Detecting emergent continuous symmetries at quantum criticality

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New or enlarged symmetries can emerge at the low-energy spectrum of a Hamiltonian that does not possess the symmetries, if the symmetry breaking terms in the Hamiltonian are irrelevant under the renormalization group flow. In this letter, we propose a tensor network based algorithm to numerically extract lattice operator approximation of the emergent conserved currents from the ground state of any quantum spin chains, without the necessity to have prior knowledge about its low-energy effective field theory. Our results for the spin-1/2 J-Q Heisenberg chain and a one-dimensional version of the deconfined quantum critical points (DQCP) demonstrate the power of our method to obtain the emergent lattice Kac-Moody generators. It can also be viewed as a way to find the local integrals of motion of an integrable model and the local parent Hamiltonian of a critical gapless ground state.

Introduction.—Low-energy physics can show different symmetries from the Hamiltonian. In the thermodynamic limit, the continuous symmetry of a Hamiltonian can be spontaneously broken in its ground state, or new symmetries that the Hamiltonian does not possess can emerge in its low-energy spectrum. The latter phenomenon of emergent symmetries is prevalent at the critical point of many quantum and classical phase transitions, provided the symmetry breaking terms in the Hamiltonian are irrelevant under the renormalization group (RG) flow. The most prominent example might be the deconfined quantum critical point (DQCP) [1,2], a direct continuous phase transition between two distinct spontaneous symmetry broken phases without fine-tuning, beyond the Landau-Ginzburg-Wilson paradigm.

The emergent symmetry which reconciles the incompatible order parameters thus becomes the smoking gun to determine whether such a phase transition is really a DQCP. Another example is the extended symmetry in the low-energy eigenstates of a one-dimensional (1D) critical Hamiltonian with an internal semi-simple Lie group symmetry, when its low-energy physics is described by a conformal field theory (CFT) [3,4]. In this case, the microscopic symmetry and the emergent symmetries can be recombined to form two independent symmetries acting respectively on the left- and right-moving fields, with the corresponding conserved charges being the zero modes of the Kac-Moody algebra [5,6].

Plenty of numerical efforts [7–10] have been devoted to confirming the existence of emergent symmetries. In the case of DQCP, the identity between the scaling dimensions of the critical fluctuations related by emergent symmetries would be an indication [8,11]. Other approaches include order parameter histograms [11,12] and level-crossing analysis [13]. A more direct probe of emergent symmetries is to check if the scaling dimensions of the effective lattice operators for the conserved currents in the field theory are equal to the space dimension [8,9]. However, identification of lattice operators to the currents in the continuum limit requires involved field theory and symmetry analysis [8,14]. Moreover, the identification is usually only approximate and also not unique.

Instead, tensor networks [15–18] provide us with much more information than simply a measurement outcome of the correlation function for given operators. Instead, rather than derive from field theory analysis, we are able to read out the lattice operator for the emergent conserved currents from a tensor network state in a straightforward way. Upon feeding a variationally optimized tensor network ground state [19,20], our algorithm returns the optimal lattice approximation of the conserved current operators truncated to a given interaction range, which systematically approximates the exact symmetry generators as $N$ increases.

Algorithm.—If a state $|\psi\rangle$ is symmetric under a global continuous symmetry transformation $U = e^{i\phi O}$, then $U|\psi\rangle = e^{i\phi} |\psi\rangle$. After absorbing the phase factor into the definition of $O$, i.e. $O = O - \phi I$, we have $e^{i\phi O}|\psi\rangle = |\psi\rangle$, and its linearization gives

$$O|\psi\rangle = 0,$$

or $\langle \psi | O^\dagger O |\psi\rangle = 0$. For an internal symmetry with local generators, $O = \sum_n e^{i\eta_n} G_{n,n+1,\ldots,n+P}$, where $\eta$ is the momentum and $G_{n,n+1,\ldots,n+P}$ is a $P$-site operator starting at the $n$th site. Given a state $|\psi\rangle$ and a momentum $\eta$, if we aim to obtain an exact or approximate conserved quantity of this form which the state has, we can consider the optimization problem

$$\min_G f(G,G^\dagger) = \min_G \frac{\langle \psi | O^\dagger O |\psi\rangle}{V \text{Tr}[G^\dagger G]}$$

with the normalization constraint $||G||^2 = \text{Tr}[G^\dagger G] = 1$, where $V$ is the system size. Note that this cost function has a physical interpretation of the static structure factor of $G$ at momentum $\eta$. The unitarity of $U$ requires $O$, and thus $G$, to be Hermitian. In that case, the optimum of $f$ is reached when $\frac{\partial f}{\partial G} = 0$, i.e.

$$\langle \psi | \frac{\partial O^\dagger}{\partial G} O |\psi\rangle + \langle \psi | O^\dagger \frac{\partial O}{\partial G} |\psi\rangle = 2 \frac{\langle \psi | O^\dagger O |\psi\rangle}{\text{Tr}[G^\dagger G]} G.$$
which, after vectorizing $G \rightarrow \mathbf{g}$, becomes an eigenvalue problem

$$(\mathcal{F} + \mathcal{F}^T) \cdot \mathbf{g} = 2\lambda_{\min} \mathbf{g}, \quad (4)$$

where the eigenvalues are guaranteed to be non-negative real numbers due to the positive semi-definite quadratic form of the cost function $f$, and it can be proved [21] that the eigenvectors $G$ are guaranteed to be Hermitian up to an arbitrary overall phase. For an eigenvector $G$, the associated eigenvalue $\lambda$ naturally measures how accurate the corresponding symmetry is.

For an infinite matrix product state (MPS) $|\psi\rangle$, this eigenvalue problem can be solved by adapting MPS techniques used in other contexts; readers not interested in these details can skip this paragraph. Take $|\psi\rangle$ as an infinite uniform MPS with one-site unit cell parameterized by tensors $A_L, A_R,$ and $A_C$ in the mixed gauge. The application of $\mathcal{F}$ to $\mathbf{g}$, and similarly $\mathcal{F}^T \cdot \mathbf{g}$, can be implemented by observing that [22] it is the same as calculating the static structure factor of $G$ except that a hole is dug in all the terms, i.e.

$$\mathcal{F} \cdot \mathbf{g} = \langle \psi | \frac{\partial O^\dagger}{\partial G} O | \psi \rangle$$

where the last “...” means sum over all diagrams with $1 \leq |n - m| \leq N - 2$, $E_L^T$ and $E_R^T$ are the left- and right-gauge MPS transfer matrices, and $(\cdot)^P$ denotes the pseudo-inverse resulting from the infinite geometric series [20] of all relative positions between $G$ and the hole without overlap, which includes a regularization procedure effectively removing the disconnected part of the correlation functions and thus is automatically consistent with the phase factor absorption mentioned previously. We can then use an iterative eigensolver [23] to obtain the lowest several solutions [24].

In principle, the algorithm works for any MPS [25]. Particularly, we are interested in applying it to the variational uniform MPS (VUMPS) [19] approximation of the gapless ground state of 1D critical Hamiltonians. Since an MPS with finite bond dimension is always gapped [20], it can never exactly represent a critical ground state of infinite correlation length and thus can never exactly capture the symmetry of a critical lattice Hamiltonian or of its low-energy effective field theory in the infrared limit. However, we may use the principle of entanglement scaling [20][23] and treat the finite bond dimension $\chi$ as a relevant perturbation, which enables us to identify the exact or emergent symmetries exclusively from the MPS through an extrapolation in the correlation length $\xi$, as shown by the benchmark results below.

**Benchmarks for exact symmetries.**—As a warming up, we first consider a critical model whose ground state has an exact U(1) symmetry [29]—the spin-1/2 isotropic quantum XY chain

$$H = -\sum_n (X_n X_{n+1} + Y_n Y_{n+1}), \quad (6)$$

where $X_n, Y_n,$ and $Z_n$ are the Pauli matrices at site $n$. The U(1) symmetry is generated by $O = \sum_n Z_n$ that satisfies $[H, \sum Z_n] = 0$. The model is integrable and thus has infinitely many local conserved quantities in the thermodynamic limit $\mathcal{O}[33]$. The critical low-energy physics is described [34] by the U(1)$_4$ CFT of free bosons with central charge $c = 1$.

