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RAPID COMMUNICATION

Structure of continuous matrix product operator for transverse field Ising model: An analytic and numerical study

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We study the structure of the continuous matrix product operator (cMPO)[1] for the transverse field Ising model (TFIM). We prove TFIM's cMPO is solvable and has the form $T = \mathrm{e}^{-\frac{1}{2}\hat{H}_\mathrm{F}}$. $\hat{H}_\mathrm{F}$ is a non-local free fermionic Hamiltonian on a ring with circumference β, whose ground state is gapped and non-degenerate even at the critical point. The full spectrum of $\hat{H}_\mathrm{F}$ is determined analytically. At the critical point, our results verify the state–operator-correspondence[2] in the conformal field theory (CFT). We also design a numerical algorithm based on Bloch state ansatz to calculate the low-lying excited states of general (Hermitian) cMPO. Our numerical calculations coincide with the analytic results of TFIM. In the end, we give a short discussion about the entanglement entropy of cMPO's ground state.

Keywords: continuous matrix product operator, transverse field Ising model, state–operator-correspondence

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1. Introduction

Tensor network approaching thermal states has a long history. Back in the age of the density matrix renormalization group, the transfer matrix renormalization group[3] based on Trotter decomposition has been developed to calculate thermodynamic quantities of low-dimensional strongly correlated systems. Recently, a new tensor structure named continuous matrix product operator (cMPO)[1] has been developed. Different from previous methods, cMPO eliminates imaginary-time discretization error.

Before going to the theme, we should give a brief review of cMPO to familiarize readers with the relevant notations and more importantly, to show the mechanism behind cMPO. For simplicity, we consider a Hamiltonian with nearest interaction (although in general, cMPO method is suitable for more complex interactions, even for long-range interactions[1])

$$\hat{H} = -\sum_i L_i R_{i+1} - \sum_i Q_i, \tag{1}$$

where i is the label of lattice site. Q_i, L_i, and R_i are local operators living on the Hilbert space of the single site i. Considering the evolution operator $\mathrm{e}^{-\tau\hat{H}}$, the first-order approximation $1-\tau\hat{H}$ can be represented as a matrix product operator (MPO) whose unit cell is an infinitesimal tensor parameterized by τ, as shown in Figs. 1(a) and 1(b),

$$t_{ij} = \begin{pmatrix} \mathbf{1}+\tau Q & \sqrt{\tau}L \\ \sqrt{\tau}R & \mathbf{0} \end{pmatrix}_{ij}, \tag{2}$$

where τ is the infinitesimal discretization step, and ij are index of the auxiliary space. The transfer matrix T is given by tracing out the physical index of the product of the unit cells t vertically (along β direction). At the same time, we consider a matrix product state (MPS) $|\Phi\rangle$ whose unit cell is $\varphi_i = \begin{pmatrix} \mathbf{1}+\tau Q_\mathrm{b} \\ \sqrt{\tau}R_\mathrm{b} \end{pmatrix}_i$, where the subscript b means boundary to distinguish with tensor elements of t_{ij}. For the same reason, the sandwich structure (φ, t, φ), a three sites MPO with open boundary condition, can be viewed as the first-order approximation of evolute operator $\mathrm{e}^{-\tau\hat{H}_\mathrm{aux}}$, where $\hat{H}_\mathrm{aux} = -\bar{Q}_\mathrm{b}\otimes 1\otimes 1 - 1\otimes Q\otimes 1 - 1\otimes 1\otimes Q_\mathrm{b} - \bar{R}_\mathrm{b}\otimes R\otimes 1 - 1\otimes L\otimes R_\mathrm{b}$ is an auxiliary three-site Hamiltonian with open boundary condition. As shown in this paper,[1] by taking $\tau\to 0$, the overlap $\lim_{\tau\to 0}\langle\Phi|T|\Phi\rangle = \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{H}_\mathrm{aux}}$ has a well-defined limit, where the infinitesimal parameter τ eliminates, see Fig. 1(c). When $\tau\to 0$, the (discrete) MPS $|\Phi\rangle$ becomes a continuous matrix product state (cMPS)[4] while the (discrete) transfer matrix becomes a cMPO, named by the authors in Ref. [1], as shown in Fig. 1(d),

$$T = \lim_{\tau\to 0}\mathrm{Tr}[\otimes t], \tag{3}$$

which can be viewed as a continuous transfer matrix without discretization error. The corresponding partition function is the product of cMPO: $Z = \mathrm{Tr}[T^L]$, if we assume the system has L sites. In the thermodynamic limit $L\to\infty$, the free energy per site f is determined by the dominate eigenvalue Λ_0 of cMPO: $\beta f = -\ln\Lambda_0$.

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In cMPO's framework, the key point is, under the assumption the dominate eigenstate $|\Phi\rangle$ (we name it the ground state in the following) of transfer matrix T can be approximated by a matrix product state (MPS) in some sense, when taking discretization step τ to be zero, the overlap $\langle\Phi|T|\Phi\rangle$ is well-defined and at the same time the ground state $|\Phi\rangle$ is parameterized as a cMPS, as we have explained above.

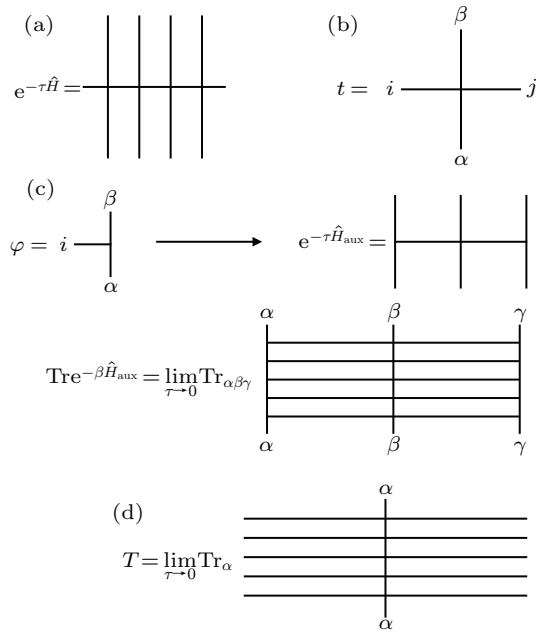


Fig. 1. The graphic representation of cMPO. (a) The unit cell of cMPO can be constructed from the corresponding infinitesimal evolution operator $e^{-\tau\hat{H}}$. (b) The graphic representation of cMPO 's unit cell tensor t, where $\{ij\}$ is the virtual index, while $\{\alpha\beta\}$ is the physical index. (c) By introducing a cMPS $|\Phi\rangle$ with unit cell tensor φ, the sandwich structure $\langle\Phi|T|\Phi\rangle$ is well-defined when $\tau\to0$ in cMPO method. The auxiliary hHamiltonian $\hat{H}_{\rm aux}$ is independent of τ. (d) cMPO is a transfer matrix by taking $\tau\to0$ if the continuum limit truly exists.

However, strictly speaking, although the existence of the overlap $\langle\Phi|T|\Phi\rangle$ at continuum limit $\tau\to0$ is enough for numerical calculation in cMPO method, the existence of cMPO T at the operator level as the continuum limit of certain (discrete) MPO, which has been defined in Eq. (3), remains to be verified. In another word, we could ask whether the transfer matrix T is a well-defined (continuous) operator when taking discretization error to be zero? As we have pointed out in the last paragraph, cMPO seems to be an intermediate notation in practical calculation: if we assume $|\Phi\rangle$ is a cMPS, then the overlap $\langle\Phi|T|\Phi\rangle$ is well-defined, no matter whether T can exist individually as an operator or not when discretization step τ to be zero.

