

Numerical Investigations of SO(4) Emergent Extended Symmetry in Spin-1/2 Heisenberg Antiferromagnetic Chains

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The antiferromagnetic Heisenberg chain is expected to have an extended symmetry, $[\text{SU}(2) \times \text{SU}(2)]/\mathbb{Z}_2$, in the infrared limit, whose physical interpretation is that the spin and dimer order parameters form the components of a common 4-dimensional pseudovector. Here we numerically investigate this emergent symmetry using quantum Monte Carlo simulations of a modified Heisenberg chain (the J-Q model) in which the logarithmic scaling corrections of the conventional Heisenberg chain can be avoided. We show how the two- and three-point spin and dimer correlation functions approach their forms constrained by conformal field theory as the system size increases and numerically confirm the expected effects of the extended symmetry on various correlation functions.

I. INTRODUCTION

The development of the theory of deconfined quantum criticality [1] has reignited interest in critical quantum systems which show an extended symmetry in the thermodynamic limit [2–4]. An example of the same can be seen in the spin-1/2 Heisenberg antiferromagnetic chain, where it is expected [5, 6] that the microscopic $\text{SU}(2)$ symmetry extends to an $[\text{SU}(2) \times \text{SU}(2)]/\mathbb{Z}_2$ symmetry. The ground state of this Hamiltonian is known to be critical and has been shown to have scale invariant behavior analytically [7] and numerically [8]. In this work, the emergence of the extended symmetry is connected to the behavior of two- and three-point correlation functions thus providing a bridge between the continuum field theory and lattice correlation functions.

Here we first connect the emergent symmetry to lattice correlation functions, then numerically study these and show that they reflect the emergent symmetry. The correlation functions have strict functional forms which are controlled by the 2D conformal field theory which describes the emergent physics. The emergent $[\text{SU}(2) \times \text{SU}(2)]/\mathbb{Z}_2$ symmetry is manifested in the three components of the Néel order parameter and the dimer order parameter (which quantifies the spin-Peierls order) forming an $\text{SO}(4)$ symmetric pseudovector [9]. The \mathbb{Z}_2 reduction to the $\text{SU}(2) \times \text{SU}(2)$ is required as it is a “double cover” of $\text{SO}(4)$ [10], i.e, there are two sets of $\text{SU}(2)$ matrices which generate the same $\text{SO}(4)$ rotation. The three-point functions of these order parameters can yield useful information about the emergent symmetry but must be treated with care, as a naive addition of scaling dimensions to infer the exponent of the power-law decay fails. An example of this will be presented here with the spin-spin-dimer three point function in the Heisenberg chain. We discuss how the connections between the continuum and lattice version of the correlation functions have to be carefully considered in order to predict the correct power-law decay of the three-point function.

The outline of the paper is as follows: In Sec. II we review the predictions from Renormalization Group (RG) analysis and examine how the extended symmetry affects the correlation functions of the continuum versions of the

lattice spin and dimer operators. In Sec. III, we present the manifestation of a CFT description on the correlation functions and benchmark these findings against numerical simulations of the Transverse Field Ising Model (TFIM) on a periodic chain. We stitch together the results of these two sections in Sec. IV and predict the complete functional forms for the correlation functions and then present numerical evidence to support the same. We briefly summarize the study and discuss possible future applications of numerical CFT tests in Sec. V.

II. EMERGENCE OF $[\text{SU}(2) \times \text{SU}(2)]/\mathbb{Z}_2$ SYMMETRY

The spin-1/2 Heisenberg chain, with the Hamiltonian

$$H = \sum_{i=1}^N \vec{S}_i \cdot \vec{S}_{i+1} \quad (1)$$

can be transformed into a system of interacting spinless fermions of two species using the transformation $\vec{S}_n = \frac{1}{2} \psi_n^\dagger \vec{\sigma}_i^j \psi_{nj}$ [5, 6], where ψ_n^i is a spin doublet and repeated indices imply summation over the range of values that the index can take (as we will use throughout this work). To take the continuum limit, we will reiterate the series of arguments presented in [5, 6] and will use this process to define some quantities that we will use later. Each fermion in the doublet can be rewritten as two new fermions,

$$\psi_n^j \simeq [i^n \psi_L^j(n \pm \frac{1}{2}) + (-i)^n \psi_R^j(n \pm \frac{1}{2})], \quad (2)$$

(plus and minus for even and odd n , respectively) which is an exact transformation up to an overall factor. This is motivated by the expectation that the free-fermion ground state would have all states with $|k| < \pi/2a$ occupied and thus only Fourier modes with $k \simeq \pm\pi/2a$ would be important [11]. Thus, we understand the left (L) and right (R) fermion operators to be “locally” constant and to be slowly varying at the scale of lattice separation. These will ultimately form the operators of the continuum field theory. We can now write the

spin operator on the lattice, using current operators ($\vec{J}_L = \psi_L^\dagger \vec{\sigma}_i^j \psi_{Lj}$, $\vec{J}_R = \psi_R^\dagger \vec{\sigma}_i^j \psi_{Rj}$) and a fermion bilinear ($\mathbf{G}_j^i = \psi_L^\dagger \psi_{Rj}$) as

$$\mathbb{S}_n^i = a(J_L^i + J_R^i) + (-1)^n a \text{Tr}[(\mathbf{G} - \mathbf{G}^\dagger) \sigma^i]. \quad (3)$$

Here we have used script letters for lattice operators and bold font for matrices and we will continue to maintain these conventions throughout this text. The operators $\vec{J}_L, \vec{J}_R, \mathbf{G}$ are defined at the same lattice position n as the spin operator but this is not explicitly indicated to keep the equations unencumbered. This form of the spin operator can be substituted into the Hamiltonian of Eqn (1), which upon coarse graining has the following continuum limit,

$$H = (a/2) \int dx [\vec{J}_L \cdot \vec{J}_L + \vec{J}_R \cdot \vec{J}_R + 2\vec{J}_L \cdot \vec{J}_R] + \dots, \quad (4)$$

where a is the lattice spacing[5].