Applying our algorithm to MPS of various bond dimensions yields the local conserved quantities up to $N = 3$. The full spectrum (after removing the trivial solutions) of the eigenvalue problem in Eq. (4) are shown in Fig. [4] and

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**Diagram Explanation:**

The diagrams represent the transfer matrices of the MPS in the mixed gauge. The left- and right-gauge MPS transfer matrices, $E_L^T$ and $E_R^T$, are involved in the calculation of the static structure factor of $G$. The hole in the diagram effectively removes the disconnected part of the correlation functions. The process is repeated for all relative positions between $G$ and the hole without overlap, which includes a regularization procedure to remove the disconnected part. The resulting expression is a pseudo-inverse of the infinite geometric series of all relative positions, which is automatically consistent with the phase factor absorption. The final result is the eigenvalue problem (4) for $G$.
the eigenvectors $G$ associated with the decaying eigenvalues are shown in Table I. For $p = 0$, there are 1, 3, 5 eigenvalues decaying with the correlation length for $N = 1, 2, 3$, respectively; for $p = \pi$, there are 0, 2, 4 eigenvalues decaying with the correlation length for $N = 1, 2, 3$, respectively. The eigenvector $G = XX + YY$ corresponds to the Hamiltonian in Eq. (3), so as a byproduct our method is also able to determine the local parent Hamiltonian $\mathbb{H}_\text{local} = XX + YY$ solely from its ground state. We notice that the decay has a power-law scaling $\lambda \sim \xi^{-\eta'}$ and the exponents are listed in Table I. All other eigenvalues increase or stay constant with the increasing correlation length. The $G$'s associated with the decaying $\lambda$'s are local integrals of motion since $\lambda$ is extrapolated to 0 at infinite correlation length. While the conserved quantities in Table I and more conserved extrapolated to 0 at infinite correlation length. While

Extended symmetries by emergent symmetries.—The ground state of the spin-1/2 antiferromagnetic Heisenberg chain is expected to have an emergent symmetry in addition to the microscopic SU(2) symmetry of the lattice Hamiltonian, and thus the symmetry is extended to SO(4) = [SU(2)$_L \times SU(2)_R$]/$\mathbb{Z}_2$ in Ref. [20]. Here, we consider

![FIG. 1. Log-log plot of the eigenvalue spectrum of $\frac{1}{\lambda} (\mathcal{F} + \mathcal{F}^T)$ versus the correlation length $\xi$ for the spin-1/2 isotropic quantum XY chain. The correlation length of an MPS with a certain bond dimension is calculated by Eq. (40) in Ref. [20]. Notice that in (e) there is one decaying $\lambda$ hidden in the bulk of larger eigenvalues but it becomes visible at larger correlation lengths.](image)

| $p$ | $N$ | $G$ | $\eta'$ |
|-----|-----|-----|--------|
| 0   | 1   | $Z$ | 1.009  |
| 2   | $XX + YY$ | 1.985 |
|     | $XY - YX$ | 1.933 |
| 3   | $XX + YY$ | 1.008 |
|     | $XY - YX$ | 1.939 |
| $\pi$ | 1   | —   | —      |
| 2   | $XX - YY$ | 2.005 |
|     | $XY + YX$ | 2.008 |
| 3   | $XX + YY$ | 2.046 |
|     | $XY + YX$ | 2.063 |

TABLE I. Local conserved quantities in the spin-1/2 isotropic quantum XY chain up to $N = 3$. Smaller-$N$ solutions reappear at larger $N$ and we only show the new solutions at each $N$. The $\eta'$ is obtained from the scaling of $\langle \psi | O^T O | \psi \rangle$ with $\xi$, which is slightly different from the slope of the decaying eigenvalues in Fig. [1] since different solutions can mix with each other and their form also become more accurate as $\xi$ increases.

the $J$-$Q$ model—a modified Heisenberg chain at whose transition point still exists the extended symmetry

$$H = -J \sum_n P_{n,n+1} - Q \sum_n P_{n,n+1} P_{n+2,n+3}$$

where $P_{n,n+1} = 1/4 - S_n \cdot S_{n+1}$ with $S_n = (S^x_n, S^y_n, S^z_n)$ = $1/2 (X_n, Y_n, Z_n)$. The dimer order enforced by strong four-site interaction transitions to a critical phase when $Q/J \lesssim 0.84831$ in Ref. [41, 42], at which the effective description is the $c = 1$ SU(2)$_{1/2}$ Wess-Zumino-Witten (WZW) CFT in Ref. [3, 40].

Fig. 2 shows the eigenvalues of our optimization problem after imposing the time reversal, parity, and spin flip symmetries of the microscopic Hamiltonian at the transition point. The eigenvectors associated with all the eigenvalues shown in Fig. 2 except the faded ones are lattice operator approximation for the conserved currents of the extended symmetry to different precision, which could be confirmed by checking [21] that their scaling dimension is one [5]. To identify the eigenvalues that associate with the same $G$'s at different $\xi$, we search for the eigenvectors at smaller $\xi$'s which have the largest overlap with each of the lowest several eigenvectors at the largest $\xi$ reached, as tracked by the colored lines in Fig. 2. The dots connected by blue and red lines at the bottom of the spectrum are the best approximation among all of the solutions. Different from the exact symmetries, eigenvalues corresponding to the emergent symmetries will finally saturate at some correlation length, because it is only a $N$-site truncated approximation of the exact emergent lattice generator.

We observe that three approximately conserved charges (red curves in Fig. 2), $M^a = \sum_n m_n^a \ (a \in \{x, y, z\})$, coming from the emergent symmetries, begin to appear at $N = 2$ in addition to the three exact microscopic SU(2) symmetry generators (blue curves in Fig. 2) $Q^a = \sum_n S_n^a$, and they become more conserved as $N$
increases, which is obvious from the drop of the corresponding eigenvalues. At $N = 2$, $m_{n,\alpha} = \epsilon_{\alpha\beta\gamma}S^\beta_n S^\gamma_{n+1}$ with $\epsilon_{\alpha\beta\gamma}$ the Levi-Civita symbol; at $N = 3$, next-nearest neighbor term shows up and we have $m_{n,\alpha} = \epsilon_{\alpha\beta\gamma}(w_1 S^\beta_n S^\gamma_{n+1} + w_2 S^\beta_n S^\gamma_{n+2} + w_3 S^\beta_n S^\gamma_{n+3})$ and $m_{n,\alpha}^3 = \epsilon_{\alpha\beta\gamma}[u_1 S^\beta_n S^\gamma_{n+3} S_{n+1} + S_{n+2}] + (S^\beta_n S^\gamma_{n+1} S_{n+3} + S_{n+2 + 3}]$, with $w_2/w_1 \approx 0.3557$, $w_3/w_1 \approx 0.4467$, $u_3/w_1 \approx 0.1577$, $u_4/w_1 \approx -0.099666$, $u_5/\pi^2 \approx 0.08169$. Considering that it is even under time reversal and odd under parity, $M^{\alpha} \sim J_0^0 - J_0^0$, where $J_0^0$ is the zero mode of the Kac-Moody generators, which form the ordinary Lie algebra $\mathfrak{su}(2)_L (\mathfrak{su}(2)_R)$ [50]. Since $Q^\alpha \sim J_0^0 + J_0^0$, $M^{\alpha}$ and $Q^\alpha$ can then be linearly combined to construct $J_0^0$ and $J_0^0$, and other modes of the Kac-Moody generators can be constructed by the Fourier transform of the currents [6].

Emergent symmetries at a DQCP.—The following spin-1/2 chain, studied by Jiang and Motrunich [52],

$$H = \sum_n (-J_x X_n X_{n+1} - J_z Z_n Z_{n+1})$$

$$+ \sum_n (K_{2x} X_n X_{n+2} + K_{2z} Z_n Z_{n+2}),$$

has an onsite $Z_2 \times Z_2$ spin-flip symmetry. It undergoes a direct continuous transition from a valence bond solid to a ferromagnetic order at $K_{2x} = K_{2z} = 1/2$, $J_x = 1$, $J_z \approx 1.4645$ [8], which has been proposed to be a DQCP with an emergent $U(1) \times U(1)$ symmetry [8,52] that is also generated by the zero modes of the Kac-Moody algebra.

