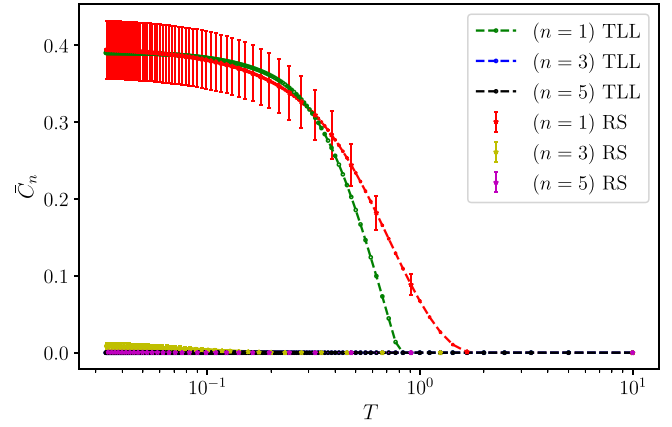
C. The low-temperature growth of multipartite entanglement is a useful probe

We saw that the zero-temperature QFI, Fig. 4, predicts both the TLL and RS phase to be multipartite entangled. Thus, stating whether a phase is m -partite or some other is l -partite is not a very useful probe if we want to distinguish them experimentally. Instead, we propose to investigate the low-temperature behavior of multipartite entanglement witness measures. We employ the equal-time structure factor for this task. As evident in Fig. 7, the growth of entanglement at low temperatures is qualitatively quite different. For the TLL, the low-temperature scaling behavior is well known [100]:

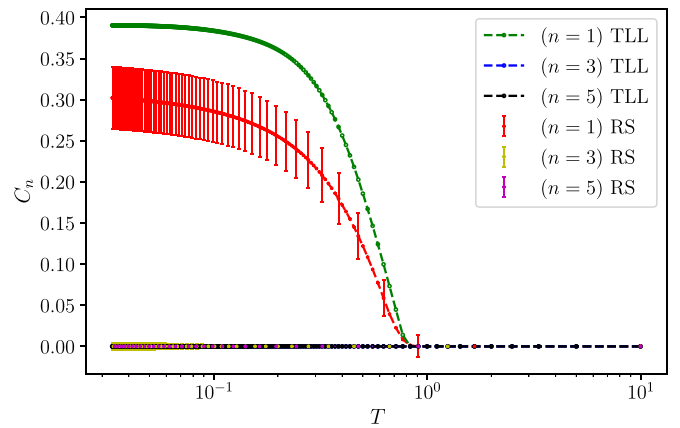
$$4S^{zz}(q = \pi, \beta) = D \log(T_0 \beta)^{3/2}. \quad (55)$$

We confirm in Fig. 7(b) that

$$D \approx 0.46, \quad T_0 \approx 10, \quad (56)$$



(a) Disorder-averaged Concurrence at finite temperature



(b) Concurrence from disorder-averaged spin correlations

FIG. 5. Demonstrating how the order of disorder average affects the concurrence distribution in the random singlet (RS) phase. (a) Disorder-averaged concurrence observed for 1st, 3rd, and 5th neighbors as a function of temperature for $N = 20$. (b) Concurrence, obtained from disorder-averaged spin correlations, observed for the 1st, 3rd, and 5th neighbors as a function of temperature. For (a), concurrence is evaluated using Eq. (13) for every disorder realization and then averaged. On the other hand, for (b), concurrence is evaluated using Eq. (47), in which case the pairwise entanglement distribution of the RS phase mimics the Tomonaga-Luttinger liquid (TLL) phase, i.e., becomes nearest neighbored. To help read the plots, some of the error bars coming from disorder averages have been suppressed.

and up to a range of temperatures, our results match very well with Eq. (55); however, at lower temperatures, we do observe finite-size effects for the different spin chain sizes we explore.

On the other hand, we find the growth of entanglement to be quite slow in our disorder-induced phase. We propose the following empirical behavior,

$$4S^{zz}(q = \pi, \beta) = a\beta^b + d, \quad (57)$$

which we found for

$$a \approx -1.5, \quad b \approx -0.6, \quad d \approx 3.1 \quad (58)$$

describes our data Fig. 7(c) very nicely. These parameter values are system-size and strength-of-disorder dependent, however.