Note also that at this stage we have only one SU(2) symmetry which comes along with the 3D rotation symmetry that the microscopic model has. This is manifest in each of $\vec{J}_{L/R}$ but they are not free to turn through different arbitrary angles due to the $\vec{J}_L \cdot \vec{J}_R$ term which keeps the relative angle between them fixed. Assuming that this Hamiltonian flows to the free fermion fixed point, which has the Hamiltonian

$$H_{fixed} = \int dx [\vec{J}_L \cdot \vec{J}_L + \vec{J}_R \cdot \vec{J}_R], \quad (5)$$

it can be shown that the term that couples left and right currents is irrelevant under RG flow [5, 6] for this particular fixed point. This is not true for all perturbations to the fixed point Hamiltonian and thus was checked explicitly [5, 6] for the $\vec{J}_L \cdot \vec{J}_R$ term. Thus we see that this line of reasoning leads us to believe that in the thermodynamic limit we should be left with the free fermion fixed point, which is also described by the $k = 1$ Wess-Zumino-Witten (WZW) conformal field theory [12].

To understand how this decoupling of the currents affects correlation functions of spin and dimer operators, we must first connect the primary operators of the CFT to these order parameters. Once we have done this, we can use the constraints that the extended symmetry places on the correlation functions of the primary operators to understand the correlations of the measurable orders.

The primary operators of the $k = 1$ WZW theory that we are going to be interested in are $[\mathbf{J}_L, \mathbf{J}_R, \mathbf{g}]$, which are the left and right currents and the primary field with scaling dimension 1/2. These are all SU(2) matrices, although the currents form matrices which belong to the Hermitian subset of SU(2), which are described by SO(3) vectors. This can be seen by observing that $\vec{J}_{L/R}$ in the fixed point Hamiltonian [Eq. (5)] are SO(3) vectors and thus the matrices to represent these must be written as

$$\mathbf{J}_{L/R} = J_{L/R}^a \sigma^a, \quad (6)$$

where $J_{L/R}^a$ form the components of $\vec{J}_{L/R}$. This structure is also justified by the framework of the 2D CFT, which requires independent generators of translations for z and \bar{z} (conjugate variables in the complex plane). In the Virasoro algebra of the 2D CFT [13], these would usually be called $J(z)$ and $\bar{J}(\bar{z})$ and in the case of the left(right) fermion, $z = x + it$ ($\bar{z} = x - it$) would encode its space-time position.

The primary field \mathbf{g} is made out of the continuum versions of the lattice operators which we shall denote as (S^a, D) . The components S^a form the continuum spin operators and D represents the continuum dimer operator. These together form an SO(4) pseudovector which is embedded in \mathbf{g} through

$$\mathbf{g} = S^a i\sigma^a + DI, \quad (7)$$

as any general SU(2) matrix can be expanded in this manner. The continuum versions of spin and dimer will be mapped back to the lattice variables in the next section.

As mentioned earlier, the left and right currents can turn through different arbitrary angles at the fixed point and these SO(3) rotations can be written in terms of transformations on the SU(2) matrices as

$$\mathbf{J}_L = J_L^a \sigma^a \rightarrow \mathbf{L} \mathbf{J}_L \mathbf{L}^\dagger = J_L^a \sigma^a, \quad (8)$$

$$\mathbf{J}_R = J_R^a \sigma^a \rightarrow \mathbf{R} \mathbf{J}_R \mathbf{R}^\dagger = J_R^a \sigma^a, \quad (9)$$

where L and R are the SU(2) rotation matrices. It is important to note here that these rotations do not mix left and right currents and keep the 2D conformal structure intact. The field \mathbf{g} depends on z and \bar{z} by construction[13] and thus is affected by both left and right rotations. These rotations are reflected in (S^a, D) through

$$\mathbf{g} = S^a i\sigma^a + DI \rightarrow \mathbf{L} \mathbf{g} \mathbf{R}^\dagger = S'^a i\sigma^a + D' I, \quad (10)$$

which creates the new set (S'^a, D') . The matrices $(\mathbf{g}, \mathbf{J}_L, \mathbf{J}_R)$ live on the complex plane formed by space-time and so do their components. The correlation functions of these components (which are the continuum spin, dimer, and current operators) on the complex plane are of interest to us as they tell us what to expect for the correlation functions of the lattice operators, which we will investigate numerically later. We would also like to point out here that all the correlation functions that we consider in this text are connected correlation functions as they are the ones which the CFT predicts. From this point on, we will not explicitly mention that we are only considering connected correlation functions. For the continuum operators, the connected correlation functions we consider are the same as the naive correlation functions as all the operators have a zero single body expectation (enforced by the CFT) value and this implies nothing needs to be subtracted from the naive correlation function to get the connected one.