Applying our algorithm to the critical point, we find a single solution $G = Z$ for $N = 1$. From $N = 2$, we require the eigenvectors to transform the same as $Z$ under the spin flip symmetry when solving the eigenvalue problem, and find two solutions at $p = \pi$ as shown in Fig. 3(a,b,c). For $N = 2$, the lowest solution (blue) is $G_1 = ZI - IZ$ (i.e., a staggered $Z$), and the second solution (red) is $G_2 = XY + YX$, which satisfies $[G_1, G_2] = 0$; these are indeed precisely the same effective lattice operators identified as conserved currents for the emergent $U(1) \times U(1)$ symmetry through bosonization [8]. At $N = 3$, the corresponding eigenvalues for $G_1$ and $G_2$ improve by almost one and two orders of magnitude, respectively. The form of both solutions modifies...
significantly by 3-site terms as compared to \( N = 2 \)—and thus compared to the field theory prediction—\( G_1 \) becomes \( \frac{3}{2}(−ZII + ZIZ - IIZ) + v_2ZZZ + v_3(YYZ + ZYY) + v_4(XZX + ZXX) + v_5XZX + v_6YIZY, \) with \( v_2/v_1 \approx 0.1615, v_3/v_1 \approx 0.0988, v_4/v_1 \approx 0.0882, v_5/v_1 \approx 0.0410, \) and \( v_6/v_1 \approx −0.1399; \) \( G_2 \) becomes \( w_1[(XY + YX)I − I(YY + YX)] + 2w_2(XIY − YIX), \) with \( w_2/w_1 \approx 0.3908 \) (Fig. 3(d)). When pushing to \( N = 4 \), longer-ranged terms further dress \( G_1 \) and \( G_2 \) \[21\]. Our algorithm hence allows us to decorate upon the bare form of the lattice operators for emergent symmetry generators found through field theory analysis, and therefore to obtain a more precise picture of the microscopic nature of the emergent symmetries.

Conclusions.—We have presented a novel general method to numerically detect emergent continuous internal symmetries in critical systems. The bottom line is that emergent symmetries do not just reveal themselves indirectly in the long-distance behavior of correlation functions—which has been the sole detection mechanism before our work—but are actually realized surprisingly accurately on the lattice, albeit with spatially extended generators. We have illustrated this by rediscovering the theory-predicted lattice operators for the emergent conserved currents at a 1D DQCP and sharply improving them with newly discovered correction terms. We have also identified the effective lattice operators of the conserved charges for the extended SO(4) symmetry in the J-Q chain with Yangian generators truncated to local terms, which were unknown before. The ability of our method to crack the explicit form of these lattice generators allows us to construct the emergent lattice Kac-Moody generators to unprecedented accuracy for both Abelian and non-Abelian symmetries \[53\] in generic settings.

Outlook.—This method could in principle be generalized to 2D, to extract emergent lattice conserved currents in the projected entangled pair states (PEPS) \[55,57\], which would be of particular use for the study of higher-dimensional DQCP. A variant version with a larger unit cell can be easily derived. It is also worth exploring if a similar algorithm works for finite systems with periodic or other boundary conditions, for the low-energy excited states \[58\], or for classical systems. Adjusting this method to find unconventional symmetries of the weakly-entangled higher excited states \[59,60\] or the emergent space-time symmetry \[61\] would be also interesting directions.

The complexity of the eigenvalue problem scales exponentially with \( N \). To reduce the complexity of solving for \( G \) of larger size, we could resort to the density matrix renormalization group (DMRG) \[15,16\] by treating \( G \) as an \( N \)-site finite matrix product operator (MPO) \[62,63\], and the tricky part will be removing the trivial solutions efficiently \[21,24\]. It would also be desirable to include terms with long-range tails by representing \( O \) as an infinite MPO \[64\], though its implementation encounters some technical difficulties \[21\].

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Notice that $J_\alpha + \bar{J}_\alpha$ also satisfies the $\mathfrak{su}(2)$ algebra, but $J_\alpha - \bar{J}_\alpha$ does not.

Strictly speaking, from bosonization one knows that $S^\alpha(x) \sim (J_\alpha^0(x) + \bar{J}_\alpha^0(x)) + (-1)^x$ (term with scaling dimension 1/2), however, the latter staggered part would cancel out upon sum over $x$ and we get only $J_\alpha^0 + \bar{J}_\alpha^0$.

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https://github.com/mingruyang/EmergentSymmetry
Supplementary material for “Detecting emergent continuous symmetries at quantum criticality”

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I. IMPOSING HERMITICITY

In the main text, we mentioned that it can be proved that the eigenvectors $G$ are guaranteed to be Hermitian up to an arbitrary overall phase. In the following, we will explain why this is true.

To make $U = e^{-iO}$ unitary, $O$ must be Hermitian. For $p = 0$ or $p = \pi$, $G$ should also be Hermitian. Supposing $G_n$ is a $N$-site Hermitian operator starting at site $n$, then

$$G_n = \sum_{\alpha = 1}^{d^2 N} c_\alpha v_{n,\alpha},$$  \hspace{1cm} (S1)

where $c_\alpha$ is real and $v_\alpha$ is a $N$-site Kronecker product of the 1-site Hermitian basis operators $\{ \frac{1}{\sqrt{2d}} I, T_1, \cdots, T_{d^2-1} \}$, with $d$ the dimension of the 1-site Hilbert space and $T_i$ the SU($d$) generator in the fundamental representation.

Let’s take $p = 0$ as an example. In this case, we have $O = \sum_n G_n$. The cost function will then become

$$f = \frac{\langle \psi | O^{\dagger} O | \psi \rangle}{V \text{Tr}[G^\dagger G]} = \frac{\sum_{n,m} \sum_{\alpha,\beta} c_\alpha c_\beta \langle \psi | v_{n,\beta} v_{n,\alpha} | \psi \rangle}{V \sum_{\alpha,\beta} c_\alpha c_\beta \text{Tr}(v_{\alpha} v_{\beta})} = \frac{2^N \sum_n \sum_{\alpha,\beta} c_\alpha c_\beta \langle \psi | v_{0,\beta} v_{n,\alpha} | \psi \rangle}{\sum_{\alpha} c_\alpha^2} = \frac{2^N c^T \cdot M \cdot c}{c^T \cdot c},$$  \hspace{1cm} (S2)

where we have used the fact that $\text{Tr}(v_{\alpha} v_{\beta}) = \frac{1}{2d} \delta_{\alpha\beta}$ and translational invariance, with

$$M_{\beta\alpha} = \sum_n \langle \psi | v_{0,\beta} v_{n,\alpha} | \psi \rangle.$$  \hspace{1cm} (S3)

Then the first derivative becomes

$$\frac{\partial f}{\partial c_\gamma} = 2^N \left( \frac{\sum_{\beta} c_\beta \langle \psi | v_{0,\beta} v_{n,\gamma} | \psi \rangle + \sum_{\alpha} c_\alpha \langle \psi | v_{0,\gamma} v_{n,\alpha} | \psi \rangle}{\sum_{\alpha} c_\alpha^2} - \frac{\sum_{\alpha,\beta} c_\alpha c_\beta \langle \psi | v_{0,\beta} v_{n,\alpha} | \psi \rangle (2c_\gamma)}{(\sum_{\alpha} c_\alpha^2)^2} \right)$$

$$= \frac{2^N (c^T \cdot M)_{\gamma} + (M \cdot c)_{\gamma}}{c^T \cdot c} - \frac{2(c^T \cdot M \cdot c)c_\gamma}{(c^T \cdot c)^2}.$$  \hspace{1cm} (S4)
If we let $\frac{\partial f}{\partial c_\gamma} = 0$, we will get

$$ (c^T \cdot M)_{\gamma} + (M \cdot c)_\gamma = \frac{2(c^T \cdot M \cdot c)}{c^T \cdot c} c_\gamma, \quad (S5) $$

or

$$ [(M^T + M) \cdot c]_\gamma = \frac{c^T \cdot (M^T + M) \cdot c}{c^T \cdot c} c_\gamma. \quad (S6) $$

