Finite Size Scaling at the Topological Transition: Bilinear-Biquadratic Spin-1 Chain

Yuting Wang\(^1\) and Alex Kamenev\(^1,2\)

\(^1\)School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA and
\(^2\)William I. Fine Theoretical Physics Institute, University of Minnesota, Minneapolis, MN 55455, USA

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We consider a finite size scaling across a topological phase transition between dimerized and Hal-dane phases in bilinear-biquadratic spin-1 chain. To this end we perform high-accuracy variational matrix product state simulations. We show that the scaling function, expressed in terms of \(L/\xi\), where \(L\) is the chain length and \(\xi\) is the correlation length, coincides with that of three species of non-interacting massive Majorana fermions. This is in agreement with the fact that the critical theory of the model has central charge \(c = 3/2\). On the other hand, the correlation length \(\xi\) exhibits a non-trivial dependence on parameters of the model.

I. INTRODUCTION

Topological states of matter continue to attract ever increasing attention of the community\(^1\)\(^2\) vis-a-vis their peculiar electric and thermal transport properties as well as applications in quantum computing. Yet, surprisingly little attention was payed to the most basic thermodynamical quantities and their scaling properties close to topological phase transitions. Though hard to measure, they exhibit a remarkable universality and provide a conceptual framework to distinguish between different universality classes.

In this paper we discuss a finite-size scaling of a many-body ground state energy across topological phase transitions in 1+1 dimensions. Critical points of such models are described by conformal field theories (CFT)\(^3\) characterized by central charge \(c\). The finite-size, \(L\), scaling of the ground state energy \(E(L,\infty)\) for an open system at criticality was shown to be\(^4\)\(^5\)

\[
E(L,\infty) = L \bar{\epsilon}(\infty) + b(\infty) - \frac{c}{L} \frac{\pi}{24} + O(L^{-2}),
\]

where \(\bar{\epsilon}(\infty)\) is the average bulk energy density, \(b(\infty)\) a size-independent boundary term and argument \((\infty)\) specifies the exact critical point where the correlation length \(\xi \to \infty\). Here velocity of excitations (“Fermi” velocity) is put to be one. The \(1/L\) term appears to be universal and depends only on \(c\) — the central charge of the Virasoro algebra.

A relevant perturbation drives the system away from criticality, creating a spectral gap \(\Delta\) and a corresponding correlation length \(\xi = 1/\Delta\). One may generalize the CFT expansion Eq. (1) as

\[
E(L,\xi) = L \bar{\epsilon}(\xi) + b(\xi) - \frac{c}{L} \frac{\pi}{24} f\left(\frac{L}{\xi}\right) + O(L^{-2}).
\]

The first two terms on the right hand are well defined for any fixed \(\Delta\) or \(\xi\) by studying the asymptotic limit \(L \gg \xi\) (we will see that in this limit \(f(L/\xi)\) is exponentially small). Once \(\bar{\epsilon}(\xi)\) and \(b(\xi)\) are known one may study the double scaling \(\lim_{L \to \infty} L/\xi = \text{const}\) (we will see that in this limit \(f(L/\xi)\) is exponentially small). Once \(\bar{\epsilon}(\xi)\) and \(b(\xi)\) are known one may study the double scaling \(L \rightarrow \infty\) and \(\xi \rightarrow \infty\), while \(w = L/\xi = \text{const}\). The scaling function \(f(w)\) is defined then as

\[
 cf(w) = \lim_{w \xi = L \to \infty} L \left( L \bar{\epsilon}(\xi) + b(\xi) - E(L,\xi) \right).
\]

According to Eq. (1), \(f(0) = \pi/24\). Universality of the scaling function \(f(w)\) for \(w \neq 0\) and its ability to distinguish between topological sectors is the subject of this work.