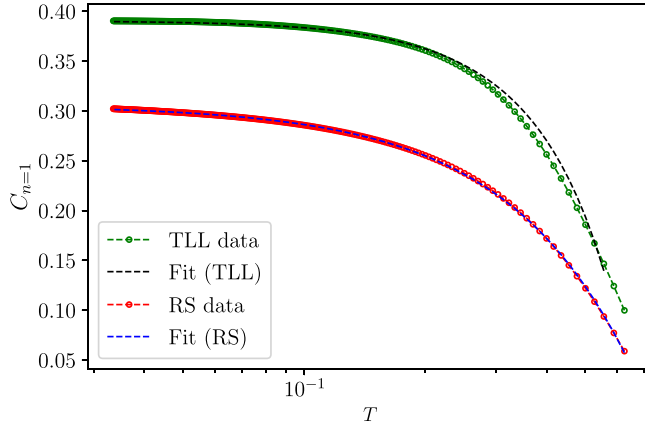


FIG. 6. Extracting central charge information from the low-temperature behavior of concurrence for the Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phase, respectively. The plots here are evaluated for the $N = 20$ spin chain. For the TLL phase, we make use of Eqs. (48) and (49) to fit the observed low-temperature behavior. For the RS phase, we make use of Eqs. (48) and (52) for the observed low-temperature behavior. Note that here we are evaluating the concurrence from disorder-averaged spin correlations [Eq. (47)], as one would access in experiments like inelastic neutron scattering (INS). For ease of viewing, the error bars have been suppressed.

VIII. DISCUSSION

A. Multipartite entanglement localization and understanding RS “phase”

Within the SDRG approach, the RS phase is pictured as a tensor product of singlets formed out of effective spins per disorder realization, Fig. 8(a) [65]. On the other hand, both RT Fig. 3 and QFI Fig. 4, point to the RS phase to be multipartite entangled. Is there an apparent contradiction here? No, there isn’t. The key here is to realize that the singlets in the SDRG picture are between effective spins [65]. The short-range physics is scaled away in the renormalization procedure, and it is this short-length-scale physics that contributes to our observation of multipartite entanglement.

The SDRG framework provides an extremely good description of the long-wavelength behavior of a disordered spin chain [99,101]. However this long-wavelength picture, in which correlations are controlled by an infinite-disorder fixed point, should be understood to come into play above a crossover length, L_c [101]. This crossover can be observed in Fig. 4(a), as the momentum

$$q_c = \pi - \frac{2\pi}{L_c} \quad (59)$$

below which the RS phase and the TLL are practically indistinguishable. What this means is that at distances shorter than L_c , spins can be entangled in clusters that contribute to the observed multipartite entanglement, as illustrated in Fig. 8(b). However, for distances $\gg L_c$, these “multipartite” clusters are completely suppressed, where now the dominant entanglement is at most 2-partite. At short length scales, the multipartite entanglement plays a role, as witnessed by the QFI density [Fig. 4(a)]. We understand this as the *localization of the multipartite entanglement*.

We can turn this observation into a bound on QFI density. If the RS phase, as understood within the SDRG, is at most 2-partite entangled, this places a limit on the entanglement contributed by long length scales. We therefore expect

$$\bar{f}_Q(q = \pi) - \bar{f}_Q(q = q_c) \leq 2. \quad (60)$$

A violation of this inequality would rule out the RS phase.

To summarize the above discussion: The RS phase contains multipartite entanglement at short length scales. This is not in contradiction with the SDRG approach, where multipartite entanglement information is absorbed within effective spin-1/2 moments, which go on to form singlets at long length scales. And as we have documented, the multipartite entanglement found in numerical simulations of disordered spin chains originates in contributions below a crossover scale, i.e., from short-range physics. In short, while multipartite entanglement is not relevant to correlations at the longest length scales, which are controlled by the SDRG fixed point, it does exist. As a consequence, the observation of finite multipartite entanglement using QFI cannot be used to rule out a RS phase.