Therefore, in order to minimize $f$, we need to solve the eigenvalue problem

$$ (M^T + M) \cdot c = 2\lambda_{\min} c \quad (S7) $$

with the constraint that $c$ is a real vector, which is automatically satisfied. This could be proved as the following. By utilizing translational invariance and the Hermiticity of $v_{n,\alpha}$, we can get that $M$ is Hermitian, i.e.

$$ M^{\ast}_{\alpha\beta} = \sum_n \langle \psi | v_{0,\alpha} v_{n,\beta} | \psi \rangle^* = \sum_n \langle \psi | v_{-n,\alpha} v_{0,\beta} | \psi \rangle^* = \sum_n \langle \psi | v_{n,\alpha} v_{0,\beta} | \psi \rangle^* = \sum_n \langle \psi | v_{0,\beta} v_{n,\alpha} | \psi \rangle = M_{\beta\alpha}. \quad (S8) $$

So

$$ M^{\ast}_{\alpha\beta} + M^{\ast}_{\beta\alpha} = M_{\beta\alpha} + M_{\alpha\beta}, \quad (S9) $$

or

$$ (M^T + M)^\ast = M + M^T, \quad (S10) $$

i.e. $M^T + M$ is a real symmetric matrix, and hence it is guaranteed that it has real eigenvectors. Thus the $G$ we obtain in this way will be automatically Hermitian operators.

Alternatively, we do not need to explicitly write $G_\alpha$, in the form of Eq. (S11) and solve the eigenvalues and eigenvectors of $M^T + M$. Instead, we could simply solve the eigenvalue problem of $\mathcal{F}^T + \mathcal{F}$, as stated in the main text, and its eigenvectors will be guaranteed to be Hermitian operators up to an arbitrary overall phase, which can be proved as follows. One could see that $M^T + M$ and $\mathcal{F}^T + \mathcal{F}$ are mapped to each other by

$$ (M^T + M)_{\alpha\beta} = v_\alpha^T \cdot (\mathcal{F}^T + \mathcal{F}) \cdot v_\beta, \quad (S11) $$

where $v_\alpha$ is a $N$-site Hermitian basis operator defined previously. Therefore, the eigenvalue problem of $M^T + M$ in Eq. (S7) is equivalent to

$$ U^T (\mathcal{F}^T + \mathcal{F}) U \cdot c = 2\lambda_{\min} c \quad (S12) $$

or

$$ (\mathcal{F}^T + \mathcal{F}) U \cdot c = 2\lambda_{\min} U \cdot c, \quad (S13) $$

where $\lambda_{\min} = 2^N \tilde{\lambda}_{\min}$ and $U = (v_1, \ldots, v_{d^N})$ is a basis transformation in the $d^N$-dimensional complex space. Thus $U \cdot c$ gives the $G$ in Eq. (S11). Because $c$ is real and $v_\alpha$ is Hermitian, the eigenvectors of $\mathcal{F}^T + \mathcal{F}$ are guaranteed to be Hermitian.

**II. IMPOSING MICROSCOPIC SYMMETRIES**

Imposing the symmetries of the microscopic Hamiltonian will help to largely reduce the number of variational parameters and thus lower the complexity of the eigenvalue problem.

If the critical one-dimensional system is described by a CFT, the emergent conserved charges will be the zero modes of the Kac-Moody generators, $J_0^a$ and $\tilde{J}_0^a$. For $J_0^a + \tilde{J}_0^a$, it would be time reversal odd and parity even; for $J_0^a - \tilde{J}_0^a$, it would be time reversal even and parity odd. In addition, quantum spin Hamiltonians usually also have spin flip symmetries, and both $J_0^a$ and $\tilde{J}_0^a$ will transform in the same way under the spin flip.

If we write $G$ in the form of Eq. (S11) and solve the eigenvalue problem of $M^T + M$ to optimize $c$, it will be easy to impose microscopic symmetries. For example, if $d = 2$, since $T \sigma T^{-1} = -\sigma$, to impose time-reversal symmetry, we can require the sum in Eq. (S11) to only include $v_\alpha$ with odd (even) number of Pauli matrices to make $G$ odd (even).
under the time reversal; to impose parity symmetry, we can require the coefficients \( c_\alpha \) to be \(-c_\beta \) (or \( v_\alpha \) parity \( v_\beta \)) to make \( G \) odd (even) under the parity transformation.

If we use the \( F^T + F \) formalism, in principle we could restrict the entries in \( G \) similarly. But a more convenient way to impose microscopic symmetries when \( N \) is not large is to apply projection operators. For example, to make the eigenvector time-reversal even, one could solve the eigenvalue problem of \( \mathcal{P}_+ (F^T + F) \mathcal{P}_+ \) instead, where \( \mathcal{P}_+ \) is the projection operator onto the time-reversal even subspace. The operation \( \mathcal{P}_+ \cdot x \) could be implemented by mapping \( x \) to \( x + T x \). In this way, all the time-reversal odd \( G \) will move to the null space. When \( N \) is not large, we can solve all the eigenvalues from the largest magnitude until we reach the null space and obtain the associated eigenvectors, and by the way we also exclude all the trivial solutions.

### III. REMOVING TRIVIAL SOLUTIONS

As mentioned in footnote [24] of the main text, there is an issue to be remembered—the number of trivial solutions is large, i.e. \( d^{2(N-1)} \), where \( d \) is the dimension of the local Hilbert space, so it would be desired to remove those trivial solutions.

It is easy to remove the trivial solutions in the \( M^T + M \) formalism by restricting the operator strings \( v_a \) involved in Eq. (S1). We first need to exclude the \( N \)-site identity in Eq. (S1). To further avoid the \( p = 0 \) trivial solutions of the form \( X \otimes I - I \otimes X \) (similarly for \( p = \pi \)), we can fix the coefficient in front of the term \( X \otimes I \) and \( I \otimes X \) in Eq. (S1) to be the same, without losing any generality, since it simply means that those terms can only appear as \( N - 1 \) site \( G = X \) in a symmetric form in the \( N \)-site \( G \).

In the \( F^T + F \) formalism, as mentioned in the last section, when \( N \) is small, one could simply solve all the eigenvalues above the null space to exclude the trivial solutions. More generally, one could get rid of these trivial solutions by lifting those trivial solutions to the top of the spectrum, i.e. \( F \to F + \alpha \mathcal{P}_{\text{trivial}} \), where \( \alpha \) is some positive real number larger than \( \lambda_{\text{max}} \) of \( F \) and \( \mathcal{P}_{\text{trivial}} \) is the projection operator onto the trivial solution subspace. To obtain \( \mathcal{P}_{\text{trivial}} \), we can consider the following problem to find the projection of a given operator \( G \) onto the trivial solution subspace, i.e.

\[
\min_X \| G - (X \otimes I - I \otimes X) \|_2, \tag{S14}
\]

where \( X \otimes I - I \otimes X \) is the form of the trivial solution at \( p = 0 \). By differentiating with respect to \( X \), we get

\[
X = \frac{1}{2d} \left( \begin{array}{cc} G & \cdots \\ \cdots & \cdots \end{array} \right) - \frac{1}{2d} \left( \begin{array}{cc} \cdots & \cdots \\ \cdots & \cdots \end{array} \right), \tag{S15}
\]

which gives us a linear equation for \( X \). If we map an operator \( X \) to a state \( |X\rangle \), the above equation becomes

\[
A |X\rangle = |b\rangle, \tag{S16}
\]

where

\[
A = \left( \begin{array}{cc} \cdots & \cdots \\ \cdots & \cdots \end{array} \right) - \frac{1}{2d} \left( \begin{array}{cc} \cdots & \cdots \\ \cdots & \cdots \end{array} \right), \tag{S17}
\]

and

\[
|X\rangle = \left( \begin{array}{cc} \cdots & \cdots \\ \cdots & \cdots \end{array} \right), \tag{S18}
\]

and

\[
|b\rangle = \frac{1}{2d} \left( \begin{array}{cc} \cdots & \cdots \\ \cdots & \cdots \end{array} \right). \tag{S19}
\]

\( A \) has a null vector \( |I\rangle \) since \( A |I\rangle = 0 \). But \( I \otimes I - I \otimes I = 0 \), so in the solution we can let the coefficient in front of the null vector to be zero without losing any generality. As a result, we get \( |X\rangle = \text{pinv}(A) |b\rangle \), where \( \text{pinv}(A) \) is the pseudo-inverse of \( A \). Finally, the projection operator onto the trivial solution subspace should be

\[
\mathcal{P}_{\text{trivial}} = \frac{1}{2d} \left( \begin{array}{cc} \text{pinv}(A) & \cdots \\ \cdots & \cdots \end{array} \right) - \frac{1}{2d} \left( \begin{array}{cc} \cdots & \cdots \\ \cdots & \cdots \end{array} \right). \tag{S20}
\]
Then we can perform $\mathcal{F} \rightarrow - (\mathcal{F} + \alpha \mathcal{P}_{\text{trivial}})$ to shift the trivial solution subspace to the top and reverse the spectrum so that the problem transforms to solving for the largest eigenvalues. $\mathcal{P}_{\text{trivial}}$ is model independent, so for each $N$ we only need to solve for $\text{pinv}(A)$ once.