In this work, we try to answer the above question in some sense by studying a simple model: the transverse field Ising model (TFIM). Our answer is yes, at least for TFIM, cMPO has the form $T=e^{-\frac{1}{2}\hat{H}_{\rm F}}$, where $\hat{H}_{\rm F}$ is some physical Hamiltonian on a ring with length β. The operator formalism of cMPO contains more physical information. Not only the ground state is important, from which we can calculate the free energy and local thermodynamic quantities of TFIM; the low-lying excited states are also useful, which encode information of different kinds of correlation lengths. Especially at the critical point, for quantum Hamiltonian on a ring, the spectrum of low-lying eigenstates corresponds to critical exponents according to the state–operator-correspondence in CFT.[2] Since TFIM's cMPO is solvable, we analytically analyze the cMPO's critical behavior and read out the conformal data explicitly, which verifies the CFT's description. Based on the analytic analysis of TFIM, we develop a more general numerical algorithm for excitation calculation, which is suitable for general Hermitian cMPO. We use TFIM's analytic results as a benchmark. In the end, we also give a short discussion about the entanglement entropy of the ground state. We find that the entanglement entropy is finite even at the critical point for TFIM. This result may explain the rationality of the cMPS approximation of the ground state.

This paper is organized as follows. In Section 2, we show the solvability of TFIM's cMPO through building an exact map to free fermion at arbitrary discrete trotter step τ and then taking continuum limit. The explicit form of cMPO is given in fermion representation: $T=e^{-\frac{1}{2}\hat{H}_{\rm F}}$, where $\hat{H}_{\rm F}$ is a non-local free Hamiltonian. In Section 3, we analyze the cMPO's structure at the scaling limit, where non-local Hamiltonian $\hat{H}_{\rm F}$ reduces to the free Majorana quantum field theory (QFT). At the critical point, the central charge $c=1/2$, critical exponents of spin and energy $x_\sigma=1/8, x_\varepsilon=1$ are explicitly calculated from the analytic spectrum, which coincides with the description of Ising CFT. In Section 4, we review the techniques of cMPS and Bloch state ansatz for excitation.[5] A numerical algorithm based on Bloch state ansatz is stated, which can be used to calculate cMPO's excitation for the general model. A benchmark for TFIM's analytic results is provided. In Section 5, we numerically calculate the entanglement entropy of cMPO's ground state both at critical and off-critical points by diagonalizing the subsystem's correlation matrix under the small trotter step.[6,7] Taking the trotter step to be zero, we could also derive an integral equation as the continuum limit of the correlation matrix. Finally, in Section 6, we give a summary and outlook.

We leave the tedious technical details in the Appendix. In Appendix A, we review the diagonalization procedure of the transfer matrix for arbitrary trotter step τ. In Appendix B, we show how to take the continuum limit to get the operator formalism of TFIM's cMPO. In Appendix C, we show the detailed calculation of the correlation matrix and the corresponding integral equation as its continuum limit. In Appendix D, we give the analytic expressions of the ground state's correlations at the continuum limit for TFIM's cMPO. In Appendix E, we prove at classical Ising limit $h=0$, cMPO's ground state has a simple cMPS representation. In Appendix F, we explain the explicit tensor constructions for our numerical algorithm.

2. Operator formalism of cMPO

The Hamiltonian of the 1D transverse field Ising model is

$$\hat{H} = -J\sum_i \sigma_i^x \sigma_{i+1}^x - h\sum_i \sigma_i^z \tag{4}$$

as a special case of Eq. (1), the corresponding cMPO's unit cell is

$$t = \begin{pmatrix} \mathbf{1}+\tau h\sigma^z & \sqrt{\tau J}\sigma^x \\ \sqrt{\tau J}\sigma^x & \mathbf{0} \end{pmatrix}. \tag{5}$$

In this section, we prove TFIM's cMPO defined above has the following operator formalism:

$$T = \mathrm{e}^{-\frac{1}{2}\hat{H}_{\mathrm{F}}}, \tag{6}$$

where $\hat{H}_{\mathrm{F}}$ is a free fermionic Hamiltonian living on a ring of length β. $\hat{H}_{\mathrm{F}}$ is diagonal in $\{\eta_k\}$ representation, which is the momentum space representation following a Bogoliubov transformation. The explicit expression of $\hat{H}_{\mathrm{F}}$ is given in Eq. (14). The corresponding spectrum and Bogoliubov angle are given in Eqs. (15)–(17). We can use Eq. (19) to find the coordinate space representation of $\hat{H}_{\mathrm{F}}$, which is a non-local QFT.

We prove Eq. (6) in two steps. In the first step, we solve the transfer matrix T under arbitrary trotter step τ. In the second step, we take τ to be zero to find the continuum limit of T. While in the first step, an important trick is employed: instead of using t in Eq. (5), we can use $\tilde{t}$ in Eq. (11) as the unit cell of cMPO, since $\tilde{t}$ and t are the same infinitesimal tensor up to the first order of τ: $\tilde{t} = t + \mathcal{O}(\tau^2)$. When $\tau \to 0$, $T = \mathrm{Tr}[\otimes t]$ and $\tilde{T} = \mathrm{Tr}[\otimes \tilde{t}]$ will correspond to the same cMPO, if the continuum limit truly exists.

We divide this section into two parts. In part I, we construct $\tilde{t}$, which is the same infinitesimal tensor as t when $\tau \to 0$, from the MPO representation of infinitesimal evolution operator $\mathrm{e}^{-\tau\hat{H}}$ and prove the solvability of transfer matrix $\tilde{T} = \mathrm{Tr}[\otimes\tilde{t}]$ at arbitrary trotter step τ. In part II, we show the operator formalism of cMPO T truly exists at the continuum limit and give its explicit form analytically.

2.1. Solvability at arbitrary trotter step τ

2.1.1. construct unit cell $\tilde{t}$

Motivated by the paper,[8] we consider the second order trotter approximation $\mathrm{e}^{-\tau\hat{H}} = V(\bar{K}_1, K_2) + \mathcal{O}(\tau^3)$, with

$$\begin{aligned} V(\bar{K}_1, K_2) &= V_1^{\frac{1}{2}}(\bar{K}_1) V_2(K_2) V_1^{\frac{1}{2}}(\bar{K}_1), \\ V_1(\bar{K}_1) &= \exp\left(\bar{K}_1 \sum_{j=1}^{N} \sigma_j^z\right), \\ V_2(K_2) &= \exp\left(K_2 \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x\right), \end{aligned} \tag{7}$$

where the trotter step τ is defined by $\beta = N\tau$, and $\bar{K}_1 = \tau h$, $K_2 = \tau J$. The functional relation between K and $\bar{K}$ is defined as $\bar{K} = \frac{1}{2}\ln(\coth K)$. As the result, we have $\bar{K}_2 = \frac{1}{2}\ln(\coth K_2)$ and $K_1 = \frac{1}{2}\ln(\coth \bar{K}_1)$, which will be used in the following.

As shown in Refs. [8,9], $V(\bar{K}_1, K_2)$ can be written as a MPO

$$V(\bar{K}_1, K_2) = \sum_{\{i\}} \tilde{t}_{i_1 i_2}^{\alpha_1\beta_1} \tilde{t}_{i_2 i_3}^{\alpha_2\beta_2} \cdots \tilde{t}_{i_N i_1}^{\alpha_N\beta_N}(K_1, K_2) \tag{8}$$

whose unit cell is denoted as $\tilde{t}$,

$$\begin{aligned} &\tilde{t}_{ij}^{\alpha\beta}(K_1, K_2) \\ &= \sqrt{\frac{2}{\sinh 2K_1}}\hat{O}_{ij}(K_2)\hat{O}_{\alpha\beta}(K_1) + \sqrt{\frac{\sinh 2K_2}{2}}\sigma_{ij}^x\sigma_{\alpha\beta}^x, \end{aligned} \tag{9}$$

where we define the matrix function $\hat{O}(K) = \begin{pmatrix} \cosh K & 0 \\ 0 & \sinh K \end{pmatrix}$ and σ^x is the x-component of Pauli matrix.