B. Infinite disorder and thermodynamic limit

Until now we focused on a setting where we considered a box distribution as specified in Eq. (44) with $\Delta = 1.0$. How does the understanding change for some other distribution? To make this question more concrete, let us consider the following family of distributions:

$$P(J; \delta) = \begin{cases} A\delta^{-1}J^{\delta-1-1} & \text{for } 0 \leq J < J_{\max} \\ 0 & \text{otherwise,} \end{cases} \quad (61)$$

where

$$A = 1/J_{\max}^{1/\delta}. \quad (62)$$

Note that for $\delta = 1$ and $J_{\max} = 2$, we recover the boxed distribution Eq. (44). In the limit $\delta \rightarrow \infty$, one obtains the infinite randomness fixed point (IRFP) of the SDRG method. For starters, an increasing δ reduces the observed entanglement depth at the $q = \pi$ point as seen in Fig. 9. This in turn moves the crossover momentum q_c , Eq. (59), further away from π . Thus, Eq. (60) remains valid for increasing δ as well. The disorder parameter δ controls the crossover length, which consequently bounds the maximum length of the multipartite cluster l_{mc} ,

$$l_{mc} \leq L_c, \quad (63)$$

such that the role of these clusters become increasingly negligible above the crossover length. What does one expect in the thermodynamic limit? At least, for a finite δ , say below $\delta \leq \delta^* = 2.5$, from our results, we do expect to observe an entanglement depth greater than 2,

$$\lim_{\delta \rightarrow \delta^*} \lim_{N \rightarrow \infty} f_Q(q = \pi) = C_* > 2, \quad (64)$$

where C^* is some constant. For real materials, a finite δ would already imply an entanglement depth larger than 2. For instance, in [102] it was reported that $\text{Ba}_5\text{CuIr}_3\text{O}_{12}$ single crystals can characterize a RS phase with a $\delta \approx 2.5$.