**IV. FINITE-SYSTEM DMRG TO OPTIMIZE $G$**

In the $\mathcal{F}^T + \mathcal{F}$ formalism, if we treat $G$ as a single big tensor, the complexity of the optimization problem will grow exponentially as $N$ increases. Alternatively, we can write $G$ as a finite matrix product operator (MPO) and use the density matrix renormalization group (DMRG) \cite{15, 16} to optimize it. Note that if we transform to the $M^T + M$ formalism, i.e. using the operator string $v_\alpha$ basis, the coefficient $c_\alpha$ can also be expressed as an MPO, and the advantage of using this basis is that the eigenvalue problem can be solved within real numbers.

Now let’s take $N = 5$ as an example. A 5-site finite MPO is illustrated as

$$G = \begin{array}{c}
W_1 \quad W_2 \quad W_3 \quad W_4 \quad W_5
\end{array}. \quad (S21)$$

Different from treating $G$ as a single big tensor, at each iteration we assume all but one site tensor $W_i$ constant and differentiate the cost function $f$ with respect to $W_i$ only. If we let $G$ in its canonical form, just like an MPS, we will get an eigenvalue problem for $W_i$ at each iteration. Solve for the lowest eigenvalue at each iteration, and after several DMRG sweeps through the 5 sites we get a $G$ corresponding to $\lambda_{\text{min}}$. Then we can construct a projection operator $\mathcal{P} = |G\rangle\langle G|$.

Removing the large number of trivial solutions is essential for doing DMRG efficiently. In principle, we could do the same thing as in the last section. However, performing efficient DMRG requires us to have $\text{pinv}(A)$ either in the form of an MPO or decomposition of some local operators, while we currently do not have a good approach to efficiently calculate $\text{pinv}(A)$ when $N$ becomes larger.

**V. THE INFINITE UNIFORM MPO FORMALISM**

A more natural representation for $O$, which is able to hold long-range interacting terms in the summation, would be the finite state automaton \cite{62, 63}, which can be translated to an infinite uniform MPO. This formalism also helps to reduce the complexity of the problem by solving for only one MPO site tensor and restricting the form of $G$ to certain combination of Pauli strings. Here, we explain how to optimize a MPO for $O$ of bond dimension $\chi_W = 2$, and show that the optimization for this MPO gives the same eigenvalue problem as in the main text. However, generalization from $\chi_W = 2$ to $\chi_W > 2$ is non-trivial and we leave it as an open question.

The MPO representation of $O$ is

$$O = \ldots \begin{array}{c}
W \quad W \quad W \quad W \quad W
\end{array} \ldots, \quad (S22)$$

where $W$ is an operator-valued matrix given by

$$W = \begin{bmatrix}
1 & G \\
0 & 1
\end{bmatrix}. \quad (S23)$$

Then

$$\langle \psi | \frac{\partial O^\dagger}{\partial G} | O |\psi \rangle = \begin{bmatrix}
A_{1} \\
W \\
1 \\
A_{2}
\end{bmatrix} \begin{bmatrix}
A_{1} \\
W \\
1 \\
A_{2}
\end{bmatrix} = D^{12,11}W_{11} + D^{12,12}W_{12} + D^{12,21}W_{21} + D^{12,22}W_{22} = D^{12,11}1 + D^{12,12}G + D^{12,22}1. \quad (S24)$$
Therefore we only need to calculate the fixed points \((L_{1,1}^{[WW]}), |R_{1,2}^{[WW]}|, (L_{1,2}^{[WW]}), |R_{2,2}^{[WW]}|\), which are defined as

\[
(L_{a,b}^{[WW]}) = \sum_{(a', b') \leq (a, b)} (L_{a', b'}^{[WW]}) \left(T_{a', b'}^{[WW]}\right)_{a', b', a, b, \ldots} \quad |R_{a,b}^{[WW]}| = \sum_{(a', b') \geq (a, b)} (T_{a,b}^{[WW]})_{a, b, a', b'} |R_{a', b'}^{[WW]}|,
\]

where

\[
(T_{L/R}^{[WW]})_{a', b'; a, b} = \sum_{s, s'} A^{s'}_{L/R} \otimes W_{a', a}^{s'} \otimes W_{b', b}^{s'} \otimes A^s_{L/R}.
\]

Notice that \(\bar{W} \otimes W\) is still upper-triangular and there are two additional identities in the diagonal elements, i.e.

\[
\bar{W} \otimes W = \begin{bmatrix}
1 & G & 0 & 1 & 1
0 & 1 & 0 & G^\dagger & 0
0 & 0 & 1 & G & 0
0 & 0 & 0 & 1 & 0
\end{bmatrix}.
\]

From the definition, substituting the form of \(W\), we get \((L_{1,1}^{[WW]}) = (L_{1,1}^{[WW]})_T\), where \(T_L\) is the transfer operator of the MPS \(|\psi[A_L]\rangle\), so we have \((L_{1,1}^{[WW]}) = |1\rangle\), where \(|1\rangle\) is the left fixed point of \(T_L\). We can then get \((L_{1,2}^{[WW]}) = (L_{1,2}^{[WW]})_T + (Y_{1,2})\), where

\[
(Y_{1,2}) = \begin{bmatrix}
A_L \\
G \\
A_L
\end{bmatrix}.
\]

To remove the divergence from \((O)\), one needs instead to solve the linear equation

\[
(L_{1,2}^{[WW]})_T (1 - T_L + |R\rangle\langle 1|) = Y_{1,2} - (Y_{1,2} |R\rangle\langle 1|
\]

to get \((L_{1,2}^{[WW]})\). Similarly we can get \(|R_{1,2}^{[WW]}|\) = \(|1\rangle\) and

\[
(1 - T_R + |1\rangle\langle 1|) R_{1,2}^{[WW]} = |Y_{2,1}\rangle - |1\rangle L |Y_{2,1}\rangle,
\]

where

\[
|Y_{2,1}\rangle = \begin{bmatrix}
A_R \\
G \\
A_R
\end{bmatrix}.
\]

Therefore \(D^{12,11}\) and \(D^{12,22}\) are proportional to \(G\) and \(D^{12,12}\) has no \(G\) dependence. It is easy to see that \(D^{12,11} \mathbb{I} + D^{12,12}G + D^{12,22} \mathbb{I}\) is equivalent to \(\mathcal{F} : g\) in the main text. If we require the normalization \(\text{Tr}[G^\dagger G] = 1\), then we get the same eigenvalue problem as in the main text. So the \(\chi_W = 2\) MPO formalism is equivalent to representing \(O\) as a summation of local terms in the case that \(G\) is one-site.