To extract the correlation functions of (S^a, D) , we look at

$$\langle \text{Tr}[\mathbf{g}_{z_1} \mathbf{g}_{z_2}^\dagger] \rangle = \langle S^a S^a \rangle + \langle DD \rangle \quad (11)$$

and see that the right hand side is non-zero as the arbitrary transformations \mathbf{L} and \mathbf{R} leave the two point function of \mathbf{g} , as defined here, unchanged through Eq. (10) due to the cyclicity of the trace and as $\mathbf{R}^\dagger \mathbf{R} = \mathbf{L}^\dagger \mathbf{L} = I$. Similarly, if we look at the transformation of the three point function,

$$\begin{aligned} \langle \text{Tr}[\mathbf{g}_{z_1} \mathbf{g}_{z_2}^\dagger \mathbf{g}_{z_3}] \rangle \rightarrow \\ \langle \text{Tr}[\mathbf{L} \mathbf{g}_{z_1} \mathbf{R}^\dagger \mathbf{R} \mathbf{g}_{z_2}^\dagger \mathbf{L}^\dagger \mathbf{L} \mathbf{g}_{z_3} \mathbf{R}^\dagger] \rangle, \end{aligned} \quad (12)$$

we see that the only way to keep this invariant under arbitrary \mathbf{L} and \mathbf{R} would be to have this vanish. The vanishing of the three point function then implies that all three point functions of (S^a, D) (which could be either of $\langle S^a S^a D \rangle$, $\langle S^a D S^a \rangle$, $\langle D S^a S^a \rangle$, $\langle D D D \rangle$) would vanish. This can be seen by writing down all the possible three point functions of \mathbf{g} and \mathbf{g}^\dagger and solving for the spin and dimer correlation functions.

When discussing the lattice spin and dimer correlation functions, we will also need the continuum versions of the correlation functions of the currents and operators. The expressions which are of interest to us and robust against arbitrary \mathbf{L} and \mathbf{R} transformations are

$$\langle \text{Tr}[\mathbf{J}_L \mathbf{J}_L] \rangle \sim \langle J_L^a J_L^a \rangle, \quad (13)$$

$$\langle \text{Tr}[\mathbf{J}_L \mathbf{g} \mathbf{g}^\dagger] \rangle \sim \langle J_L^a S^a D \rangle + \langle J_L^a D S^a \rangle, \quad (14)$$

and permutations of the second equation with \mathbf{J}_L in different positions. These equations also apply for the right currents by just switching all $L \rightarrow R$. The non-vanishing nature of these correlation functions can be seen again using the cyclicity of the trace and transformation equations (8), (9) and (10).

III. CFT AND CORRELATION FUNCTIONS

Due to the mapping to massless fermions, the spin-1/2 Heisenberg chain is a 2D CFT and we can use the constraints the 2D CFT puts on the correlation functions to understand their precise forms. A 2D CFT is defined on the complex plane and the constraints that conformal symmetry requires restricts the two point and three point correlation functions of primary operators to behave as [13]

$$\langle O_i O_j \rangle \sim \frac{\delta_{ij}}{|z|^{2\Delta_{ij}}}, \quad (15)$$

$$\langle O_i O_j O_k \rangle \sim \frac{1}{|z_{ij}|^{\Delta_{ij}} |z_{jk}|^{\Delta_{jk}} |z_{ki}|^{\Delta_{ki}}}, \quad (16)$$

where O_i are the primary operators of the CFT and Λ_i are their scaling dimensions and $\Delta_{ij} = \Lambda_i + \Lambda_j - \Lambda_k$. The scaling dimension of a primary operator is made up of two numbers h_i and \bar{h}_i which indicate the scaling in z and \bar{z} respectively. These correlation functions can be factorised into two pieces, where one depends on z , and the other on \bar{z} and the Λ_i 's are replaced by $h_i(\bar{h}_i)$. This is useful when $h_i \neq \bar{h}_i$, which may be the case for current operators, which generate translations in either z or \bar{z} . For operators with $h_i = \bar{h}_i$, we do not mention each of them separately, but only indicate the total scaling dimension $\Lambda_i = h_i + \bar{h}_i$.

As these relations are valid on the infinite complex plane and our simulations are done on a periodic chain, we must use a mapping from the cylinder to the infinite plane to understand the correlation functions. In our simulations, we use ground state projector quantum Monte Carlo (QMC) simulations, which means that we project on a trial state with a large number of Hamiltonians, effectively for a long imaginary time. This implies that we are using a cylinder whose circumference is system size and length is infinite for all practical purposes. The system can then be mapped to the infinite plane through the transformations $\tau \rightarrow r$ and $x \rightarrow \theta$ [14] which results in two spatially separated points on the periodic chain having a conformal distance between them of

$$|z_{ij}| = L \sin\left(\pi \frac{x}{L}\right), \quad (17)$$

where x is the separation on the ring. This substitution into the correlation functions on the plane tells us what we should expect on the cylinder. In some cases, the correlation function on the plane may have different dependence on z and \bar{z} and may not be expressible in $|z|$, but the mapping to the cylinder correlation functions reverses this [13, 14] and they only depend on the conformal distance given by Eq.(17), which must be the case as they are real. For the case of the two point function, this has already been checked for the spin-1/2 Heisenberg chain and the TFIM chain [15].