FIG. 1: (Color online) The solid line is the scaling function \(f\). Here \(w > 0\) (< 0) represents the topological non-trivial (trivial) side of the transition (the edge states exist for \(w > 1\), see the main text). Symbols are numerical results for lattice models of non-interacting fermions in five symmetry classes; after Ref. [9].

The scaling function was studied\(^6\) for the class of 1+1D topological models of non-interacting fermions. It was shown that it is universal for all symmetry classes, admitting non-trivial topology in 1D\(^1\)\(^2\)\(^3\)\(^4\)\(^5\)\(^6\)\(^7\)\(^8\)\(^9\)\(^10\)\(^11\)\(^12\) AIII, DIII, CI, where \(c = 1\) and BDI and D, where \(c = 1/2\), see Fig. 1. Moreover, it was shown that the corresponding \(f(w)\) may be derived from the Dirac Hamiltonian, e.g. in AIII symmetry class \((c = 1)\), \(H = m \sigma_1 + i \partial_x \sigma_2\), where the Pauli matrices act in sublattice \(A/B\) space. The model is equivalent to two copies of \(c = 1/2\) Majorana fermions.
Assuming that outside of the interval $0 < x < L$ the gap is very large and, e.g., negative one derives the boundary conditions $\Psi_A(0) = \Psi_B(L) = 0$. The quantized values of momentum $k > 0$ are then given by

$$\cos(kL + \delta(k)) = 0; \quad \tan \delta(k) = \frac{m}{k L}. \quad (4)$$

As a result the spectrum is determined by the condition $w \equiv L m = k_n L \cot(k_n L)$ and the energies are given by $\epsilon_{\pm}(k_n) = \pm \sqrt{m^2 + k_n^2}$. At $w = 1$ two of its real solutions collide and switch to purely imaginary ones for $w > 1$. Those correspond to the topological edge states, decaying into the bulk of the system.

The total ground state energy is given by $E(L, \xi) = \sum_n \epsilon_{\pm}(k_n)$, which, using the argument principle, may be written as

$$E(L, \xi) = \frac{1}{2} \int \frac{dk}{2 \pi i} \epsilon_{\pm}(k) \partial_k \ln [\cos(kL + \delta(k))], \quad (5)$$

where the contour runs in the complex $k$-plane encircling all solutions of Eq. (4). The bulk and boundary terms are given by $L c + b = \{ (dk/2\pi) \epsilon_{\pm}(k) [L + \partial_k \delta(k)] \}$, where $L + \partial_k \delta(\xi)$ are bulk and boundary parts of the continuous density of states. To find the scaling function $f(w)$ one employs Eq. (3), deforms the integration contour to run along the branch cut of $\sqrt{m^2 + k^2}$ and rescales the integration variable as $z = ik L$. As a result, one finds [9]

$$f(w) = -\int_0^\infty \frac{dz}{\pi} \frac{\sqrt{z^2 - w^2}}{\partial_z \ln [1 + e^{-2z - 2\delta_w(z)}]}, \quad (6)$$

where $\delta_w(z) = -\arctanh(w/z)$. This expression is plotted as a solid line in Fig. 1.

One may see that the scaling function is markedly asymmetric between the topological non-trivial, $w > 0$, and topological trivial, $w < 0$, sides. This is a feature of an open system. Indeed, similar calculation for periodic boundary conditions results in a symmetric function. [9]

On the other hand, a specific shape of the boundary (e.g., a shape of the gap $m(x)$ near the boundary) does not change the scaling function. This suggests that the asymmetry is due to the presence of the edge states on the topological non-trivial side of the transition. This is corroborated with the fact that the maximum of the scaling function (i.e., maximum sensitivity to the finite size effects) occurs at $w = 1$, i.e. $\xi = L$, which is exactly the point where the edge states (wave function $e^{i k_n x}$ with purely imaginary wavenumber $k_n$) appear. Glancing at the scaling function, one would be hard-pressed to locate the point of the bulk phase transition. However, a more accurate look reveals a non-analytic behavior of the form $f(w) \approx \frac{\pi}{2x} - \frac{\pi}{2} \log |w|$ close to $w = 0$, marking the bulk transition point.