However, this equivalence could not be generalized to \(\chi_W > 2\). For example, the most generic form for \(\chi_W = 3\) is

\[
W = \begin{bmatrix}
\mathbb{I} & A & B \\
0 & D & C \\
0 & 0 & \mathbb{I}
\end{bmatrix}.
\]

If we want there to be some exponentially decaying interacting term, then \(D = \kappa \mathbb{I}\) with \(\kappa < 1\). There are several issues to optimize \(W\). First, considering the simplest case with \(D = 0\), the \(O\) generated by \(W\) would be \(\sum_n (A_n C_n + B_n)\), and \(\langle \psi | O^\dagger O | \psi \rangle\) contain terms linear in \(A, B,\) and \(C\), so taking its derivative with respect to \(A, B,\) or \(C\) would not give us an eigenvalue problem, but one might be able to use the gradient descent method. The second question would be how to choose a proper normalization condition for \(W\), especially when there is an exponentially decaying term. Simply requiring \(A, B,\) and \(C\) each to be individually normalized does not make sense. Probably the canonical form [64] for such Hamiltonian-like MPO might help.
VI. METHOD BASED ON THE FUNDAMENTAL THEOREM OF MPS

In footnote [25] of the main text, we mentioned that solving the symmetry of the ground state of a gapped system is much easier, and another method based on the MPS fundamental theorem also works. In this section, we will discuss this alternative method for gapped systems and why it does not work well for critical systems.

If an MPS

\[ |\Psi(A)\rangle = \ldots A A A A A \ldots \]  

(S33)

is symmetric under a global on-site symmetry operation, the MPS tensor itself transforms under this operation [20]:

\[ U^g_N |\Psi(A)\rangle \propto |\Psi(A)\rangle \rightarrow U^g_A = e^{i\phi_g} V^g A V^g \dagger \]  

(S34)

If the symmetry transformation is continuous, we can write \( U^g = e^{i\epsilon G} \). After absorbing the phase factor \( e^{i\phi_g} \) into the definition of \( G \), the infinitesimal version becomes

\[ 1 + i\epsilon G_A = 1 + i\epsilon K_1 - i\epsilon K_A \]  

(S35)

or

\[ G_A = K_1 - K_A \]  

(S36)

After vectorizing \( G \mapsto \mathbf{g} \) and \( K \mapsto \mathbf{k} \), the above equation becomes

\[ \begin{bmatrix} P & Q & R \end{bmatrix} \begin{bmatrix} \mathbf{g} \\ \mathbf{k} \end{bmatrix} = 0, \]  

(S37)

where \( P_{\alpha\beta,\gamma} = \delta_{ij} A^i_{\alpha\beta} \), \( Q_{\alpha\beta,\gamma\rho} = \delta_{\rho\beta} A^i_{\alpha\gamma} \), and \( R_{\alpha\beta,\gamma\rho} = \delta_{\alpha\gamma} A^i_{\rho\beta} \). The equation can be transformed into a least square problem

\[ \min_{\mathbf{x}} \| M \cdot \mathbf{x} \| \]  

(S38)

with constraint \( \| \mathbf{x} \|_2 = 1 \), where \( M = [P \; Q - R] \) and \( \mathbf{x} = [\mathbf{g} \; \mathbf{k}]^T \). This problem can be solved by either quadratic programming or singular value decomposition (SVD) \( M = USV^\dagger \), where \( S = \text{diag}(\lambda_1, \ldots, \lambda_{d^2+D^2}) \) and \( V = (v_1, \ldots, v_{d^2+D^2}) \).

While it works for gapped systems, this way to solve for the symmetries is numerically unstable for the critical systems. In the benchmarks for the 1D isotropic XY model, it was observed that the singular vector \( v_i \) whose first \( d^2 \) components best approximate the symmetry generator \( S_z \) does not always correspond to the second lowest singular value \( \lambda_{d^2+D^2-1} \) (the trivial solution is the lowest one). In addition, the SVD only requires the orthogonality

\[ [\mathbf{g} \; \mathbf{k}]^\dagger [\mathbf{g}' \; \mathbf{k}'] = 0 \]  

(S39)

but not necessarily \( \mathbf{g}'^\dagger \mathbf{g}' = 0 \), so there are many \( v_j \)'s that have nonzero overlap with \( (S_z, K) \). Also, we didn’t see a clear scaling of the singular values with the correlation length.

Furthermore, \( M \) is not gauge invariant and so are its singular values. If we work in the mixed gauge, the infinitesimal version of the fundamental theorem becomes

\[ A_C = -K A_R - A_L - K \]  

(S40)
with \( A_C = LAR, A_L = LAL^{-1}, \) and \( A_R = R^{-1}AR. \) Notice that the trivial solution now becomes \((G, K) = (0, C),\) where \( C = LR.\) In the benchmarks for the 1D isotropic \( XY \) model, we could see a clear scaling of the singular values with the correlation length \( \xi.\) However, the problems are only partially solved by utilizing the mixed gauge. \( g \) in the singular vectors is still not orthogonal to each other. As a result, we observed that the number of singular values that scales to zero with increasing correlation length is much larger than the number of symmetries the system actually has, though there is a gap between the lowest ones and the higher ones. The \( D^2 \) useless degrees of freedom for \( K \) also increase the complexity of the problem and make the solution quickly become unreachable as \( N \) and \( D \) increases. In addition, the singular values are not very physical, since they are still gauge dependent. In conclusion, for critical systems one should resort to the variational method in the main text.

Note that the on-site symmetry \( \otimes_n U_n = \exp(-\text{i} \sum G_n) \) can be generalized to a continuous symmetry \( U = \exp(-\text{i}O) \) generated by a summation of \( N \)-site local Hermitian operators \( O = \sum G_{n \ldots n+\eta_N}, \) which takes a similar form to a local Hamiltonian. If the state is invariant under the transformation, i.e. \( \exp(-\text{i}O)|\psi\rangle = |\psi\rangle \) (the phase factor has been absorbed into the definition of \( O \)), it implies equivalently \( O|\psi\rangle = \sum G_{n \ldots n+\eta_N} |\psi\rangle = 0, \) or

\[
\begin{array}{c}
\begin{array}{c}
A_L \\
... \\
A_{i-1} \\
G \\
A_{i+1} \\
... \\
A_R
\end{array}
\end{array}
= -
\begin{array}{c}
\begin{array}{c}
A_L \\
... \\
A_{i-1} \\
K \\
A_{i+1} \\
... \\
A_R
\end{array}
\end{array}
= -
\begin{array}{c}
\begin{array}{c}
K \\
A_{i+1} \\
... \\
A_L \\
G \\
A_{i-1} \\
... \\
A_R
\end{array}
\end{array}
\tag{S41}
\]

for injective MPS, where \( G \) is a \( N \)-site operator and \( K \) is a \( N - 1 \)-site tensor. Now there are \( d^{2(N-1)} \) trivial solutions, which take the form \( G = X \otimes I - I \otimes X, \) where \( X \) is a \( N - 1 \)-site operator and \( I \) is the one-site identity operator.

VII. CONSERVED QUANTITIES IN THE SPIN-1/2 ISOTROPIC QUANTUM \( XY \) CHAIN

In this section, we review the master symmetry \([30]\) technique to obtain the conserved quantities in the spin-1/2 isotropic quantum \( XY \) chain.

The Hamiltonian of the spin-1/2 isotropic quantum \( XY \) chain can be written as

\[
H = \sum_i h_i \tag{S42}
\]

where \( h_i = X_iX_{i+1} + Y_iY_{i+1}. \) Obviously, \( H \) has a \( U(1) \) symmetry and thus \( [H, Q_0] = 0, \) where \( Q_0 = \sum Z_i. \) Each term in the conserved quantity \( Q_1 = \sum_i (X_iY_{i+1} - Y_iX_{i+1}) \) can be obtained by Eq. (46) in Ref. \([6]\), i.e. \( 2i(X_iY_{i+1} - Y_iX_{i+1}) = [h_i, Z_i]. \) If we denote \( H_0 = H, \) each term in level-\( n \) conserved quantities \( H_n = \sum_i h_{n,i} \) and \( Q_n = \sum_i q_{n,i} \) can be constructed recursively up to a constant by

\[
\begin{align}
&h_{n+1,i} \propto [h_i, H_n], \quad \text{if } n \geq 0; \tag{S43a} \\
&q_{n+1,i} \propto [h_i, Q_n], \quad \text{if } n \geq 1. \tag{S43b}
\end{align}
\]

For example, we have \( H_1 = \sum_i (X_iZ_{i+1}Y_{i+2} - Y_iZ_{i+1}X_{i+2}), \) and \( Q_2 = \sum_i (X_iZ_{i+1}X_{i+2} + Y_iZ_{i+1}Y_{i+2}). \) One can verify that

\[
[H_n, H_m] = [H_n, Q_m] = [Q_n, Q_m] = 0. \tag{S44}
\]