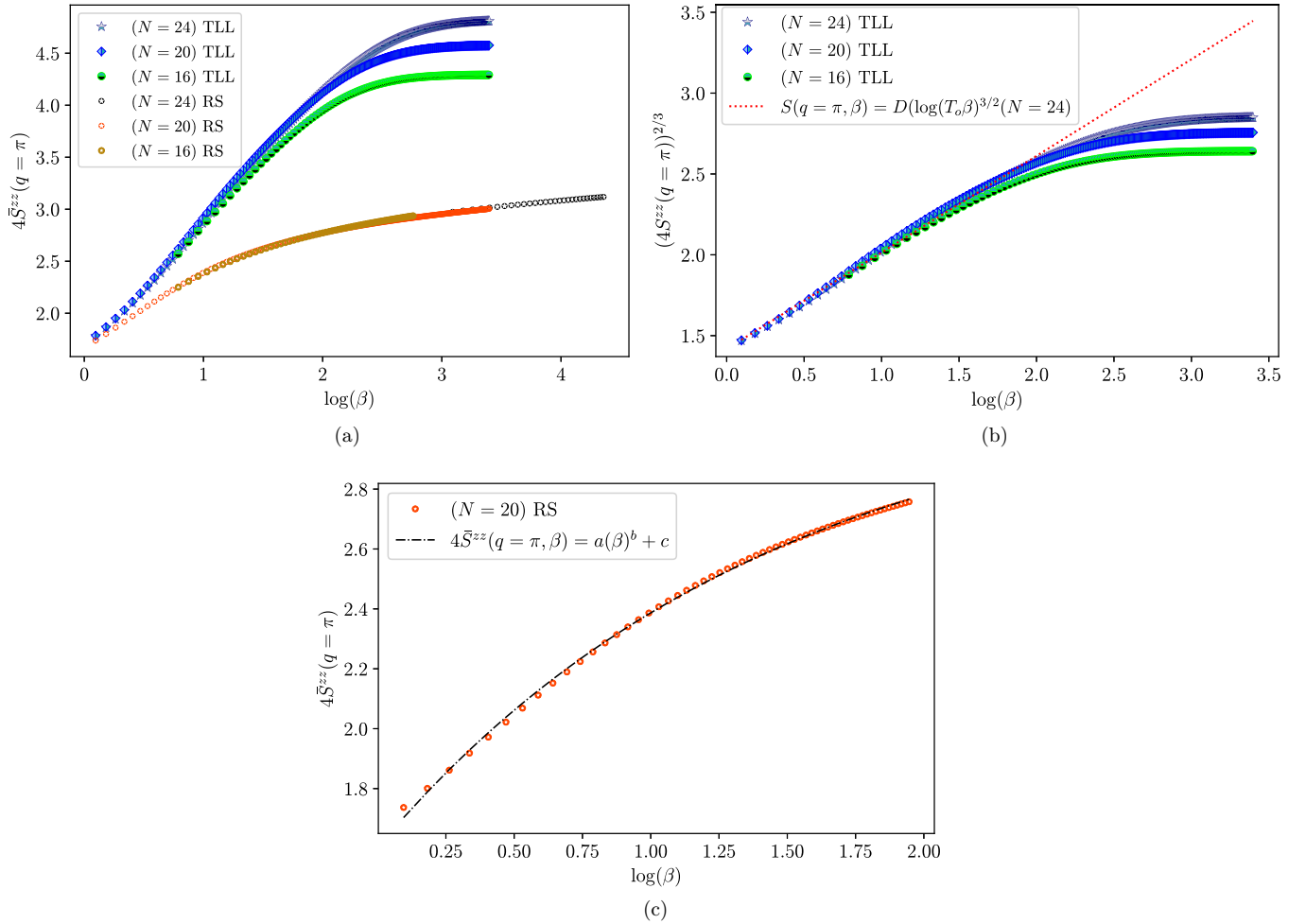


FIG. 7. Comparison of the low-temperature behavior of the equal-time structure factor for the Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phase. (a) Equal-time structure factor of both the TLL and RS phases observed as function of $\log(\beta)$ for $N = 16, 20, 24$ chains. (b) Testing the low-temperature behavior of equal-time structure factor for the TLL against the analytic prediction Eq. (55). (c) Testing the low-temperature behavior of equal-time structure factor for the RS against the ansatz Eq. (57) for the $N = 20$ spin chain. The fitting parameters are given in Eqs. (56) and (58). The fits were checked within a fixed interval $0.09 < \log(\beta) < 1.9$ for both the TLL and RS phases. This choice was made owing to the finite-size effects in the TLL phase for temperatures below the lower bound. For ease of viewing, the error bars have been suppressed.

C. Experimentally ruling out RS phase is a subtle business

The RS phase is multipartite entangled. This could have been inferred from the results in [94,103], in hindsight. While the 2-partite entanglement of this phase may indeed be the relevant entanglement setting to understand the effects of disorder, it does also have a multipartite contribution from length scales below the crossover length. Even though the multipartite nature of the phase may not be relevant to understand the effects of disorder at long length scales, these contributions do not simply disappear either. Consequently, ruling out RS phase under the assumption that it has only 2-partite entanglement is incorrect. Furthermore, we showed how one might be misled into ruling out RS phase by the absence of any concurrence beyond the nearest neighbors. One might incorrectly conclude the absence of long-range singlets from such an observation.

Convex roof measures like concurrence depend quite a lot on the way the disorder average is performed. This is due to

the presence of the “max” function in the definition Eq. (10). The operation of averaging over disorder realizations does not commute with the max operation. Whether one takes the disorder average inside the max function or outside it, the end results are completely different. Why is this important? For quenched disordered systems, the spin correlations are already disorder averaged. It follows that if concurrence is estimated from INS data using Eq. (47), the different order of average leads to profound changes in results, as can be seen by comparing Fig. 5(b) with Fig. 5(a). The former corresponds to the case when concurrence has been evaluated from disorder-averaged spin correlations, and the latter is the one where we evaluate concurrence for each disorder realization and then average it. In the former case, the RS phase shows no further neighbor concurrence, essentially mimicking the TLL phase at the 2-partite level, Fig. 2(c). In [59], the authors incorrectly ruled out the RS phase by observing vanishing concurrence and multipartite entanglement using QFI. However, both of these observations cannot rule out the RS phase as shown in