Our goal here is to verify if the scaling function Eq. (6) is applicable beyond the simple models of non-interacting fermions. To this end we evaluate it for bilinear-biquadratic spin-1 chain, using variational Matrix Product State (MPS) approach [10] and variational uniform MPS (VUMPS) algorithm [10]. The model undergoes a topological phase transition between dimerized and Haldane phases [14]. The transition is known [13] to be described by a CFT with $c = 3/2$.

We conclude that, to the best of our numerical precision, the scaling function of bilinear-biquadratic spin-1 chain is indeed in agreement with the analytical result, Eq. (6). This fully supports the theory [13,25] that the low energy physics of the model is equivalent to that of three species of massive Majorana fermions. According to our results, this correspondence goes beyond the bulk of the spectrum and encompasses the finite size physics, including the edge states. It is probably exact in the double scaling limit, Eq. (3). So far we are not aware of any counterexamples of scaling form Eq. (2) with the scaling function Eq. (6) among 1+1 D topological transitions.

The paper is organized as follows: In Section II we introduce the model and discuss our numerical results for the scaling function. In Section III we describe the variational MPS approach and VUMPS algorithm as well as details of our numerical approach.

II. THE MODEL AND SCALING FUNCTION

The model we study is the bilinear-biquadratic spin-1 chain with the Hamiltonian

$$H = \sum_{i=1}^{L} \cos \theta (\vec{S}_i \cdot \vec{S}_{i+1}) + \sin \theta (\vec{S}_i \cdot \vec{S}_{i+1})^2, \quad (7)$$

where $\vec{S}_i$ is the spin-1 operator at site $i$ and $\theta$ is a parameter that controls the relative strength between the bilinear and biquadratic interactions. This model exhibits a rich phase diagram when $\theta$ is varied between $-\pi$ to $\pi$. In particular, $\theta = 0$ is the Heisenberg point [10], and $\theta = \arctan \frac{1}{L}$ is the AKLT model [23] with a known exact ground state.
The quantum phase transition we concentrate on is between the Haldane phase: \(-\frac{\pi}{4} < \theta < \frac{\pi}{4}\) and the dimerized phase: \(-\frac{3\pi}{4} < \theta < -\frac{\pi}{4}\), (see Fig. 3). The system is gapped in the Haldane phase with a unique ground state under periodic boundary condition (PBC) and 4-fold degenerate (in the thermodynamic limit) ground states under open boundary condition (OBC). The model undergoes the topological transition at \(\theta = -\frac{\pi}{4}\) to a gapped dimerized phase with doubly degenerate ground states under PBC and a single ground state under OBC. At the critical point \(\theta = -\frac{\pi}{4}\), the model is integrable via the Bethe ansatz, and is known as Babudjan-Takhtajan model. The critical model is gapless and the spin-spin correlation function exhibits power law behavior. The low energy physics is described by the SU(2)\(_{\text{2}}\) Wess-Zumino-Witten (WZW) model, with a central charge \(c = 3/2\).

We evaluate the ground state energy and the correlation length of the model with the help of variational MPS approach and VUMPS algorithm. Details of the method and the scaling function evaluation are described in the next section. Our results are presented in Fig. 3. Even for our largest systems there is still a slow size dependence of the scaling function. It very much looks like it tends to converge to the limiting form, given by non-interacting fermions, Eq. (6).