When $\tau \to 0$, using Taylor expansion about τ, we find tensor $\tilde{t}$ coincides with t up to the first order of τ,

$$\tilde{t}_{ij} = t_{ij} + \mathcal{O}(\tau^2). \tag{10}$$

Since $\tilde{t}$ and t are the same infinitesimal tensor, TFIM's cMPO can be rewritten as $\tilde{T} = \lim_{\tau\to 0}\mathrm{Tr}[\otimes\tilde{t}]$.

2.1.2. Map $\tilde{T}$ to be free fermion

The solvability of $\tilde{T}$ is based on the following algebraic identity:[8]

$$\tilde{T} = [\sinh(2\bar{K}_1)\sinh(2K_2)]^{\frac{N}{2}} V(\bar{K}_2, K_1). \tag{11}$$

In Eq. (11), $\tilde{T}$ is factorized into operator $V(\bar{K}_2, K_1)$ and a scalar factor. Since $V(\bar{K}_2, K_1)$ is also the transfer matrix of the two-dimensional Ising model,[10] $V(\bar{K}_2, K_1)$, and $\tilde{T}$ at the same time, can be mapped to free fermion and exactly solvable.

To prove Eq. (11), we need the following dual relation, which can be easily checked from Eq. (9),

$$\tilde{t}_{ij}^{\alpha\beta}(K_1, K_2) = [\sinh 2\bar{K}_1 \sinh 2K_2]^{\frac{1}{2}} \tilde{t}_{\alpha\beta}^{ij}(K_2, K_1). \tag{12}$$

This functional relation exchanges index $\{ij\}$, $\{\alpha\beta\}$ and variable K_1, K_2 at the same time.

Equation (11) can be proved by substituting Eq. (12) into definition of $\tilde{T}$ and then comparing it with Eq. (8),

$$\begin{aligned} \tilde{T} &= \sum_{\{\alpha\}} \tilde{t}_{i_1 j_1}^{\alpha_1\alpha_2} \tilde{t}_{i_2 j_2}^{\alpha_2\alpha_3} \cdots \tilde{t}_{i_N j_N}^{\alpha_N\alpha_1}(K_1, K_2) \\ &= [\sinh(2\bar{K}_1)\sinh(2K_2)]^{\frac{N}{2}} \sum_{\{\alpha\}} \tilde{t}_{\alpha_1\alpha_2}^{i_1 j_1} \cdots \tilde{t}_{\alpha_N\alpha_1}^{i_N j_N}(K_2, K_1) \\ &= [\sinh(2\bar{K}_1)\sinh(2K_2)]^{\frac{N}{2}} V(\bar{K}_2, K_1). \end{aligned} \tag{13}$$

Technical details about the diagonalization of $V(\bar{K}_2, K_1)$ can be found in the classic paper[10] or Appendix A.

2.2. Operator formalism at the continuum limit

In the continuum limit $\tau \to 0$, cMPO has the well-defined operator formalism $T = \mathrm{e}^{-\frac{1}{2}\hat{H}_\mathrm{F}}$. Detailed calculation can be found in Appendix B. In the free fermion representation, the Hilbert space of $\hat{H}_\mathrm{F}$ splits into two sectors

$$\begin{aligned}
&\hat{H}_\mathrm{F} = \hat{H}_\mathrm{F}^\mathrm{NS}\left(\frac{1+\hat{P}_\mathrm{NS}}{2}\right) + \hat{H}_\mathrm{F}^\mathrm{R}\left(\frac{1-\hat{P}_\mathrm{R}}{2}\right),\\
&\hat{H}_\mathrm{F}^\mathrm{NS/R} = E_0^\mathrm{NS/R} + \sum_{k\in NS/R}\varepsilon_k \eta_k^\dagger \eta_k,\\
&\hat{P}_\mathrm{NS/R} = (-)^{\sum_{k\in\mathrm{NS/R}}\eta_k^\dagger\eta_k},
\end{aligned} \tag{14}$$

where $\hat{P}$ is the parity operator, as the result, $(1\pm\hat{P}_\mathrm{NS/R})/2$ is the projector which restricts the Hilbert space into even/odd particle number sector. The even particle number sector corresponds to subscript NS, named Nuven–Schwartz sector, following the CFT's convention; the odd sector corresponds to subscript R, named Ramond sector. In the NS sector, we have the anti-periodic boundary condition (APBC) and the quantum number of the translational operator is $k \in Z+\frac{1}{2}$; while in the R sector, we have the periodic boundary condition (PBC) with $k \in Z$.

The vacuum energy $E_0^\mathrm{NS/R}$ in the two sectors are

$$\begin{aligned}
\frac{1}{2}E_0^\mathrm{NS} &= -\frac{1}{\pi}\int_0^\pi \ln\left[2\cosh\left(\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}\right)\right]\mathrm{d}\theta,\\
\frac{1}{2}E_0^\mathrm{R} &= -\frac{1}{\pi}\int_0^\pi \ln\left[2\sinh\left(\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}\right)\right]\mathrm{d}\theta\\
&\quad + \frac{1}{4}(|\varepsilon_0|-\varepsilon_0),
\end{aligned} \tag{15}$$

where we have defined $\Gamma = \beta h$ and $K = \beta J$. Since $E_0^\mathrm{NS} < E_0^\mathrm{R}$, the ground state of $\hat{H}_\mathrm{F}$ corresponds to the vacuum of the NS sector.

The quasi-particle excitation spectrum ε_k is

$$\begin{aligned}
&\frac{1}{2}\varepsilon_k = \ln\left(x_k + \sqrt{x_k^2-1}\right), \quad k\neq 0,\\
&\frac{1}{2}\varepsilon_0 = \ln\frac{\Gamma}{K}, \quad k = 0,
\end{aligned} \tag{16}$$

where $x_k = \frac{\pi^2k^2}{2\Gamma K} + \frac{1}{2}\left(\frac{\Gamma}{K}+\frac{K}{\Gamma}\right)$.

The phase angle of Bogoliubov transformation is

$$\begin{aligned}
&\eta_k = \cos\phi_k c_k + \sin\phi_k c_{-k}^\dagger,\\
&\cos 2\phi_k = \frac{\pi^2k^2+(\Gamma^2-K^2)}{2\Gamma K\sqrt{x_k^2-1}},\\
&\sin 2\phi_k = \frac{\pi k}{\Gamma\sqrt{x_k^2-1}}.
\end{aligned} \tag{17}$$

We consider a general eigenstate $\prod_k \eta_k^\dagger|0\rangle_\mathrm{NS/R}$, where $|0\rangle_\mathrm{NS/R}$ is the vacuum in the NS/R sector. Any eigenstate should have even/odd fermion modes in corresponding sector. For example, state $\eta_k^\dagger|0\rangle_\mathrm{NS}$ is forbidden. The corresponding energy and momentum are

$$\begin{aligned}
&E = E_0^\mathrm{NS/R} + \sum_k \varepsilon_k,\\
&P = \sum_k \frac{2\pi k}{\beta} \equiv \frac{2\pi N}{\beta}, \quad N\in Z,
\end{aligned} \tag{18}$$

where the quantum number of momentum N is always an integer in both sectors because of the restriction of particle number parity.