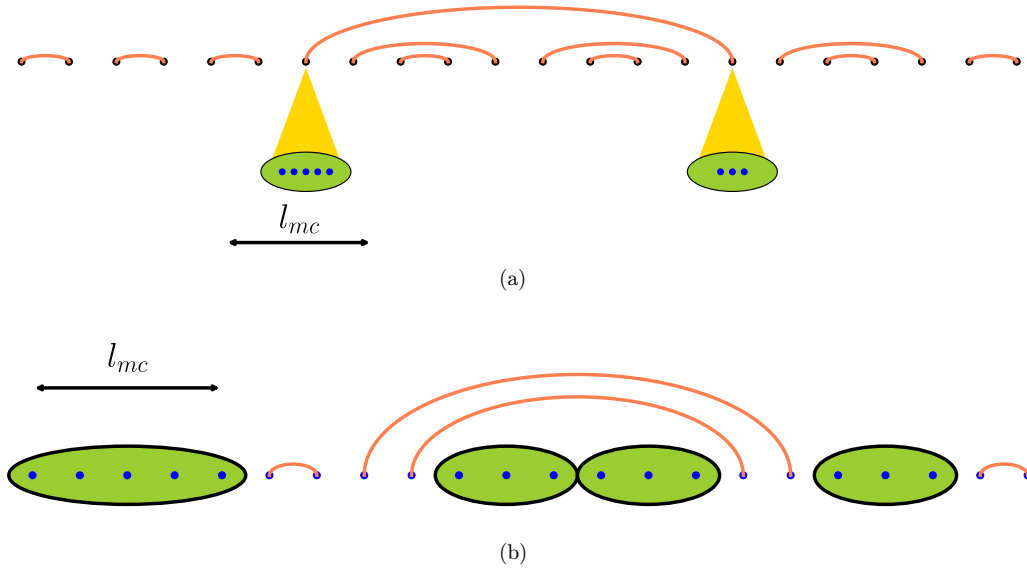


FIG. 8. An illustration of the random singlet (RS) phase. (a) The schematic picture of the RS phase, as described within the strong disorder renormalization group (SDRG), where pairs of entangled effective spins (black) are connected by orange-colored arcs. The green-shaded ovals highlight that the effective spins are made up of multiple real-space spins. (b) Schematic picture of the RS phase predicted from our results, where multiparticle clusters (mc) are represented by green-shaded ovals of size l_{mc} alongside pairwise entangled sites (blue) connected by orange-colored arcs. These mc are localized to distances below the crossover length L_c .

Secs. VIB and VII A. This point will be discussed further in a follow-up work [104].

D. What can be useful experimentally?

For 1d critical systems, the low-temperature behavior of concurrence can access central charge information. In particular, the nearest-neighbor concurrence of an $SU(2)$ symmetric phase can be related to the internal energy, and this allowed us to extract the central charge of the TLL. On the other hand, for RS phase, while the order of disorder average effects how concurrence is distributed among the sites, the universal information about the phase should still be accessible if it is contained within the 2-partite entanglement. This universal in-

formation is the effective central charge. Since experimentally the concurrence distribution for the RS phase can be nearest neighbored just as the TLL, we thought that perhaps one might be able to access the effective central charge for the RS phase. This is based on the assumption that there exists a form of generalized c-theorem for the RS phase [98]. This is what we tested in Fig. 6 and see some positive indications. However, we admit that this is conjectural at best.

On the other hand, multipartite entanglement witnesses like the QFI or the equal-time structure factor are invaluable markers for not only identifying the existence of multipartite entanglement, but also how disorder affects their growth. We saw this by the marked difference in the low-temperature behavior of the equal-time structure factor in the TLL and RS