This result is not entirely surprising. Based on Affleck-Haldane realization that the critical point is described by \(c = 3/2\) CFT, Tsvelik argues that the vicinity of the transition may be described by three species of massive Majorana spinors, \(\tilde{\chi}^a\), where \(a = 1, 2, 3\). This statement is based on the analysis of relevant perturbations around SU(2)\(_{\text{2}}\) conformal point. For level \(k\) WZW theory the primary fields are classified by their spin representation, \(j\), and have conformal dimensions \(2(j+1)/(2+k)\). For \(k = 2\), spin-1/2 field has dimension 3/8, while dimension of spin-1 perturbation is 1. The former is non-local in Majorana fields, and odd upon translation by one lattice site. As a result, it can’t be present in translationally invariant models. The spin-1 perturbation, on the other hand, is even under translations, local and quadratic in Majorana’s, \(\tilde{\chi}^a\tilde{\chi}^a\). There is also a composite marginal (dimension 2) operator allowed by the symmetries of the form \(J_a^\mu J_a^\mu\), where the chiral currents are \(J_a^\mu = i\tilde{\epsilon}^{abc}\tilde{\chi}^b\gamma_\mu\tilde{\chi}^c\) and \(\gamma_0 = \gamma_x\gamma_1 = i\sigma_y\). As a result, the low energy Lagrangian close to the transition acquires a form

\[
\mathcal{L} = i\tilde{\chi}^a\gamma_\mu\partial_\mu\tilde{\chi}^a - m\tilde{\chi}^a\tilde{\chi}^a - \lambda J_a^\mu J_a^\mu \tag{8}
\]

where the mass \(m \propto \Delta = \theta + \pi/4\) and \(\lambda\) is a marginal coupling. As shown in Ref. (22) the role of the marginal four-fermion term is to renormalize the excitation gap, \(\Delta\), as

\[
\Delta = m (1 + \lambda a \log m), \tag{9}
\]

where \(a\) is of the order of the lattice spacing. We will show in the next section that the inverse correlation length, \(1/\xi \propto \Delta\), may be indeed reasonably well fit with with this expression.

After the renormalization Eq. (9) the low-energy spectrum of the model is given by the three species of Majoranas (with the renormalized mass). Remarkably this statement goes beyond the bulk of the spectrum, but also encompasses the finite size effects, including the energies of the edge states. This illustrates a remarkable universality of \(1 + 1\) topological transitions. This universality is not limited to the transition point, but extends away from it as long as the correlation length is large. The peculiarities of individual models are packed into a number of Majoranas and a specific (non-universal) dependence of their correlation length (inverse excitation gap) on the parameters.

![Figure 3](image-url)
III. ALGORITHMS

A. Variational MPS approach

Here we provide a brief recap of the variational MPS approach\textsuperscript{13–15}. Consider a one-dimensional chain of \( L \) sites and \( d \) dimensional local state space \( | \sigma_i \rangle \) on site \( i \). For interacting systems, the Hilbert space of the chain grows exponentially with the number of sites. A generic pure many-body state is

\[
| \psi \rangle = \sum_{\sigma_1, \ldots, \sigma_L} c_{\sigma_1, \ldots, \sigma_L} | \sigma_1, \ldots, \sigma_L \rangle ,
\]

with \( d^L \) coefficients \( c_{\sigma_1, \ldots, \sigma_L} \). One can find a more local representation of the state by using singular value decomposition (SVD): for any arbitrary rectangular matrix \( M \) there exists SVD: \( M = USV^\dagger \). Suppose \( M \) is of dimension \( m \times n \), then \( U \) is of dimension \( m \times \min(m,n) \) and is left normalized, i.e. \( U^\dagger U = I \); \( V \) is of dimension \( n \times \min(m,n) \) and is right normalized, i.e. \( VV^\dagger = I \); \( S \) is a diagonal matrix of dimension \( \min(m,n) \) with non-negative entries \( s_i \), called singular values.