In the continuum limit, the field operator is defined through Fourier transformation,

$$\psi(x=\tau j) \equiv \lim_{\tau\to 0}\frac{1}{\sqrt{\tau}}c_j = \frac{1}{\sqrt{\beta}}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\sum_{k\in\mathrm{NS/R}}\mathrm{e}^{\mathrm{i}\frac{2\pi k}{\beta}x}c_k, \tag{19}$$

where the coordinate position $x\in[0,\beta)$ is defined as $x = \lim_{\tau\to 0}\tau j$. Considering $k\in Z+\frac{1}{2}$ ($k\in Z$) in the NS (R) sector, the field operator $\psi(x)$ satisfies APBC (PBC) in the corresponding sector: $\psi(x+\beta) = -\psi(x)$ ($\psi(x+\beta)=\psi(x)$).

In principle, we can transform the Hamiltonian in Eq. (14) from the momentum space to the coordinate space using Eq. (19). However, for the general parameters J and h, we will have a strongly non-local QFT in coordinate space, where the non-locality reflects $\hat{H}_\mathrm{F}$ has many irrelevant operators and is not a fixed point Hamiltonian. The non-locality of $\hat{H}_\mathrm{F}$ makes the theory ultraviolet (UV) complete and all the physical quantities can be calculated without divergence. For example, the ground state energy density $e = E_0^\mathrm{NS}/\beta$, which corresponds to the free energy density of TFIM, is well-defined.

The free energy density of TFIM determined from the dominant eigenvalue of cMPO: $f = -\frac{1}{\beta}\lim_{L\to\infty}\frac{1}{L}\mathrm{Tr}T^L = -\frac{1}{2\beta}E_0^\mathrm{NS}$ in Eq. (15) verifies the classic result in Ref. [11].

We can also use Eqs. (15) and (16) to calculate the partition function $Z(L,\beta)$ on a torus. Furthermore, to compare with the formula calculated by diagonalization of the physical Hamiltonian, we can explicitly verify the modular invariance of Ising CFT for critical TFIM in the scaling limit. A calculation can be found in Appendix B.

Finally, we should point out that, the spectrum in Eqs. (15) and (16) suggests that, for any finite β, even at the critical point $J=h$, there always exists a finite energy gap of order $1/\beta$, which indicates the finite entanglement entropy of the ground state.

3. Hamiltonian structure at the scaling limit

In this section, we analyze the Hamiltonian structure $\hat{H}_\mathrm{F}$ in Eq. (14) in the coordinate space representation at the scaling limit. To be concrete, we consider the mass perturbation $m = 2(h-J)$ near the critical point $h_\mathrm{c} = J_\mathrm{c} = 1$ at the low temperature limit, where $\beta\gg 1$ and $\beta m = \mathrm{const.} < \infty$.[12] Under such perturbation, we have $\Gamma = \beta(1+\frac{1}{4}m)$ and $K = \beta(1-\frac{1}{4}m)$.

We divide this section into two parts. In the first subsection, we show that the Hamiltonian $\hat{H}_{\rm F}$ is equivalent to the familiar free Majorana QFT at the scaling limit. Although, in general, the Hamiltonian is non-local as explained in Section 2. In the second subsection, we verify the state–operator-correspondence from the Hamiltonian structure explicitly.

3.1. Map to Majorana QFT

In the scaling limit, the short-distance feature washes out. We only care about the behavior at the low-energy scale of order $1/\beta$ corresponding to the long-wavelength limit. We can expand the excitation spectrum and phase angle in Eqs. (16) and (17) at $\beta\to\infty$ to the first order of $1/\beta$,

$$\begin{aligned}
&\varepsilon_k=\sqrt{p^2+m^2}+\mathcal{O}\left(\frac{1}{\beta^2}\right),\quad k\neq 0,\\
&\varepsilon_0=m+\mathcal{O}\left(\frac{1}{\beta^2}\right),\quad k=0,\\
&\sin 2\phi_k=\frac{p}{\sqrt{p^2+m^2}}+\mathcal{O}\left(\frac{1}{\beta^2}\right),\\
&\cos 2\phi_k=\frac{m}{\sqrt{p^2+m^2}}+\mathcal{O}\left(\frac{1}{\beta^2}\right),
\end{aligned}\tag{20}$$

where $p=2\pi k/\beta$ is the momentum mode labeled by k.

We substitute Eq. (20) into the Hamiltonian $\hat{H}_{\rm F}=\sum_k\varepsilon_k:\eta_k^\dagger\eta_k$, and use Eq. (19) to transform the Hamiltonian from momentum space representation into coordinate space representation,

$$\begin{aligned}
\hat{H}_{\rm F}\;=\;&m\int_0^\beta {\rm d}x:\psi^\dagger(x)\psi(x)\\
&-\frac{1}{2}\int_0^\beta {\rm d}x[:\psi^\dagger(x)\partial_x\psi^\dagger(x)-:\psi(x)\partial_x\psi(x)],
\end{aligned}\tag{21}$$

where slightly different from the expression in Eq. (14), we put vacuum energy $E_0^{\rm NS/R}$ to be zero and use the normal order to avoid UV divergence.

Therefore, as shown in Eq. (21), the Hamiltonian $\hat{H}_{\rm F}$ is reduced to a local QFT at the scaling limit. Furthermore, Eq. (21) is nothing but the familiar 1D Majorana QFT. To see this, we introduce the Majorana representation:[12] $\psi(x)=\frac{{\rm e}^{-{\rm i}\frac{\pi}{4}}}{\sqrt{2}}(\chi_2(x)+{\rm i}\chi_1(x))$ and define the real spinor field $\chi(x)=(\chi_1(x),\chi_2(x))$. In this new representation, the Hamiltonian becomes

$$\hat{H}_{\rm F}=\frac{1}{2}\int_0^\beta {\rm d}x:\chi\gamma^0[\gamma^1(-{\rm i}\partial_1)+m]\chi,\tag{22}$$

where $\gamma^0=\sigma^y$, $\gamma^1=-{\rm i}\sigma^x$, which satisfies Dirac's spinor algebra: $\{\gamma^\mu,\gamma^\nu\}=2g^{\mu\nu}$. Here $g^{\mu\nu}=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ is the metric in 1+1D Minkowski space–time.

In the R sector, $\hat{H}_{\rm F}$ has an extra correction $(\varepsilon_0-|\varepsilon_0|)\eta_0^\dagger\eta_0$ in Eq. (22) because of the zero mode.

It is well-known that the effective theory of TFIM is the Majorana QFT. We find the Hamiltonian $\hat{H}_{\rm F}$ of cMPO in Eq. (22) is also the Majorana QFT. This fact reflects the rotation symmetry of Euclidean field theory.

3.2. State–operator-correspondence at $m=0$

When $m=0$, $\hat{H}_{\rm F}$ is critical and restores the conformal symmetry, which can be described by Ising CFT on a cylinder.[13,14]

The state–operator-correspondence[2] relates the central charge c and critical exponents x with the eigenvalues of the transfer matrix $T(u)={\rm e}^{-\hat{H}u}$, which is the evolution operator of time interval u, and $\hat{H}$ is the CFT's Hamiltonian on the cylinder. The central charge c is a universal object in CFT, which corresponds to the ground state energy E_0 through the formula $E_0-e_0l=\frac{\pi c}{6l}$, where l is the system size and e_0 is the ground state energy density at $l\to\infty$. The basic fields in CFT are primary operators $\hat{\phi}_i$, whose correlation functions are algebraic decay with critical exponents x_i on the plane: $\langle\phi_i(x_1)\phi_j(x_2)\rangle\sim\delta_{ij}/|x_1-x_2|^{2x_i}$. For every primary field $\hat{\phi}$, there exists an eigenstate of $\hat{H}$, whose eigenvalue corresponds to the critical exponent x: $E_n-E_0=2\pi x/l$. For Ising CFT, the central charge is $1/2$ and we have three primary fields: identity (1), spin (σ) and energy (ε), which correspond to critical exponents $x_1=0$, $x_\sigma=1/8$ and $x_\varepsilon=1$.[13]