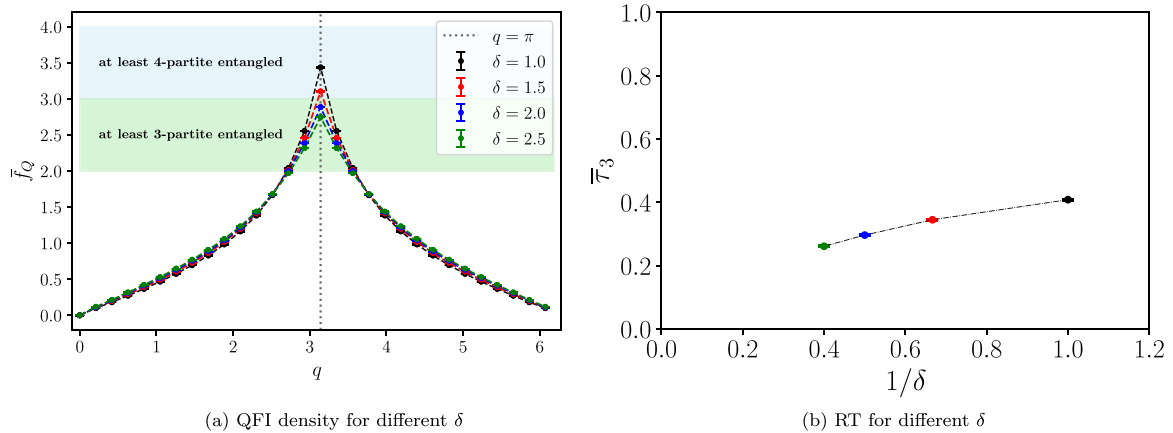


FIG. 9. Observing the decreasing entanglement depth with increasing δ in the random singlet (RS) phase. (a) Quantum Fisher information (QFI) density as function of q for $\delta = 1.0, 1.5, 2.0, 2.5$ in a $N = 30$ spin chain. (b) Residual tangle (RT) as a function of $\frac{1}{\delta}$ for $N = 30$ chain, where the line is used as a guide. While an increasing δ reduces the entanglement depth, for the $\delta = 2.5$ and $N = 30$ spin chain the QFI density at $q = \pi$ still detects a multipartite entangled RS phase.

phase. This behavior can be experimentally useful in identifying the role of disorder in spin chains.

E. Limitations to detection of multipartite entanglement

Measures like QFI, when accessed via the dynamic structure factor, can only detect multipartite entanglement if the underlying phase shows correlations peaked around specific $\mathbf{q}$ points. Due to the sum rule, this structure constraints the visibility of multipartite entanglement detection at other $\mathbf{q}$ points. However, such peaked structure factors are not universal. For instance, in Kitaev and Kagome QSLs, there are no special $\mathbf{q}$ points with sharp features [105–107]. Therefore, multipartite entanglement cannot be accessed using INS in these cases. This does not imply the absence of multipartite entanglement in these phases; rather, it suggests that the multipartite entanglement could be spread among nonlocal correlations, rendering the operator used to access this information insufficient.

IX. CONCLUSIONS

While there are no perfectly clean samples in nature, none are infinitely disordered either. In this work we set out to understand how one can experimentally access the effects of disorder on the entanglement of ground states within condensed-matter systems. We utilized the quantum spin chain as a representative example to investigate the impact of bond disorder. In this setting we focused on distinguishing between Tomonaga-Luttinger liquid (TLL) and random singlet (RS) phases through experimentally accessible entanglement measures, such as concurrence, residual-tangle (RT), and quantum fisher information (QFI).

We saw that both the TLL and RS phases are multipartite entangled. For the TLL, the observed multipartite entanglement is a consequence of the uninhibited growth of correlations. On the other hand, such correlations are completely suppressed for the RS phase. Consequently, the observation of multipartite entanglement in the RS phase is a consequence of the localization of multipartite clusters up to a crossover length scale. Beyond this length scale, our calculations of QFI find no evidence of further multipartite entanglement, and are therefore consistent with the SDRG picture. To better characterize the effect of disorder, we introduced the inequality, Eq. (60), which we found is also in agreement for the larger system sizes that were accessed in [94,103].

For quenched disorder, the order of average matters for convex roof measures. In particular, the distribution of pairwise entanglement, as characterized by concurrence, depends on how one performs the average. For the RS phase, this distribution can transform from being shared between distant sites, Fig. 5(a), to only among nearest neighbors, Fig. 5(b), as is the case in TLL. Since in INS one would access disorder-averaged correlations, it is the latter that one would observe rather than the former.

For the TLL, it is well established that it can be described by a conformal field theory. We leveraged this connection to extract the associated central charge from the low-temperature behavior of concurrence. Conversely, for the RS phase, we extracted the effective central charge from the low-temperature

behavior of concurrence by employing disorder averaging accessible in experiments. This relies on appreciating that the order of disorder averaging alters the distribution of pairwise entanglement while preserving the universal information encoded within it. However, the existence of an effective central charge for the RS phase remains conjectural, based on the assumption of a generalized c-theorem [98].