![Graphical representation of (a) a general matrix product state (b) a general matrix product operator. Solid circles/squares represent local tensors. Vertical bonds represent physical indices while horizontal bonds represent auxiliary indices.](image)

By applying successive SVDs to the array of coefficients, the quantum state in Eq. (10) can be represented as a product of local tensors, or the so-called matrix product state:

\[
| \psi \rangle = \sum_{\sigma_1, \ldots, \sigma_L} M^{\sigma_1} M^{\sigma_2} \cdots M^{\sigma_{L-1}} M^{\sigma_L} | \sigma_1, \ldots, \sigma_L \rangle .
\]

The tensor \( M^{\sigma_{i-1}, a_i} \) on site \( i \) has 3 indices. Here \( \sigma_i \) is a physical index, which corresponds to the dimension of local state space \( d \). While \( a_{i-1}, a_i \) are two auxiliary indices. They count the left and right bonds through which the local state is connected to the left and right neighboring sites. The dimension of the bonds blow up exponentially with the distance to the edges: \( \text{dim}(\text{bond } a_i) = \min(d^i, d^{L-i}) \), which means the decomposition itself does not reduce the complexity of calculation. In order to avoid exponential growth, it is demanded that the bond dimensions have a ceiling of \( D \). The auxiliary space can be truncated due to the fact that the singular values of matrix \( M^{\sigma_i} \) decay very fast. Therefore the exact SVD can be replaced by an approximate one: \( M_{a_{i-1}, a_i} \approx \sum_{a=1}^D U_{a_{i-1}, a} S_{a} V_{a, a_i}^\dagger \). Note that the summation index \( a \) runs over the largest \( D \) singular values instead of \( \min(d\text{dim}(\text{bond } a_{i-1}), \text{dim}(\text{bond } a_i)) \). With this approximation, the bond dimension of the MPS representation is limited by \( D \). The fast decay of singular values is guaranteed by the area law for gapped systems; in critical systems, the decay is slower and the choice of \( D \) depends on the system size. Also one should keep in mind that in general tensor \( M^\sigma \) are different on each site.

![Graphical representation of the eigenvalue problem for optimization of a single-site tensor. The unknown tensor is circled with red color. Usually two-sites tensors are used in practical calculations.](image)
B. VUMPS algorithm

We now recap the variational uniform MPS (VUMPS) algorithm[12], which deals with systems in the thermodynamic limit $L \to \infty$. In this case, the ground state approximation is constructed by a translation invariant uniform MPS, i.e. same single MPS tensor $M^\sigma$ (or a unit cell of several tensors) on all sites:

$$|\psi\rangle = \sum_\sigma (\cdots M^{\sigma_{i-1}} M^{\sigma_i} M^{\sigma_{i+1}} \cdots) \mid \sigma \rangle. \quad (14)$$

By local gauge transformation, the above state can be brought into a left/right canonical representation with left/right normalized tensors $A/B$ that satisfy:

$$\sum_\sigma A^{\sigma\dagger} A^{\sigma} = 1, \quad \sum_\sigma A^{\sigma} \rho_A A^{\sigma\dagger} = \rho_A,
\sum_\sigma B^{\sigma\dagger} B^{\sigma} = 1, \quad \sum_\sigma B^{\sigma} \rho_B B^{\sigma\dagger} = \rho_B. \quad (15)$$

Here $\rho_A$ and $\rho_B$ are the reduced density matrices of the bipartited system.

With the help of left and right normalized tensors, we cast the state into a mixed canonical representation:

$$|\psi\rangle = \sum_\sigma (\cdots A^{\sigma_{i-1}} M^{\sigma_i}_C B^{\sigma_{i+1}} \cdots) \mid \sigma \rangle, \quad (16)$$

where the center site tensor $M^\sigma_C$ is related to the left/right normalized tensor by a bond matrix $C$:

$$M^\sigma_C = A^\sigma C = C B^\sigma. \quad (17)$$

In fact, bond matrix $C$ relates the left and right normalized tensor $A$ and $B$ by a gauge transformation $A^\sigma = C B^\sigma C^{-1}$ and allows the arbitrary shift of center site tensor on the chain. Furthermore, by applying the normalization condition and fixed point relation in Eq. (15), one can verify that $\rho_A = C C^\dagger$ and $\rho_B = C^\dagger C$.