Here we will check that the functional form of the three point function matches the CFT prediction for the TFIM as we will be using three point functions in the next section to point out features of the extended symmetry. The CFT of the TFIM is made up of three primary operators, namely the identity I , the spin σ and the ferromagnetic part of the energy density ϵ , with scaling dimensions 0, 1/8 and 1 respectively [12, 16]. With these operators, the non-vanishing three point function with the smallest scaling dimension is $\langle \epsilon \sigma \sigma \rangle$. We must also note here that the CFT only tells us the behavior of the connected three point function and due to this, we compare the CFT expectation to $\langle \epsilon \sigma \sigma \rangle_c = \langle \epsilon \sigma \sigma \rangle - \langle \epsilon \rangle \langle \sigma \sigma \rangle$. We will not carry the subscript c for connected correlation functions as they make the symbolic expressions cumbersome.

Using the conformal distance and Eq. (16), the three

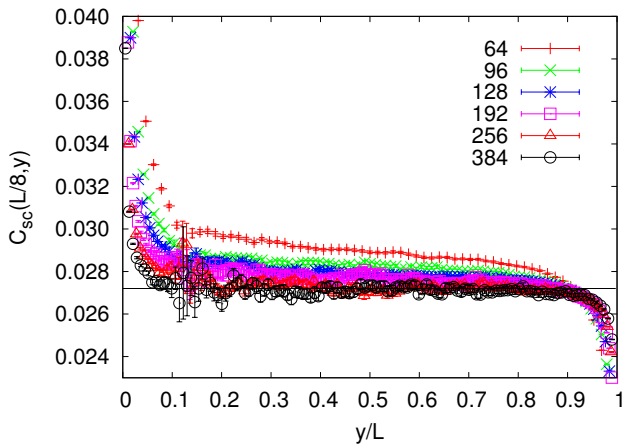


FIG. 1. Scaled three-point function for the critical periodic TFIM chain as defined in Eq. (19) flows to a constant for $x = L/8$. The constant line is a guide to the eye and the same value for the constant is used in Fig. 2.

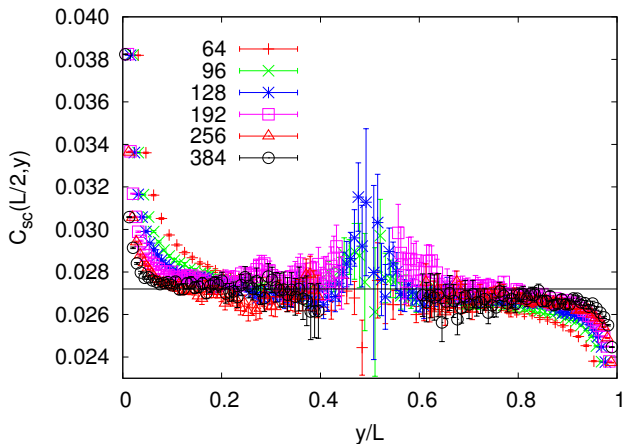


FIG. 2. Scaled three-point function for the critical TFIM chain as defined in Eq. (19) flows to a constant for $x = L/2$. We only exclude data around $y/L = 0.5$ for large sizes as the correlation function vanishes quickly as $x \sim y \sim L/2$ and this means the numerical signal is very weak.

point correlation function on the ring should be

$$\langle \epsilon_0 \sigma_x \sigma_y \rangle \sim \frac{[L \sin(\pi \frac{|y-x|}{L})]^{3/4}}{[L \sin(\pi \frac{x}{L})][L \sin(\pi \frac{y}{L})]}. \quad (18)$$

To compare numerical data to this expression, we define a scaled correlation function $C_{sc}(x, y)$ which is the raw correlation function multiplied by the inverse of the expected form as shown below:

$$C_{sc}(x, y) \sim \langle \epsilon_0 \sigma_x \sigma_y \rangle \times \frac{[L \sin(\pi \frac{x}{L})][L \sin(\pi \frac{y}{L})]}{[L \sin(\pi \frac{|y-x|}{L})]^{3/4}} \quad (19)$$

If the expression matches, we should expect the scaled correlation function to be a constant as a function of x

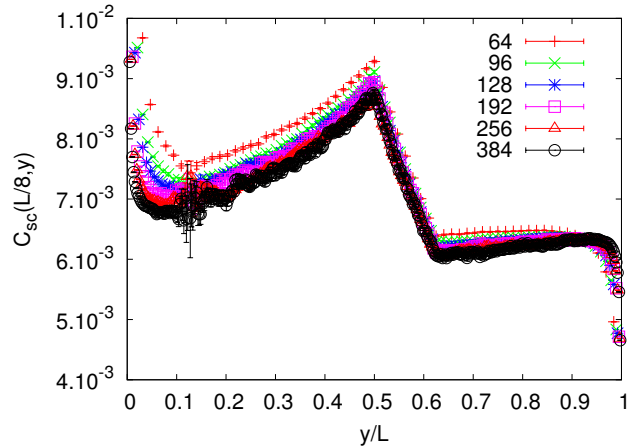


FIG. 3. Three-point function for the critical TFIM periodic chain scaled using the lattice distance rather than the conformal distance as shown in Eq. (20). We see strong disagreement with Eq. (18) for $x = L/8$.

and y . In Figs. 1 and 2, we plot the scaled correlation function for two different values of x and the whole range of y and see that for large sizes, we get a constant and the only deviations occur when two out of the three operators get close, where the coarse grained description does not hold anymore. It is important to note here that we must use the conformal distances when predicting the functional form due to the cylinder to plane conformal transformation that we have used. We can also define the scaled correlation function using just the lattice distances instead of the conformal distance as

$$C_{sc}(x, y) \sim \langle \epsilon_0 \sigma_x \sigma_y \rangle \times \frac{[s(0, x)][s(0, y)]}{[s(x, y)]^{3/4}} \quad (20)$$

where $s(a, b)$ is the shortest distance between a and b along the ring. This way of defining the scaled correlator results in a disagreement with the expected constant form for the scaled correlation function, as can be seen in Fig. 3, although the curves for different sizes still show data collapse as the correct scaling dimension is being used even in this correlator. This manner of using scaled correlation functions has already been used in previous work [15] for the two point spin correlation function and will also be used in the next section to show agreement to the predictions of Sec. II.