For \( p = \pi \) we could get in a similar way the conserved quantities that take a staggered pattern in the summation, \( K = \sum_i (-1)^i k_i. \)

VIII. EXPLANATION OF THE CRITICAL EXPONENTS OF THE CONSERVED QUANTITIES IN THE SPIN-1/2 ISOTROPIC QUANTUM \( XY \) CHAIN

For a correlation function \( C(r, \xi) = \langle \psi|G_{n+r}^\dagger G_n|\psi\rangle \) near the critical point, it takes the form \([25]\)

\[
C(r, \xi) = r^{-\eta} g(r/\xi), \tag{S45}
\]

where \( \eta = 2\Delta \) is double the scaling dimension of the operator \( G. \) Since the effect of finite bond dimension is like a relevant perturbation which deforms the MPS away from the exact critical point, the correlation function calculated
with MPS should also take this form. In the continuum limit, the static structure factor \( S \) at momentum \( p = 0 \) is given by

\[
S(\xi) = 2 \int_0^\infty \! dr r^{-\eta} g(r/\xi),
\]

which should be invariant under a change of integration variable \( x = \lambda r \), i.e.

\[
S(\xi) = 2\lambda^{\eta-1} \int_0^\infty \! dx x^{-\eta} g(x/(\lambda \xi)) = \lambda^{\eta-1} S(\lambda \xi).
\]

Therefore, we have \( S(\lambda \xi) = \lambda^{-(\eta-1)} S(\xi) \), which yields

\[
S(\xi) \sim \xi^{-\eta},
\]

i.e. the critical exponent for \( S(\xi) \) is given by the critical exponent for the corresponding correlation function minus one, and to make \( S(\xi) \) decay with increasing \( \xi \) it requires \( \eta > 1 \).

However, we find the above argument is oversimplified and thus does not generally hold. In TABLE I, one could observe that generally \( \eta' \neq \eta - 1 \) except for \( Z \) and \( XYZ + YZ \). Actually, the value of \( \eta' \) is extracted from calculation not in the continuum limit but within the discrete lattice, so

\[
S(\xi) = 2 \sum_{r=1}^\infty C(r, \xi) + C(0, \xi).
\]

For \( XX + YY \) at \( p = 0 \), since \( C(r, \xi = \infty) \sim (-1)^r + r^{-2} \), for terms at large \( r \) the sum reduces to

\[
\sum_r C(r, \xi) \sim \sum_{\text{odd } r} \left[ \frac{1}{r^2} - \frac{1}{(r+1)^2} \right] = \sum_{\text{odd } r} \frac{1}{r^2} \left[ 1 - \left( \frac{1}{r+1} \right)^2 \right] \approx \sum_{\text{odd } r} \frac{2}{r^2}. \tag{S50}
\]

Therefore effectively \( \eta \) becomes 3 and thus the relation \( \eta' = \eta - 1 \) still holds. For \( XX + YY \) and \( XY + YY \) at \( p = \pi \), it could be argued similarly.

In fact, we found that \( \eta' \) depends on the behavior of the correlation function calculated with MPS not only in the infrared limit but at all distances. For a MPS, \( C(r, \xi) \sim r^{-\eta} e^{-r/\xi} \) \cite{28} is only true when \( r \) is much larger than the lattice spacing, and thus there is a certain range \( \Lambda < r < \xi' \) where \( C(r, \xi) \sim r^{-\eta} \). At short distance \( r < \Lambda \), the behavior of \( C(r, \xi) \) relies on microscopic details. At sufficiently large distance \( r \gg \xi' \), we have \( C(r, \xi) \sim e^{-r/\xi} \). As a result, weird cancellation can happen to give the final value of \( \eta' \) for \( XYZ - YZX, ZXX - XYZ, YZX + YZ \), and it does not follow the previous simple argument.

Notice that the correlation length manifested in the correlation function calculated with MPS can be different from the correlation length obtained by the formula \( \xi = \frac{1}{\log(\lambda_2/\lambda_1)} \), where \( \lambda_i \) is the \( i \)th largest eigenvalue of the MPS transfer matrix \( T = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i| \). Define

\[
(G) = \begin{pmatrix}
A_L & \cdots & A_L \\
\vdots & \ddots & \vdots \\
A_L & \cdots & A_L
\end{pmatrix}. \tag{S51}
\]
The reason is that \((G|\lambda_i)\) can be zero for the first several \(\lambda_i\)'s, depending on the charge \(G\) carries, and thus the correlation length will be instead given by \(\xi = \exp[\frac{1}{\lambda_i}]\), where \(\lambda_i\) is the largest eigenvalue of \(T\) that satisfies \((G|\lambda_i) \neq 0\). Nevertheless, we find that \(\lambda_i = \lambda_{2i}^2\) for \(i > 2\), which will only bring a constant prefactor \(a_i\) to the correlation length and therefore will not affect the scaling.

IX. MORE RESULTS OF THE SPIN-1/2 \(J-Q\) MODEL

At the transition point \(Q/J \approx 0.84831\), we first use VUMPS with 1-site unit cell to obtain the ground state for various bond dimensions from \(\chi = 10\) to \(\chi = 400\) until the gradient converges to \(10^{-12}\) and then apply our algorithm to these uniform MPS. When doing VUMPS, we only require the MPS to be real so as to impose time-reversal symmetry but not impose any other microscopic symmetries. When applying our algorithm to the MPS obtained by VUMPS from \(N = 2\), we impose the time-reversal, parity, and spin-flip symmetries as mentioned in the previous section. Since the one-site unit cell enforces translational invariance, we would get a (non-injective) equal weight superposition of all translational symmetry broken MPS ground state approximation, if it energetically favors a translational symmetry broken ground state within finite bond dimension, and thus it would limit the precision VUMPS can reach [19]. To avoid this, we perform a sublattice spin rotation around the \(z\)-axis by angle \(\pi\) when doing VUMPS, which is important for it to converge. Due to this sublattice rotation, the \(x\) and \(y\) components of the generators move to \(p = \pi\).

As a supplemental, here we also show the data for \(N = 1\), where we obtain the three generators for the microscopic \(\text{SU}(2)\) symmetry. For \(p = 0\), we get only one decaying solution, \(G = Z\) (blue curve in Fig. S1(a)); for \(p = \pi\), we get two decaying solutions corresponding to the other microscopic \(\text{SU}(2)\) generators \(X\) and \(Y\) (blue curve and scattered points below it in Fig. S1(b)). Notice that most of those scattered points are well below \(10^{-8}\) and not shown.

![Graph](image-url)

FIG. S1. Log-log plots of the non-trivial eigenvalue spectrum (without imposing microscopic symmetries) of \(\mathcal{F}\) versus the correlation length \(\xi\) for the spin-1/2 \(J-Q\) chain at \(Q/J \approx 0.84831\) when \(N = 1\).

The conservation of currents in \(1 + 1d\) implies their scaling dimension must be \(1\) [5], which means their correlation functions should decay as \(r^{-2}\). This is indeed the case as shown in Fig. S2, which plots the correlation function of \(q_z\) and \(m_z\) for different \(N\), where \(Q_z = \sum_x q_z(x)\) and \(M_z = \sum_x m_z(x)\) are the zero modes of the Kac-Moody generators. We can see that

\[
\langle q_z(0)q_z(r) \rangle \sim c_1(1^{-}\r_{-1} + c_2r^{-2}, \quad \langle m_z(0)m_z(r) \rangle \sim r^{-2}. \quad (S52)
\]

Notice that \(\langle q_z(0)q_z(r) \rangle \sim r^{-2}\) for even \(N\) because of the cancellation of the staggered part due to terms like \(G \otimes I + I \otimes G\), where \(G\) is a \(N - 1\)-site operator, as listed in Table III. This cancellation can be explained as follows. If \(\langle G(0)G(r) \rangle \sim c_1(-1)^{r_{-1} + c_2r^{-2}}\), then

\[
\langle (G \otimes I + I \otimes G)(0)(G \otimes I + I \otimes G)(r) \rangle
= \langle G(0)G(r) \rangle + \langle G(0)G(r + 1) \rangle + \langle G(1)G(r) \rangle + \langle G(1)G(r + 1) \rangle
= 2[c_1(-1)^{r_{-1} + c_2r^{-2}}] + c_1(-1)^{r_{-1} + c_2r^{-2}} + c_2(r + 1)^{-2} + c_1(-1)^{r_{-1} + c_2r^{-2}} + c_2(r - 1)^{-2}
\sim 4c_2r^{-2}. \quad (S53)
\]

Note that although for \(q_\alpha\) at \(N > 2\) we got longer-range decoration to the 1-site spin operator \(S_\alpha\) from terms in higher even-level Yangian generators. Those decorations will finally vanish as the correlation length goes to infinity, as shown in Fig. S3.