In order to find the ground state in the thermodynamic limit, we again apply the Hamiltonian to the uniform MPS we constructed in Eq. (16) and solve the effective eigenvalue problem. But instead of sweeping through the entire chain (which destroys the translational symmetry of the state), we only solve for the center site tensor $M^\sigma_C$ and the bond matrix $C$. We then compute the left and right normalized tensors by Eq. (17) and update the state globally. Convergence is considered to be reached when the tensor $M^\sigma_C$ no longer changes.

IV. DETAILS OF THE SIMULATIONS

The ground state energy of finite size system is calculated by regular variational MPS approach with truncation error at order $10^{-12}$. To obtain the average bulk energy density $\bar{\epsilon}$, we consider the ground state energy of uniform MPS at different bond dimension $D$. By plotting the energy density $\epsilon$ as a function of inverse bond dimension and fitting the relationship using a power law, $\bar{\epsilon}$ is extrapolated by letting bond dimension $D \to \infty$, see Fig. 7. The average ground state energy per spin, $\bar{\epsilon}$, is plotted as a function of tuning parameter $\theta/\pi$ in Fig. 8 (similar result was obtained in Ref. [32]). At criticality, $\theta/\pi = -1/4$, the ground state energy is known[24,25] from the Bethe ansatz to be $\bar{\epsilon} = -2\sqrt{2} = -2.828427$; our numerical result is $-2.828426$.

![Fig. 7: Log-log plot of the variational ground state energy of uniform MPS as a function of inverse bond dimension.](image)

The blue "+" symbols represent for numerical data (at $\theta = -\pi/4 + 0.3$). The plot follows a power law fit $\epsilon(D^{-1}) = \bar{\epsilon} + a(D^{-1})^b$ where $a$ and $b$ are fitting parameters.

The boundary term, $b$, is found by subtracting the total bulk energy from the ground state energy for some large system size. Fig. 9 shows that $E(L, \theta/\pi) - L\bar{\epsilon}(\theta/\pi)$ gets saturated as system size increases. The limit size used in this paper is $L = 512$.

The correlation length can be calculated through the eigenvalues of the transfer matrix of the uniform MPS state. The transfer matrix is defined as

$$T = \sum_\sigma \tilde{M}^\sigma \otimes \tilde{M}^\sigma, \quad (18)$$

where $\tilde{M}^\sigma$ is the repeated tensor on each site in Eq. (14). One can prove that the eigenvalue of the transfer matrix is bounded by 1 given that the wave function is
FIG. 8: The bulk energy per spin, $\bar{\epsilon}$, vs. parameter $\theta$. The critical point is at $\theta/\pi = -1/4$. Left (right) side of the critical point is the dimerized (Haldane) phase.

FIG. 9: The difference $E(L, \theta) - L\bar{\epsilon}(\theta)$ vs. $\theta$ plotted for different system sizes, $L$. As the system size increases the sub-leading term $cf(L/\xi)/L$ is negligible. The difference thus saturates to the boundary term $b(\theta)$, cf. Eq. (3).

Suppose that the eigenvalues of $T$ is sorted in descending order $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \cdots$ with $\lambda_1 = 1$ to be non-degenerate. Then the correlation function between two operators $O$ with distance $j - i$ is

$$\langle \psi | \hat{O}^{[i]} \hat{O}^{[j]} | \psi \rangle = \cdots T^{[i-1]} | T^{[j]} T^{[i+1]} \cdots T^{[j-1]} | T^{[j]} T^{[j+1]} \cdots = \sum_k \langle 1 | T^{[j]} O | k \rangle \lambda_k^{j-i-1} \langle k | T^{[j]} O | 1 \rangle. \quad (19)$$

Here $|k\rangle$ and $\langle k|$ are the right and left eigenvectors of transfer matrix $T$ which corresponds to eigenvalue $\lambda_k$. Thus the correlator is a superposition of exponentials with the decay lengths $\xi_k = -1/\ln \lambda_k$. And the MPS two-point correlation function have the generic form:

$$\frac{\langle \psi | \hat{O}^{[i]} \hat{O}^{[j]} | \psi \rangle}{\langle \psi | \psi \rangle} = c_1 + \sum_{k=2}^D c_k e^{-r/\xi_k}, \quad (20)$$

where $r = |j - i - 1|$ and $c_k = \langle 1 | T^{[j]} O | k \rangle \langle k | T^{[j]} O | 1 \rangle$.