IV. LATTICE CORRELATION FUNCTION NUMERICS

In Sec. II, we have seen that some of the correlation functions of continuum operators vanish and for the ones that do not, we can predict their functional forms based on the CFT constraints presented in Sec. III. The primary operators of the $k = 1$ WZW model are $\mathbf{J}_L, \mathbf{J}_R$

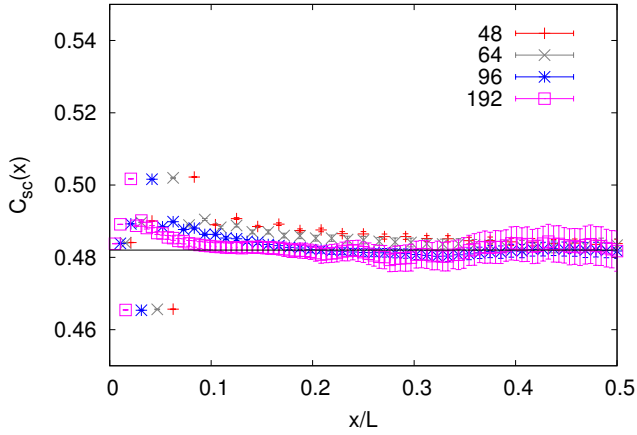


FIG. 4. Scaled dimer two-point function for the critical JQ_2 periodic chain as defined in Eq. (35) flows to a constant with increasing size. Horizontal axis only extends to 0.5 as two-point functions are symmetric about $y = L/2$.

and \mathbf{g} with scaling dimensions (h, \bar{h}) given by $(1,0), (0,1)$ and $(1/4, 1/4)$ respectively. Using these dimensions, we can infer that the correlation functions on the periodic chain must have the following forms,

$$\langle \text{Tr}[\mathbf{g}(0)\mathbf{g}^\dagger(x)] \rangle \sim \frac{1}{L \sin(\pi \frac{x}{L})}, \quad (21)$$

$$\langle \text{Tr}[\mathbf{J}_L(0)\mathbf{J}_L(x)] \rangle \sim \frac{1}{[L \sin(\pi \frac{x}{L})]^2}, \quad (22)$$

$$\langle \text{Tr}[\mathbf{J}_L(0)\mathbf{g}(x)\mathbf{g}^\dagger(y)] \rangle \sim \frac{1}{[L \sin(\pi \frac{x}{L})][L \sin(\pi \frac{y}{L})]} \quad (23)$$

and the same for $L \rightarrow R$. We can now use these expressions to understand the lattice correlation functions by writing the lattice operators in terms of their continuum versions. Inspired by the analysis leading upto Eq. (3), the spin and dimer lattice operators have been postulated [5, 9] to be

$$\mathbb{S}_n^i \sim \alpha(J_L^i + J_R^i) + (-1)^n \beta S^i, \quad (24)$$

$$\mathbb{D}_n = \vec{S}_n \cdot \vec{S}_{n+1} \sim D_0 + (-1)^n \gamma D, \quad (25)$$

where α, β, γ are UV sensitive prefactors and D_0 is a constant shift of the lattice dimer operator which must be subtracted out when calculating connected correlation functions.

Using this equivalence between the lattice and continuum operators, we can construct the lattice correlation functions that we are going to use to be

$$\langle \mathbb{D}\mathbb{D} \rangle \sim (-1)^n \langle \text{Tr}[\mathbf{g}\mathbf{g}^\dagger] \rangle + \dots, \quad (26)$$

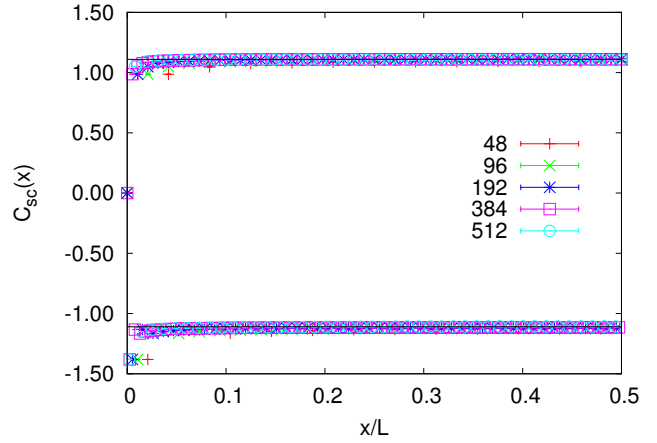


FIG. 5. Spin two-point function for the critical JQ_2 periodic chain scaled with the first term of Eq. (32) as shown in Eq. (36) and we see agreement with the expected form for large enough sizes. The two branches capture the relative sign between odd and even sites.