From the experimental point of view, a more robust characteristic is to examine the low-temperature behavior of multipartite entanglement witnesses like quantum Fisher information (QFI) or the equal-time structure factor. We made use of the equal-time structure factor to show a marked difference in the rate of growth of multipartite entanglement within the two phases Fig. 7(a). This scaling provides a clear distinction between the TLL and RS phases, which can be observed experimentally.

We would like to conclude by pointing out that in general some caution should be maintained especially when ruling out disorder-induced phases using measures based on witnesses. However, when used carefully, these can provide important information about quantum spin systems in the presence of disorder.

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APPENDIX: CONCURRENCE WITHIN PURE AND MIXED STATES

In this Appendix we consider two different ways of evaluating concurrence for a pair of qubits, one appropriate for a mixed state and one for pure state, with the aim of highlighting the difference between the two.

For a *mixed state* describing a pair of spins (qubits), concurrence is given by [67,68],

$$C_{ij}^{\text{mix}} \equiv C(\rho_{ij}^{\text{mix}}) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \quad (\text{A1})$$

where λ_v are the solutions of

$$\rho_{ij} \tilde{\rho}_{ij} |v_{\lambda_v}\rangle = \lambda_v^2 |v_{\lambda_v}\rangle, \quad (\text{A2})$$

arranged in descending order, with

$$\tilde{\rho}_{ij} = (\sigma^y \otimes \sigma^y) \rho_{ij}^* (\sigma^y \otimes \sigma^y), \quad (\text{A3})$$

where $*$ reflects complex conjugation in a computational basis defined in terms of eigenstates of σ^z (cf. Eqs. (10)–(12) of Sec. II).

In contrast, if the (reduced) density matrix describing the pair of spins reflects a *pure state*, then one can evaluate concurrence as [67,68]

$$C_{ij}^{\text{pure}} = |\langle \psi^* | \sigma_i^y \otimes \sigma_j^y | \psi \rangle|. \quad (\text{A4})$$

To see that these two definitions lead to different answers when applied to many-body states with finite multipartite entanglement, we consider a four-site Heisenberg spin chain with antiferromagnetic interactions ($J > 0$) under periodic boundary conditions:

$$\mathcal{H} = J(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_4 \cdot \mathbf{S}_1). \quad (\text{A5})$$

The ground state is of this model is

$$|\Psi\rangle = \frac{1}{\sqrt{3}}([12] \otimes [34] + [23] \otimes [41]), \quad (\text{A6})$$

where

$$[ij] = \frac{1}{\sqrt{2}}(|0_i 1_j\rangle - |1_i 0_j\rangle) \quad (\text{A7})$$

is a singlet shared between sites i and j .

We consider first the pair of sites 1 and 2. Tracing out the spins associated with sites 3 and 4, we find a reduced density

matrix describing a mixed state:

$$\rho_{12} = \begin{pmatrix} 1/12 & 0 & 0 & 0 \\ 0 & 5/12 & -1/3 & 0 \\ 0 & -1/3 & 5/12 & 0 \\ 0 & 0 & 0 & 1/12 \end{pmatrix}. \quad (\text{A8})$$

The direct application of the result for a mixed state, Eq. (A1), yields a concurrence

$$C_{12}^{\text{mix}} = \frac{1}{2}, \quad (\text{A9})$$

reflecting the fact that a singlet, with concurrence $C = 1$, and an unentangled state, with concurrence $C = 0$, occur with equal probability for this pair of spins in Eq. (A7).

If, instead, one were to blindly apply the result for a pure state, Eq. (A4), this would lead to an overestimate of the concurrence between the two spins:

$$C_{12}^{\text{pure}} = \frac{2}{3}. \quad (\text{A10})$$

Similarly, for the pair of sites 1 and 3, one should find

$$C_{13}^{\text{mix}} = 0, \quad (\text{A11})$$

since the wave function, Eq. (A7), does not support any Bell state between this pair of spins. In contrast, if we apply the result for a pure state, Eq. (A4), we find

$$C_{13}^{\text{pure}} = \frac{1}{3}, \quad (\text{A12})$$

falsely diagnosing entanglement between this pair of spins.

The message, as far as disordered spin chains are concerned, is very clear: random singlet phases involve states with finite multipartite entanglement (cf. Sec. VIB). For this reason, it is necessary to work the definition appropriate to a mixed state, Eq. (A1), when calculating the concurrence associated with any given pair of spins.

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