The correlation length is defined by the largest decay length $\xi = -1/\ln \lambda_2$. As the bond dimension $D$ of tensor $M^\sigma$ increases, the correlation length is saturated. To be more specific, the inverse of correlation length is related to the inverse of log $D$ by a power law$^{[3]}$. If we denote $\Delta = \xi^{-1}$ and $\chi = (\log D)^{-1}$, then $\Delta(\chi) = \bar{\Delta} + a\chi^b$ is shown in Fig. 10.

FIG. 10: Log-log plot of the inverse of correlation length $\Delta$ as a function of inverse of log($D$). The blue ‘+’ symbols represent for numerical data (at $\theta = -\pi/4 + 0.3$). The plot follows a power law fit $\Delta(\chi) = \bar{\Delta} + a\chi^b$ where $a$ and $b$ are fitting parameters.

FIG. 11: Inverse correlation length $\xi^{-1}$ vs. deviation from critical point $\Delta \theta = \theta + \pi/4$. Here $\Delta \theta > 0$ ($< 0$) represents Haldane (dimerized) phase.

The calculated inverse correlation length $\xi^{-1}$ vs. $\Delta \theta$ is shown in Fig. 11. In Fig. 12 we fit $(\xi \Delta \theta)^{-1}$ with $a_1 + a_2 \log \Delta \theta$, which is the expected dependence due to the renormalization by marginal composite four-Majorana operator, Eq. (9). The fit is rather satisfactory, though we do not know how to independently verify the fitting parameter $a_{1,2}$ on the two sides of the transition.

Finally we show, Fig. 13, convergence of the scaling function Eq. (3) towards the free Majorana result, Eq. (6), for small system sizes (the larger sizes are shown in Fig. 3 (a)).
FIG. 13: Scaling function $f(w)$ is plotted, where $w = L/\xi$. Points of different color represent calculations for different system sizes. The solid lines are guides for an eye. The black solid line is the analytical result Eq. (6).

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Appendix A: Details of the variational MPS approach

The MPO representation of the Hamiltonian (7) is shown below:

$\mathcal{H} = \hat{W}^{[1]} \hat{W}^{[2]} \ldots \hat{W}^{[L]}$, \hspace{1cm} (A1)

where matrix $\hat{W}^{[i]}$, $i \in [2, L - 1]$ has zero entries except first column $\hat{W}^{[i]}_{A1}$ and last row $\hat{W}^{[i]}_{L, A1}$.

$\hat{W}^{[i]}_{A1} = [ \hat{I} \hat{S}^+ \hat{S}^- \hat{S}^z \hat{S}^+ \hat{S}^- \hat{S}^z \hat{S}^+ \hat{S}^- \hat{S}^z \hat{S}^+ \hat{S}^- \hat{S}^z \hat{S}^+ \hat{S}^- \hat{S}^z ]$

$\hat{W}^{[i]}_{L, A1} = [ 0 \cos \theta / 2 \hat{S}^+ \cos \theta / 2 \hat{S}^- \cos \theta \hat{S}^z \sin \theta / 4 \hat{S}^+ \hat{S}^- \hat{S}^2 \sin \theta / 4 \hat{S}^z \sin \theta \hat{S}^2 ]$

The matrices on two ends: $\hat{W}^{[1]} = \hat{W}^{[i]}_{A1}$ is a pure row matrix and $\hat{W}^{[L]} = \hat{W}^{[i]}_{L, A1}$ is a column matrix.

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