In the cMPO's framework, we exchange the space and time, where we view β as space while the time direction is discrete and labeled by the index of lattice site i. Because of the discretion of time, the continuous evolution operator becomes the discrete cMPO: $T={\rm e}^{-\lambda\hat{H}_{\rm F}}$, where λ is some non-universal normalization factor. In the TFIM case, we will see $\lambda=1/2$ in the following as already shown in Eq. (6). To see the conformal structure of cMPO, we first determine the central charge c and critical exponent x_σ from vacuum energy shift in Eq. (15), where the identity corresponds to ground state $|0\rangle_{\rm NS}$ and the spin operator corresponds to zero mode state in the R sector $\eta_0^\dagger|0\rangle_{\rm R}$ (Remember in R sector, only odd particle number state is allowed). We will also show the energy operator corresponds to the first excited state in the NS sector. Furthermore, since the operator formalism of the free Majorana field in Eq. (22) (with $m=0$) is well known,[13,14] the entire conformal tower structure is obvious. Using transformation relation Eq. (19), we can build a dictionary between fermion representation in Eq. (14) and CFT's operator formalism explicitly.

3.2.1. Determine c and x_σ from vacuum energy shift

As we already explained at the beginning of this subsection, to determine the central charge c, we need to calculate the energy shift of the ground state: $\Delta E_0^{\rm NS}=E_0^{\rm NS}-\beta e_0=-\frac{\pi c}{6\beta}+$ higher orders, where the central charge is determined

by the leading order of $\Delta E_0^{\rm NS}$ according to the state–operator-correspondence. Since the ground state energy density e_0 of TFIM is[11]

$$\beta e_0 = -\frac{1}{\pi}\int_0^\pi \mathrm{d}\theta \sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}. \tag{23}$$

To compare it with Eq. (15), we have

$$\begin{aligned}\Delta E_0^{\rm NS} &= \lim_{\beta\to\infty}\frac{2}{\pi}\int_0^\pi \mathrm{d}\theta \ln\left[\frac{\mathrm{e}^{\kappa(\theta)}}{2\cosh\kappa(\theta)}\right]\\ &= -\frac{1}{\pi\beta}\int_0^\infty \mathrm{d}x\ln[1+\mathrm{e}^{-x}] = -\frac{\pi}{6\beta}\frac{1}{2},\end{aligned} \tag{24}$$

where, for simplicity, we define the function $\kappa(\theta) = \sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}$. In the first equality, we use Taylor expansion at π for $\kappa(\theta)$ since $\mathrm{e}^{-\kappa(\theta)} \simeq \mathrm{e}^{-\beta(\pi-\theta)}$ when $\beta \gg 1$; while in the second equality, a variable substitution $x = 2\beta(\pi-\theta)$ is used, and we instead of the upper limit of integral with $+\infty$. As the result, we determine the central charge $c = 1/2$.

Similarly, we can determine x_σ from the energy shift between vacuum energy of the R sector and ground state energy: $\Delta E^{\rm R} = E_0^{\rm R} - E_0^{\rm NS} = \frac{2\pi x_\sigma}{\beta} +$ higher orders, since for zero-mode $\varepsilon_0 = 0$,

$$\begin{aligned}\Delta E_0^{\rm R} &= \lim_{\beta\to\infty}\frac{2}{\pi}\int_0^\pi \mathrm{d}\theta \ln[\coth\kappa(\theta)]\\ &= \frac{2}{\pi\beta}\int_0^\infty \mathrm{d}x\ln[\coth x] = \frac{2\pi}{\beta}\frac{1}{8}\end{aligned} \tag{25}$$

from which we find $x_\sigma = 1/8$, which verifies Ising CFT.

The primary field of energy corresponds to state $\eta^\dagger_{\frac{1}{2}}\eta^\dagger_{-\frac{1}{2}}|0\rangle_{\rm NS}$, which is the first excited state in the NS sector with energy $E_\varepsilon = E_0^{\rm NS} + \varepsilon_{\frac{1}{2}} + \varepsilon_{-\frac{1}{2}}$, where $\varepsilon_k = \frac{2\pi|k|}{\beta} + \mathcal{O}(\frac{1}{\beta^2})$ as shown in Eq. (20) with $m = 0$. Therefore the energy shift is $\Delta E_\varepsilon = E_\varepsilon - E_0^{\rm NS} = \frac{2\pi}{\beta} + \mathcal{O}(\frac{1}{\beta^2})$ and we determine $x_\varepsilon = 1$.

Therefore, to summarize, we determine the corresponding eigenstate of three primary fields: $|1\rangle \equiv |0\rangle_{\rm NS}$, $|\sigma\rangle \equiv \eta_0^\dagger|0\rangle_{\rm R}$, and $|\varepsilon\rangle \equiv \eta^\dagger_{\frac{1}{2}}\eta^\dagger_{-\frac{1}{2}}|0\rangle_{\rm NS}$ with critical exponents $x_1 = 0$, $x_\sigma = 1/8$, and $x_\varepsilon = 1$.

3.2.2. Operator formalism in CFT

We could construct the operator formalism of free Majorana QFT explicitly by Virasoro algebra. Detailed descriptions can refer to the classic textbook.[13] Here, we only review the basic results briefly.

To introduce the complex coordinate $z = \tau + \mathrm{i}x$, the real spinor field splits into holomorphic and anti-holomorphic components: $\chi(x,\tau) \equiv \mathrm{e}^{\tau\hat{H}_{\rm F}}\chi(x)\mathrm{e}^{-\tau\hat{H}_{\rm F}} = (\chi(z),\bar{\chi}(\bar{z}))$. (We only care about the holomorphic part, since the anti-holomorphic part has a totally similar expression denoted by the notation bar.) Using mode expansion $\chi(z) = \frac{1}{\sqrt{\beta}}\sum_{n\in{\rm NS/R}} b_n \mathrm{e}^{-\frac{2\pi n}{\beta}z}$, the Hamiltonian and momentum (in fermion representation, the momentum operator is $\hat{P} = \int_0^\beta \psi^\dagger(x)(-\mathrm{i}\partial_x)\psi(x)\mathrm{d}x = \sum_{k\in{\rm NS/R}} k c_k^\dagger c_k$) of cMPO become

$$\begin{aligned}\hat{H}_{\rm F} &= \frac{2\pi}{\beta}(L_0+\bar{L}_0),\\ \hat{P} &= \frac{2\pi}{\beta}(L_0-\bar{L}_0),\end{aligned} \tag{26}$$

where $L_N = \frac{1}{2}\sum_{n\in{\rm NS/R}} n : b_{N-n}b_n$ for $N \in Z$ satisfies the Virasoro algebra. We remove the vacuum energy $E_0^{\rm NS/R}$ in Eq. (26), therefore $\hat{H}_{\rm F}|1\rangle = \hat{H}_{\rm F}|\sigma\rangle = 0$. If we set the ground state energy to be zero, we will have $\hat{H}_{\rm F} = \frac{2\pi}{\beta}(L_0+\bar{L}_0)$ in the NS sector while $\hat{H}_{\rm F} = \frac{2\pi}{\beta}(L_0+\bar{L}_0) + \frac{2\pi}{\beta}\frac{1}{8}$ in the R sector by considering the vacuum energy shift. Therefore, we have $\hat{H}_{\rm F}|1\rangle = 0$ and $\hat{H}_{\rm F}|\sigma\rangle = \frac{1}{8}|\sigma\rangle$.