In Fig. S4, we also show the extrapolation of the coefficient ratio in \(m_z\) for \(N = 4\).
FIG. S2. The absolute value of the correlation function $\langle q_z(0) q_z(x) \rangle$ and $\langle m_z(0) m_z(x) \rangle$ measured with MPS of bond dimension $\chi = 240$, where $q_z$ and $m_z$ are the optimized solution for MPS of bond dimension $\chi = 400$. The subleading part of the correlation function of the $N$-site operator $G$ is obtained by measuring the correlation function of $G \otimes I + I \otimes G$, and therefore the subleading part of the correlation function of the 1-site $q_z$ is equivalent to the correlation function of the 2-site $q_z$.

FIG. S3. (a) The weight of the part excluding $S^z$ in $q_z$ for (a) $N = 3$ and (b) $N = 4$ versus the correlation length $\xi$.

FIG. S4. (a) The ratio between the coefficients of the terms in $m_z$ for $N = 4$ versus $\xi$, similarly for $m_x$ and $m_y$. 
TABLE II. Optimal lattice operator approximation of the conserved currents for the extended symmetry in the spin-1/2 J-Q chain at \(Q/J \approx 0.84831\) up to \(N = 4\) with \(\chi = 400\). There are 3 generators associated to the exact microscopic SU(2) symmetry and the corresponding eigenvalues of \(\mathcal{F}\) decays in a power law with the the correlation length \(\xi\); Z has \(\eta' \approx 1.027\), while 0.242768X + Y and X − 0.242768Y have \(\eta' \approx 1.028\). Notice the effect on the signs from the sublattice rotation. And also notice that different (approximate) symmetry generators can be linearly combined with each other to form an eigenvector. + (−) means parity \(\mathcal{P}\) or time reversal \(\mathcal{T}\) even (odd).
X. YANGIANS IN THE HALDANE-SHASTRY MODEL

In the last section, we mentioned that the lattice form of the Kac-Moody generators in the J-Q model looks like local truncation to the Yangian generators, which are exact symmetry of the Haldane-Shastry model. In this section, we give the explicit lattice forms of the Yangian generators up to level 3.

Yangian is a Hopf algebra and its level-n generators can be defined recursively starting from the level-0 and level-1 generators [47]. For SU(2), the level-0 generators are the usual global SU(2) generators, i.e. $Q_0 = \sum_i S_i^\alpha$. The level-1 generators are

$$Q_1^\alpha = \frac{1}{2} \sum_{i \neq j} w_{ij} \epsilon^{\alpha \beta \gamma} S_i^\beta S_j^\gamma \tag{S54}$$

with $w_{ij} = (z_i + z_j)/(z_i - z_j)$ and $z_j = \exp(2\pi ij/L)$, where $L$ is the size of the system with periodic boundary condition. By utilizing the recursive relation

$$\epsilon^{\alpha \beta \gamma} [Q_1^\gamma, Q_n^\beta] = 2Q_n^\alpha, \tag{S55}$$

it can be derived that

$$Q_2^\alpha = \frac{1}{12} (N - 1)(N - 2)Q_0^\alpha - \sum_{i \neq j \neq k} w_{ij} w_{kj} S_j^\alpha S_j^\beta S_k \tag{S56}$$

and

$$Q_3^\alpha = \frac{1}{6} (N - 1)(N - 2)Q_1^\alpha + \frac{1}{2} \sum_{i \neq j \neq k \neq m} w_{ij}(w_{ml} - w_{mi})(w_{jl} - w_{ji})\epsilon^{\alpha \beta \gamma} S_i^\beta S_j^\gamma S_k \cdot S_m. \tag{S57}$$

We could see that the odd (even) level Yangian generators are odd (even) under the parity transformation.

XI. MORE RESULTS OF THE JIANG-MOTRUNICH MODEL

At $K_{2x} = K_{2z} = 1/2$, $J_x = 1$, $J_z \approx 1.4645$, we perform VUMPS [22] with 1-site unit cell from bond dimension $\chi = 10$ to $\chi = 400$ until the gradient converges to $10^{-12}$ and then apply our algorithm. We also tried two-site unit cell but did not see a notable difference in the results.

FIG. S5. The absolute value of the correlation function $\langle G_1(0)G_1(x) \rangle$ and $\langle G_2(0)G_2(x) \rangle$ measured with MPS of bond dimension $\chi = 240$, where $G_1$ and $G_2$ are the optimal solution for MPS of bond dimension $\chi = 400$. The subleading part of the correlation function of the $N$-site operator $G$ is obtained by measuring the correlation function of $G \otimes I \otimes G$, and therefore the subleading part of the correlation function of the 1-site $G_1$ is equivalent to the correlation function of the 2-site $G_1$.

In Fig. S5 we show the correlation function of $G_1$ and $G_2$ for different $N$ and confirm that their scaling dimension is pinned at one. We can see that

$$\langle G_1(0)G_1(r) \rangle \sim c_1 r^{-s/2} + c_2(-1)^r r^{-2}, \quad \langle G_2(0)G_2(r) \rangle \sim (-1)^r r^{-2}, \tag{S58}$$
where $g \approx 1.5$ is the Luttinger parameter [S]. Notice that $\langle G_1(0)G_1(r) \rangle \sim (-1)^{r-2}$ for even $N$ because of the cancellation of the non-staggered part due to terms like $G \otimes I - I \otimes G$, where $G$ is a $N-1$-site operator, as listed in Table III. This cancellation can be explained as follows. If $\langle G(0)G(r) \rangle \sim c_1 r^{-1} + c_2 (-1)^{r-2}$, then

$$\langle (G \otimes I - I \otimes G)(0)(G \otimes I - I \otimes G)(r) \rangle$$

$$= \langle G(0)G(r) \rangle - \langle G(0)G(r+1) \rangle - \langle G(1)G(r) \rangle + \langle G(1)G(r+1) \rangle$$

$$= 2[c_1 r^{-1} + c_2 (-1)^{r-2}] - c_1 (r+1)^{-1} - c_2 (-1)^{r+1}(r+1)^{-2} - c_1 (r-1)^{-1} - c_2 (-1)^{r-1}(r-1)^{-2}$$

$$\sim 4c_2(-1)^{r-2}.$$  

Here we also provide results of the eigenvalues of the optimization problem at $p = 0$ from $N = 1$ to $N = 4$. None of them have scaling dimension one, and thus none of them are emergent conserved currents.

![Graphs](image_url)

FIG. S6. Log-log plot of the non-trivial eigenvalue spectrum of $F$ (with time reversal and parity symmetry imposed) versus the correlation length $\xi$ at $p = 0$ for the Jiang-Motrunich model at $J_z = 1.4645$. The $G$'s associated with the blue (red) dots are parity even (odd) and time reversal odd (even). The green curve is the Hamiltonian.

In Table III, we list the optimal $G$'s we obtained with MPS of bond dimension $\chi = 400$ from $N = 1$ to $N = 4$ for the Jiang-Motrunich model.

| $p$ | $N$ | $\xi$ | $G$ |
|-----|-----|-------|-----|
| 0   | 1   |       |     |
| 2   |     |       |     |
| 4   |     |       |     |
| 3   |     |       |     |
| 5   |     |       |     |

TABLE III. Optimal lattice operator approximation of the emergent conserved currents in the Jiang-Motrunich model at $J_z = 1.4645$ up to $N = 4$ with $\chi = 400$. $+$ (-) means parity $P$ or time reversal $T$ even (odd).