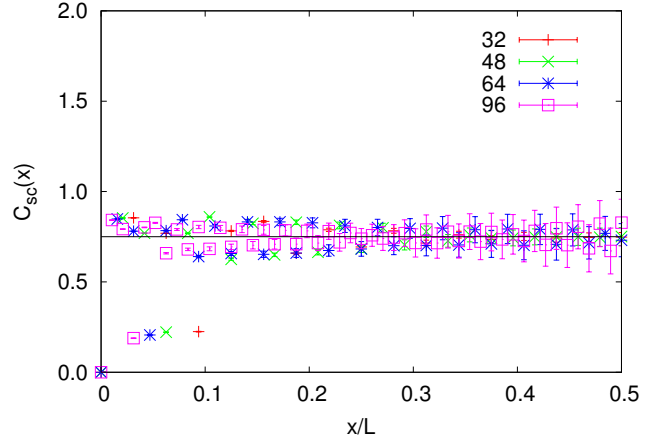


FIG. 6. Spin two-point function for the critical JQ_2 periodic chain with the first term of Eq. (32) subtracted out and scaled with the second term as shown in Eq. (37). We see agreement with the expected form.

$$\langle \mathbb{D}\mathbb{D}\mathbb{D} \rangle \sim 0 + \dots, \quad (27)$$

$$\langle \vec{S} \cdot \vec{S} \rangle \sim (-1)^n \langle \text{Tr}[\mathbf{g}\mathbf{g}^\dagger] \rangle + \langle \vec{J}_L \cdot \vec{J}_L \rangle + \langle \vec{J}_R \cdot \vec{J}_R \rangle + \dots, \quad (28)$$

$$\langle \vec{S} \cdot \vec{S}\mathbb{D} \rangle \sim \langle \text{Tr}[\mathbf{J}_L \mathbf{g}\mathbf{g}^\dagger] \rangle + \langle \text{Tr}[\mathbf{g}\mathbf{J}_L \mathbf{g}^\dagger] \rangle + (L \rightarrow R) + \dots, \quad (29)$$

where we have dropped the prefactors as they are UV-controlled parameters which are not important from the continuum perspective and to keep the equations from

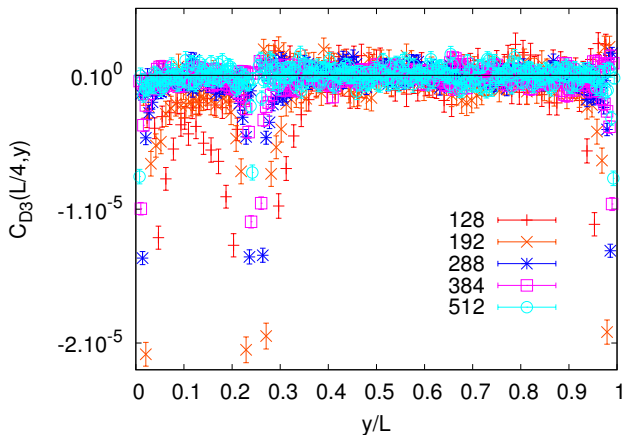


FIG. 7. Dimer three-point function for the critical JQ_2 periodic chain can be seen to vanish for large enough sizes which agrees with Eq. (30) for $x = L/4$.

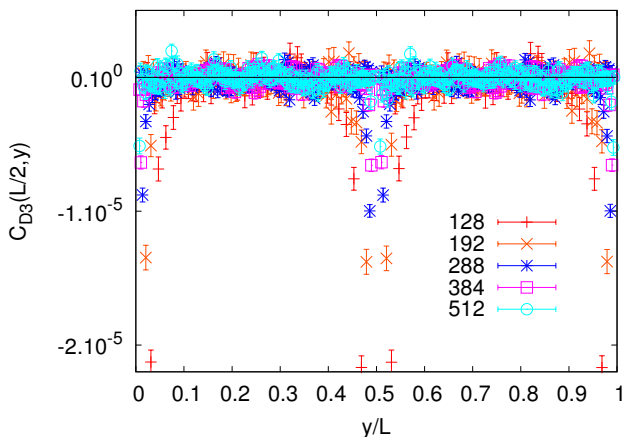


FIG. 8. Dimer three-point function for the critical JQ_2 periodic chain can be seen to vanish for large enough sizes which agrees with Eq. (30) for $x = L/2$.

becoming unnecessarily dense. The additional terms ignored in these equations are lattice corrections which occur due to finite size lattices and deviations from criticality and our simulations use sizes that are large enough to justify neglecting these terms. Now we can incorporate the results of Eqs. (21), (22) and (23) to hypothesize that the full functional forms of the connected lattice correlation functions are

$$\langle \mathbb{D}_0 \mathbb{D}_x \mathbb{D}_y \rangle \sim 0 + \dots, \quad (30)$$

$$\langle \mathbb{D}_0 \mathbb{D}_x \rangle \sim \frac{(-1)^x}{L \sin(\pi \frac{x}{L})} + \dots, \quad (31)$$

$$\langle \vec{\mathbb{S}}_0 \cdot \vec{\mathbb{S}}_x \rangle \sim \frac{(-1)^x}{L \sin(\pi \frac{x}{L})} + \frac{1}{[L \sin(\pi \frac{x}{L})]^2} + \dots, \quad (32)$$