In the CFT's operator formalism, the Hilbert space splits into $V\otimes\bar{V}$, which correspond to holomorphic and anti-holomorphic parts, respectively. According to the Virasoro algebra, every primary field corresponds to the highest weight state $|p\bar{p}\rangle$ (which is annihilated by any positive Virasoro mode: $L_n|p\rangle = 0, \forall n \in Z^+$), which satisfies the eigen-equation $L_0|p\bar{p}\rangle = p|p\bar{p}\rangle$ ($\bar{L}_0|p\bar{p}\rangle = \bar{p}|p\bar{p}\rangle$) with eigenvalue p ($\bar{p}$). (It is easy to check $|1\rangle = |0\bar{0}\rangle$, $|\sigma\rangle = |\frac{1}{16}\frac{\bar{1}}{16}\rangle$, and $|\varepsilon\rangle = |\frac{1}{2}\frac{\bar{1}}{2}\rangle$.) The Hilbert space is expanded by eigenstates generated by primary states $\prod_{\{n\},\{\bar{n}\}} L_{-n}L_{-\bar{n}}|p\bar{p}\rangle$, with eigenvalue $p+\sum_n n$ ($\bar{p}+\sum_n \bar{n}$), where $n,\bar{n} \in Z^+$.

Using the transformation relation between $\{\eta_n\}$ and $\{b_n\}$, we list the one-to-one map between the fermion representation in Eq. (14) and CFT's operator formalism in Eq. (26) in a dictionary.

Structure of Hilbert space of $\hat{H}_{\rm F}$		
Primary states: $\lvert p\bar{p}\rangle, x_p = p+\bar{p}$	Fermion representation	Virasoro algebra
$\lvert 1\rangle \equiv \lvert 0\bar{0}\rangle$	$\lvert 0\rangle_{\rm NS}$	$\lvert 0\rangle_{\rm NS}$
$\lvert\varepsilon\rangle \equiv \lvert\frac{1}{2}\frac{\bar{1}}{2}\rangle$	$\eta^\dagger_{\frac{1}{2}}\eta^\dagger_{-\frac{1}{2}}\lvert 0\rangle_{\rm NS}$	$b_{-\frac{1}{2}}\bar{b}_{-\frac{1}{2}}\lvert 0\rangle_{\rm NS}$
$\lvert\sigma\rangle \equiv \lvert\frac{1}{16}\frac{\bar{1}}{16}\rangle$	$\eta_0^\dagger\lvert 0\rangle_{\rm R}$	$(\bar{b}_0 - \mathrm{i}b_0)\lvert 0\rangle_{\rm R}$
Other excited states	$\prod_{\{k\}}\eta_k^\dagger\lvert 0\rangle_{\rm NS/R}$ $\#\{k\}=$ even in NS; $\#\{k\}=$ odd in R	$\prod_{\{n\},\{\bar{n}\}} L_{-n}L_{-\bar{n}}\lvert p\bar{p}\rangle$ $n,\bar{n}\in Z^+$, $\lvert p\bar{p}\rangle \in \{\lvert 1\rangle,\lvert\varepsilon\rangle,\lvert\sigma\rangle\}$
Energy	$E = \sum\varepsilon_k$	$E = \frac{2\pi}{\beta}(x_p + \sum n + \sum\bar{n})$
Momentum	$P = \frac{\pi}{\beta}\sum k$	$P = \frac{2\pi}{\beta}(\sum n - \sum\bar{n})$

Additionally, according to the above analysis, to make $\hat{H}_{\rm F} \pm \hat{P}$ be holomorphic (anti-holomorphic) in Eq. (26), the non-universal factor λ should be $1/2$ in TFIM's cMPO as shown in Eq. (6).

4. Numerical algorithm for excitation

Motivated by the analytic results of TFIM's cMPO and field theoretical prediction of CFT, which has been detailed discussed in previous sections, in this section, we show how to numerically calculate the low-lying excited states of cMPO for the general lattice model (with the assumption the corresponding cMPO is Hermitian) and extract critical information

from numerical data. (In history, there already exist some numerical works to verify the state–operator-correspondence by studying the low-lying excited states of the lattice Hamiltonian $\hat{H}_{\text{latt}}$.[15–17])

We first briefly review the variational cMPS method for cMPO's ground state search, which has a detailed discussion in the original paper for the cMPO method.[1] Next, we explain the method for excited states' calculation based on the Bloch state ansatz. Finally, we show the numerical results for TFIM's cMPO as a benchmark.

4.1. The cMPS ansatz for ground state

We could parameterize cMPO's ground state $|\Phi\rangle$ as a uniform cMPS with the periodic boundary condition, whose unit cell is $\begin{pmatrix}\mathbf{1}+\tau Q\\ \sqrt{\tau}R\end{pmatrix}$.[1] However, for convenience of the statement of excited state ansatz in the next, we rewrite cMPS in a more elegant form[4]

$$|\Phi(Q,R)\rangle = \mathrm{Tr}[U(0,\beta)]|0\rangle, \tag{27}$$

where we define the evolution operator $U(x,y)$,

$$U(x,y) = \mathcal{T}\exp\int_x^y [Q\otimes\mathbf{1}+R\otimes\psi^\dagger(\tau)]\,\mathrm{d}\tau, \tag{28}$$

where $\mathcal{T}$ is the path-order operator. Because of translational invariance, the parameters Q and R are τ independent. $\hat{\psi}(\tau)$ is the certain bosonic field operator living in cMPO's Hilbert space and $R\otimes\psi^\dagger$ is the shorthand of $\sum_{i=1}^d R^i\otimes\psi_i^\dagger$ since generally $R=(R^1,\ldots,R^d)$ has d components. (Although in the TFIM case, we have $d=1$ trivially, however, for the general model, for example, in the XY model, we have $d=2$).

To find the optimal cMPS ground state, we could use the variation principle for free energy $f=-\frac{1}{\beta}\ln\Lambda_0$, where Λ_0 is the dominant eigenvalue of cMPO,

$$\Lambda_0 = \frac{\langle\Phi|T|\Phi\rangle}{\langle\Phi|\Phi\rangle}. \tag{29}$$

4.2. Bloch state ansatz for excited state

Bloch state is a variational wave function in the tangent space of cMPS's manifold with certain momentum $k=\frac{2\pi n}{\beta}$, $n\in Z$,[5]

$$\begin{aligned}&|\phi_k(V,W)\rangle\\ &=\int_0^\beta \mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}k\tau}\mathrm{Tr}[U(0,\tau)(V\otimes 1+W\otimes\psi^\dagger(\tau))U(\tau,\beta)]|0\rangle,\end{aligned} \tag{30}$$

where V and W are variational parameters.

Since it is a variation problem for quadratic form, we can apply the Rayleigh–Ritz method to determine excitations by solving the following generalized eigen-equation:

$$[\rho_k - N_k]\begin{pmatrix}V\\W\end{pmatrix} = (\mathrm{e}^{-\Delta E}-1)N_k\begin{pmatrix}V\\W\end{pmatrix}, \tag{31}$$

where

$$\begin{aligned}\langle\phi_k|\mathrm{e}^{\beta f}T|\phi_{k'}\rangle &= \delta_{k,k'}(V^\dagger,W^\dagger)\rho_k\begin{pmatrix}V\\W\end{pmatrix},\\ \langle\phi_k|\phi_{k'}\rangle &= \delta_{k.k'}(V^\dagger,W^\dagger)N_k\begin{pmatrix}V\\W\end{pmatrix}.\end{aligned} \tag{32}$$

In Eq. (31), we multiply T by a factor $\Lambda_0^{-1}=\mathrm{e}^{\beta f}$ in Eq. (32) to shift the ground state energy to be zero. ρ_k and N_k are both square matrices with dimension $(d+1)\times D^2$ if the cMPS has bond dimension D and R has d components.