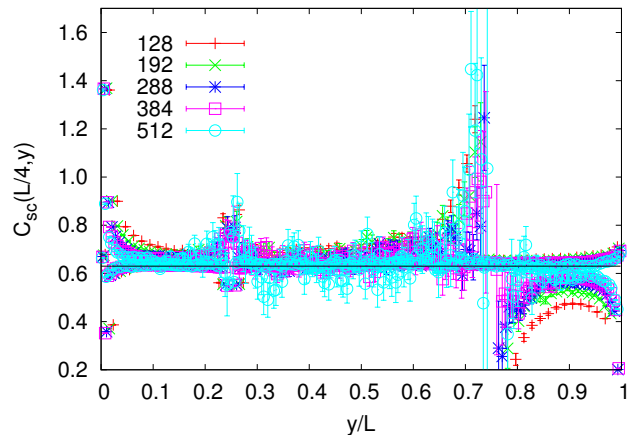


FIG. 9. Scaled dimer-spin-spin three-point function for the critical JQ_2 periodic chain as defined in Eq. (38) flows to a constant for $x = L/4$. The divergence at $y = 3L/4$ is caused due to the vanishing of the correlation function, which implies that the unscaled numerical signal is weak.

$$\langle \mathbb{D}_0 \vec{\mathbb{S}}_x \cdot \vec{\mathbb{S}}_y \rangle \sim \frac{1}{L \sin[\frac{\pi}{L}(y-x)]} \left[\frac{(-1)^x}{L \sin(\pi \frac{y}{L})} - \frac{(-1)^y}{L \sin(\pi \frac{x}{L})} \right] + \dots \quad (33)$$

The most striking effects of the extended symmetry are seen in Eqs. (30) and (33) where the vanishing of the three point function of \mathbf{g} ensures that there is no term with scaling dimension $3/2$ (three times scaling dimension of \mathbf{g}) in either of these equations. In this case, if we were to use the three point function's scaling form to infer the scaling dimensions of the operators (which imply the scaling dimensions should sum to 2), we would run into errors as we would be unable to make it consistent with the two point functions (which imply the scaling dimensions should sum to $3/2$). To see proof of this numerically, we again calculate scaled correlation functions for these expressions, except for $\langle \mathbb{D}_0 \mathbb{D}_x \mathbb{D}_y \rangle$, which is expected to be zero. If the numerics agree, we should expect to see that the scaled functions are constants with respect to x and y , as seen in Sec. III for the TFIM.

The continuum description of the Heisenberg model ground state has marginal operators which lead to log corrections to correlation functions. We shall use the JQ_2 chain which is the Heisenberg model with a four spin term that enforces dimer order when strong and tunes out the log corrections at the transition point (where the marginal operator vanishes) into the dimer phase;

$$H = -J \sum_i \mathbb{P}_{i,i+1} - Q \sum_i \mathbb{P}_{i,i+1} \mathbb{P}_{i+2,i+3} \quad (34)$$

where $\mathbb{P}_{i,j} = 1/4 - \vec{\mathbb{S}}_i \cdot \vec{\mathbb{S}}_j$. This model is an alternative to the more commonly used J_1 - J_2 (first and second neighbor interacting) Heisenberg chain [17], with the advantage that it is amenable to QMC studies without sign problems.

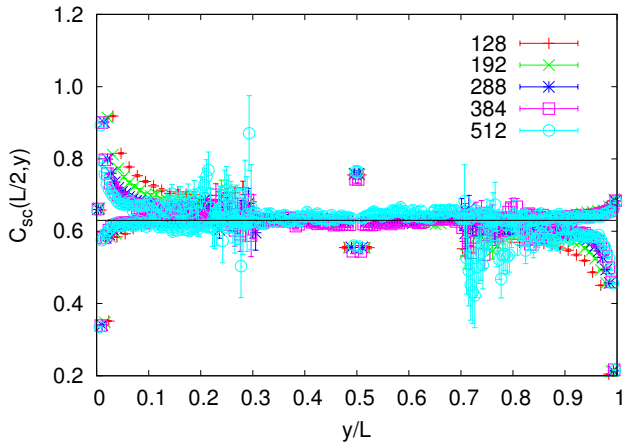


FIG. 10. Scaled dimer-spin-spin three-point function for the critical JQ_2 periodic chain as defined in Eq. (38) flows to a constant for $x = L/2$. Data for even values of y in the range $y/L \in (0.3, 0.7)$ are excluded as $\langle \mathbb{D}_0 \vec{S}_x \cdot \vec{S}_y \rangle$ tends to a 0/0 form in that range and thus the scaled correlation function is very noisy.

At a critical value of Q/J , $Q_c/J \approx 0.84831$ [18, 19], we would expect to see the correlation functions behave in the predicted forms. All our simulations of the ground state of the critical JQ_2 chain are done using a projector QMC method formulated in the valence-bond basis. The correlation functions are evaluated using loop estimators on the transition-graphs created by sampling the states in the valence-bond basis [20]. Fig. 4 illustrates the scaled correlator for $\langle \mathbb{D}_0 \mathbb{D}_x \rangle$, defined using Eq. (31) as

$$C_{sc}(x) = \langle \mathbb{D}_0 \mathbb{D}_x \rangle \times \frac{L \sin(\pi \frac{x}{L})}{(-1)^x}, \quad (35)$$

and we see that it goes to a constant for fairly small chain lengths. Fig. 5 shows the scaled version of the first term (scaling dimension of 1) of $\langle \vec{S}_0 \cdot \vec{S}_x \rangle$, again defined using Eq. (32) as

$$C_{sc}(x) = \langle \vec{S}_0 \cdot \vec{S}_x \rangle \times \left[L \sin \left(\pi \frac{x}{L} \right) \right], \quad (36)$$

which dominates the second term (scaling dimension of 2) and we see that this flows to a constant (1.11(1)) with increasing size. In Fig. 6, we subtract out the first term and present the scaled version of the second term in a scaled correlation function defined as

$$C_{sc}(x) = \left[\langle \vec{S}_0 \cdot \vec{S}_x \rangle - 1.11 \times \frac{(-1)^x}{L \sin(\pi \frac{x}{L})} \right] \times \left[L \sin \left(\pi \frac{x}{L} \right) \right], \quad (37)$$

for which we cannot go to large sizes due to insufficient data quality, and we see that it matches our expectations and flows to a constant with increasing size. In Figs. 7 and 8, we show the agreement of the three point

dimer correlation function (denoted by $C_{D3}(x, y)$ in both figures) with Eq. (30) for two different values of x and the whole range of y values. Only in the case of the three point dimer function, we present the raw correlation function without scaling as it is expected to be zero and there is no sense in which we can scale it. We show the same for Eq. (33) through Figs.9 and 10 by again defining a scaled correlator $C_{sc}(x, y)$ as

$$\langle \mathbb{D}_0 \vec{S}_x \cdot \vec{S}_y \rangle \times \left[\frac{1}{L \sin \left[\frac{\pi}{L} (y - x) \right]} \left[\frac{(-1)^x}{L \sin(\pi \frac{y}{L})} - \frac{(-1)^y}{L \sin(\pi \frac{x}{L})} \right] \right]^{-1} \quad (38)$$

and observing that it approaches a constant for large sizes. With this numerical evidence, we conclude that the signatures of the extended symmetry that we expect to see are indeed present in the spin-1/2 Heisenberg chain. Finite-size (distance) corrections can be seen clearly in our numerical data and these should be described by irrelevant operators.

V. CONCLUSION

We have shown numerical evidence of the effects of the emergent $SO(4) \equiv [SU(2) \times SU(2)]/Z_2$ symmetry in the Heisenberg chain on the correlation functions of lattice operators. This establishes the IR emergent symmetry which was theoretically expected from a variety of arguments. The three point function is discussed here as a useful tool to understand the structure of the underlying field theory and has been shown to yield useful information through not only its scaling dimension, but also its functional form, an example of which is $\langle \mathbb{D}_0 \vec{S}_x \cdot \vec{S}_y \rangle$ whose observed scaling dimension is not directly related to the leading scaling dimensions of the operators it is made out of. Here, we have also developed tests of CFT through correlation functions and these can be used to test suspected extended symmetry in higher dimensional systems [2, 3] and more broadly to test for CFT signatures in general.

In higher dimensions, an open question is what system geometry is best suited for investigating the conformal symmetry explicitly in equal-time correlation functions. In 1D, the ring geometry (infinite imaginary time, i.e., the ground state), the conformal distance naturally emerges in this case, but it does not have a direct generalization to 2D or 3D. The functional form of the correlation functions when expressed using the conformal distance in 1D provides perhaps the most striking evidence of conformal invariance in finite systems, and such a concept in higher dimensions would be very useful for lattice calculations.

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- [1] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, *Science* **303**, 1490 (2004).
- [2] A. Nahum, P. Serna, J. T. Chalker, M. Ortuno, and A. M. Somoza, *Phys. Rev. Lett.* **115**, 267203 (2015).
- [3] C. Wang, A. Nahum, M. A. Metlitski, C. Xu, and T. Senthil, *Phys. Rev. X* **7**, 031051 (2017).
- [4] Y. Q. Qin, Y.-Y. He, Y.-Z. You, Z.-Y. Lu, A. Sen, A. W. Sandvik, C. Xu, and Z. Y. Meng, *Phys. Rev. X* **7**, 031052 (2017).
- [5] I. Affleck, *Phys. Rev. Lett.* **55**, 1355 (1985).
- [6] I. Affleck and F. D. M. Haldane, *Phys. Rev. B* **36**, 5291 (1987).
- [7] T. Giamarchi and H. J. Schulz, *Phys. Rev. B* **39**, 4620 (1989).
- [8] O. A. Starykh, R. R. P. Singh, and A. W. Sandvik, *Phys. Rev. Lett.* **78**, 539 (1997).
- [9] A. M. Tsvelik, *Quantum field theory in condensed matter physics* (Cambridge university press, 2007).
- [10] R. W. Carter, I. G. MacDonald, G. B. Segal, and M. Taylor, *Lectures on Lie Groups and Lie Algebras*, London Mathematical Society Student Texts (Cambridge University Press, 1995).
- [11] F. D. M. Haldane, *Phys. Rev. Lett.* **45**, 1358 (1980).
- [12] A. A. Belavin, A. M. Polyakov, and A. B. Zamolodchikov, *Nucl. Phys. B* **241**, 333 (1984).
- [13] P. Francesco, P. Mathieu, and D. Sénéchal, Springer Science & Business Media (1997).
- [14] P. Calabrese and J. Cardy, *J. Phys. A* **42**, 504005 (2009).
- [15] P. Patil, Y. Tang, E. Katz, and A. W. Sandvik, *Phys. Rev. B* **96**, 045140 (2017).
- [16] V. G. Knizhnik and A. B. Zamolodchikov, *Nucl. Phys. B* **247**, 83 (1984).
- [17] S. Eggert, *Phys. Rev. B* **54**, R9612 (1996).
- [18] Y. Tang and A. W. Sandvik, *Phys. Rev. Lett.* **107**, 157201 (2011).
- [19] S. Sanyal, A. Banerjee, and K. Damle, *Phys. Rev. B* **84**, 235129 (2011).
- [20] K. S. D. Beach and A. W. Sandvik, *Nucl. Phys. B* **750**, 142 (2006).