However, technically, N_k is singular because of gauge freedom. To resolve the problem, we can fix the gauge to reduce the parameter space's dimension to be $d\times D^2$ and thus make N_k be full rank.[18] Under the gauge fixing, the solution of the above eigen-equation Eq. (31) gives the dD^2 lowest excited states parameterized by $\{V_n,W_n\}$ with the corresponding excitation energies $\{\Delta E_n\}$, $n\in 1,2,\ldots,dD^2$. The explicit expressions of ρ_k and N_k can be found in Appendix F.

4.3. Benchmark for TFIM

4.3.1. Excitation at the critical point

To test our algorithm for excitation, we show the numerical results of TFIM's cMPO at the critical point $h_c=J_c=1$.

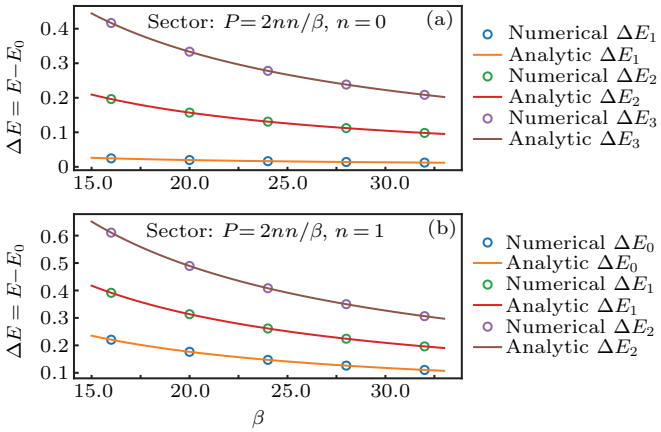


Fig. 2. (a) The first three excitations spectrum as function of β in $P=0$ sector, where the ground state energy is set to be zero. The curves are analytic results and points are numerical data. The lowest spectrum corresponds to the primary field of spin ΔE_0^{R}; the second spectrum corresponds to the primary field of energy ΔE_ε. (b) The first three excitations spectrum as the functions of β in $P=1$ sector.

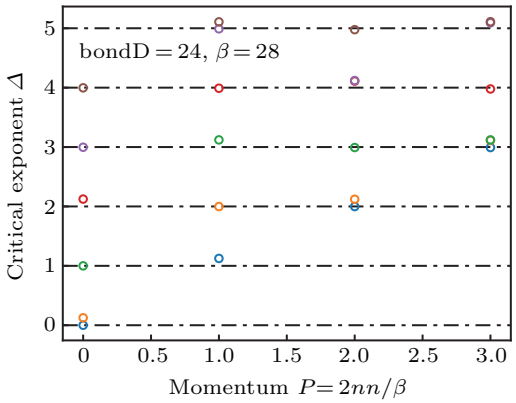


Fig. 3. Structure of conformal tower for TFIM's cMPO at $\beta=28$. The variational cMPS has bond dimension bondD = 24.

We first verify the formulas of spectrum in Eqs. (15) and (16). We plot the excitation spectrum as the function of β in the momentum sectors $P = 0$ and $P = 1$, as shown in Fig. 2, where the curves are analytic results and the points are numerical data.

We can also verify the conformal data of Ising CFT at $\beta \gg 1$. In Fig. 3, we plot the low-lying excitation spectrum at $\beta = 28$, which has the structure of conformal tower of Ising CFT, agreeing with the analytic calculation in Section 3. Using finite size scaling, at the numerical level, we confirm the central charge $c = 1/2$ and critical exponents for three primary fields $x_1 = 0$, $x_\sigma = 1/8$ and $x_\varepsilon = 1$ in Fig. 4.

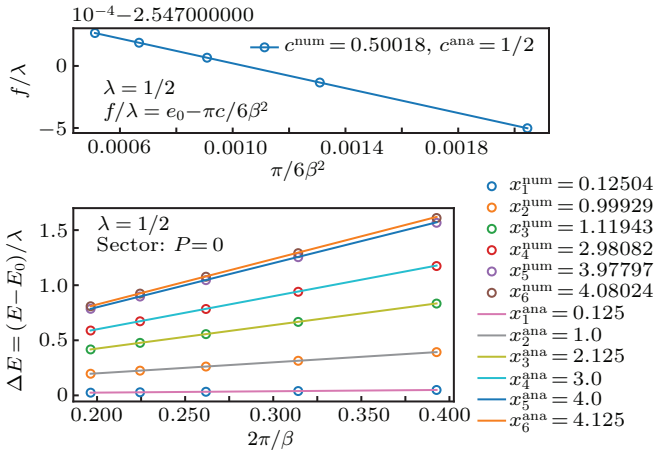


Fig. 4. (a) The central charge $c = 1/2$ from finite size scaling of the free energy. (b) The critical exponents from finite size scaling of the excitation spectrum. The superscript 'num' means numerical data and 'ana' means analytic results. The first two exponents correspond to spin and energy: $x_1 \equiv x_\sigma$, $x_2 \equiv x_\varepsilon$. The identity is trivial, which is set to be zero. The $\lambda = 1/2$ is the non-universal factor in Eq. (6).

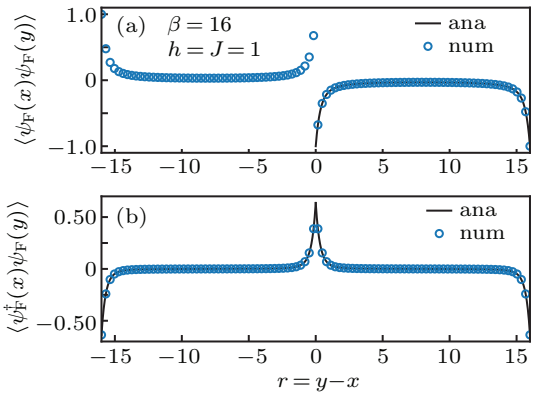


Fig. 5. Two-point correlation functions of the ground state of TFIM's cMPO. The curves are analytic solutions while the points are numerical results. We choose parameters $\beta = 16$, $h = J = 1$. The cMPS's bond dimension is bondD = 16. (a) $\langle \psi_{\rm F}(x)\psi_{\rm F}(y)\rangle$ and (b) $\langle \psi_{\rm F}^\dagger(x)\psi_{\rm F}(y)\rangle$.

4.3.2. Correlation for ground state

To finish this subsection, we also comment to explain why the underlying field $\psi(x)$ of cMPS is bosonic. Since we could view the cMPO as the continuum limit of a discrete spin model, when we take the continuum limit, the local spin (hard-core boson) operator σ_j^+ corresponds to the bosonic field operator $\psi_{\rm B}(x) \sim \sqrt{\rho(x)}\, {\rm e}^{{\rm i}\phi(x)}$ in the meaning of density-phase representation.[19,20] (Here, we use subscript B to emphasize the bosonic operator and subscript F to emphasize the fermionic operator.) For the TFIM's case, since we do the Jordan–Wigner transformation to reconstruct the original Hilbert space, the fermionic field operator $\psi_{\rm F}(x)$ in Eq. (19) then relates to the original bosonic operator $\psi_{\rm B}(x)$ by a Jordan–Wigner string[19]

$$\psi_{\rm F}(x) = {\rm e}^{{\rm i}\pi \int_0^x \rho(x')\,{\rm d}x'} \psi_{\rm B}(x). \tag{33}$$

To support the above argument, we can calculate the two-point correlation functions $\langle \psi_{\rm F}(x)\psi_{\rm F}(y)\rangle$ and $\langle \psi_{\rm F}^\dagger(x)\psi_{\rm F}(y)\rangle$ under the cMPS's framework. For bosonic cMPS, we should rewrite the fermionic operator into the bosonic operator using Eq. (33). For example,

$$\langle \psi_{\rm F}(x)\psi_{\rm F}(y)\rangle = \langle \Phi|\, {\rm e}^{\int_0^x \rho(x')\,{\rm d}x'} \psi_{\rm B}(x)\, {\rm e}^{\int_0^y \rho(x')\,{\rm d}x'} \psi_{\rm B}(y)|\Phi\rangle,$$

where $|\Phi\rangle$ is the variational cMPS ground state in Eq. (27). We compare the numerical results with the analytic results in Fig. 5, which coincides with our prediction. Additionally, results in Fig. 5 also show that the variational cMPS ground state truly captures the exact ground state of TFIM's cMPO, which is a fermionic Gaussian state and thus is completely captured by its two-point correlations.

The analytic expressions of the fermionic correlation functions can be found in Eqs. (D2) and (D3) in Appendix D. The technical details of calculating cMPS's expectation values about operators with a Jordan–Wigner string have been explained in Appendix F.

5. Entanglement entropy

In this section, we discuss the ground state entanglement entropy of cMPO based on the analysis of TFIM.

Before the concrete analysis, we could make some general comments. As we have pointed out in Section 2, the spectrum in Eqs. (15) and (16) shows that, at any finite β, the ground state is always gapped even at the critical point. The fact indicates that the entanglement entropy is always finite at any finite temperature. On the other hand, since TFIM's cMPO is the Majorana QFT as shown in Section 3, the general field theoretical analysis in Ref. [21] also predicts the finite entanglement entropy. ($S \leq$ const. at the off-critical point and $S \sim \frac{c}{3}\log\beta$ at the critical point, where $c = 1/2$ is the central charge.) The finite entanglement entropy allows us to approximate the ground state with a cMPS of finite bond dimension with enough precision, which supports the rationality of the cMPS approximation of the ground state in Ref. [1].

Although we cannot find the exact cMPS representation of the ground state for TFIM's cMPO, at the limit case $h = 0$,

the ground state is a simple cMPS with bond dimension two, see Appendix E,

$$\begin{pmatrix} \mathbf{1} \\ \sqrt{\tau J}\sigma^x \end{pmatrix}. \tag{34}$$

Its entanglement entropy is independent of the subsystem's size β' as shown in Eq. (E16): $S = \ln 2 + \delta S(\beta)$, which tends to be $S = \ln 2$ when $\beta \to \infty$. The correction term $\delta S(\beta) \sim \mathrm{e}^{-2\beta}(1-2\ln 2) < 0$ is exponential small. (We set the coupling constant to be $J = 1$ by absorbing J into β).

In the following, we first verify the finite entanglement entropy for TFIM by diagonalizing the subsystem's correlation matrix under a small trotter step[6,7] in the first subsection. We also give an integral equation as the continuum limit of the correlation matrix in the second subsection.

5.1. Entanglement entropy for TFIM: numerical results

We consider a subsystem of length β', whose ratio with the total system is $\Lambda = \beta'/\beta \in [0,1]$. We discretize the imaginary time to be $\beta = N\tau$ and $\beta' = M\tau$, where τ is a small trotter step. The sub-correlation matrix Γ^A is a $2M \times 2M$ matrix with matrix elements $\Gamma^A_{j\alpha,k\beta}$ (see Appendix C),

$$\Gamma^A_{j\alpha,k\beta} = g(j-k)\otimes\sigma^+_{\alpha\beta} - g(k-j)\otimes\sigma^-_{\alpha\beta}, \tag{35}$$

where $g(l) = \frac{2}{N}\sum_{k>0}\cos(2\phi_k + kl)$ and ϕ_k is the Bogoliubov angle of mode k.

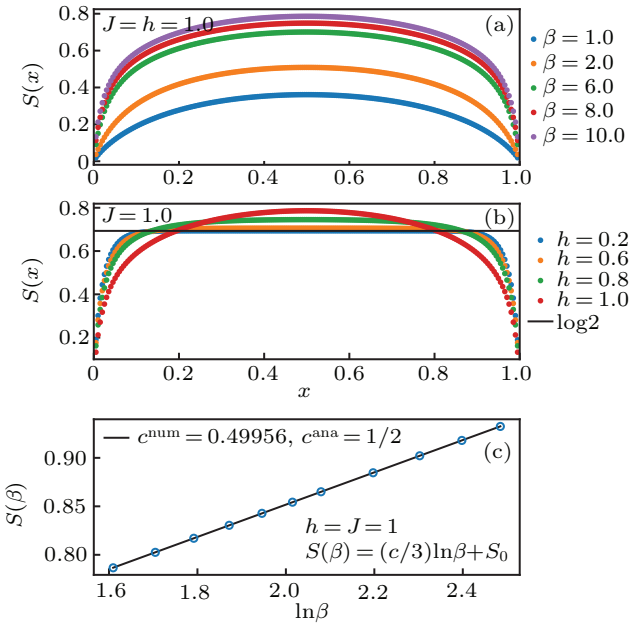


Fig. 6. (a) The critical entanglement entropy with $h = J = 1$ for different β. (b) The off-critical entanglement entropy at $\beta = 10$, which has a lower bound $S = \ln 2$. The x-axis labels the ratio $x = \beta'/\beta$, where β' is the subsystem's size. (c) The critical entanglement entropy as the function of β. We verify the central charge $c = 1/2$ from the scaling of the critical entanglement entropy.

Since Γ^A is real anti-symmetric, $\mathrm{i}\Gamma^A$ is Hermitian. If we define the 'density matrix' $\hat{\rho} = \frac{1}{2}(\mathrm{i}\Gamma^A + \mathbf{1})$, we can calculate the entanglement entropy using the following formula:

$$S_{\beta'} = -\mathrm{Tr}[\hat{\rho}\ln\hat{\rho}]. \tag{36}$$

By numerically diagonalizing $\hat{\rho}$, we can calculate entanglement entropy using Eq. (36) under certain trotter step τ. We plot the entanglement entropy as a function of ratio Λ at critical point $h_c = J_c = 1$ for different total system sizes β in Fig. 6(a). We also show the off-critical behavior of entanglement entropy for different h with fixed $J = 1$ at $\beta = 10$ in Fig. 6(b), where the entropy decreases when we decrease the magnitude of magnetic field h. The entanglement entropy has a lower bound $\ln 2$ which corresponds to the classical Ising limit. By calculating the maximum critical entanglement entropy $S(\beta' = \beta/2)$ at different β, we verify the central charge $c = 1/2$ for TFIM again from the scaling of the critical entanglement entropy: $S(\beta') = \frac{c}{3}\ln\beta' + S_0$,[21] as shown in Fig. 6(c).

5.2. Integral equation for correlation matrix

In the continuum limit $\tau \to 0$, the eigen-equation $\mathrm{i}\Gamma^A\chi_n = \lambda_n\chi_n$ becomes an integral equation with the block difference kernel, see Appendix C,

$$\int_0^\Lambda \mathrm{d}y \boldsymbol{K}(x-y)\chi_n(y) - \sigma^y\chi_n(x) = \lambda_n\chi_n(x), \tag{37}$$

where the integral kernel is

$$\boldsymbol{K}(x-y) = \begin{pmatrix} 0 & \frac{\mathrm{i}}{\pi}\int_0^\pi \mathrm{d}\theta f(\theta, x-y) \\ -\frac{\mathrm{i}}{\pi}\int_0^\pi \mathrm{d}\theta f(\theta, y-x) & 0 \end{pmatrix}$$

and the explicit expression of $f(\theta,x)$ can be found in Eq. (C39) of Appendix C.

Then the corresponding 'density matrix' $\hat{\rho}$ becomes $\rho_{\alpha\beta}(x-y) = \frac{1}{2}\begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}_{\alpha\beta}\delta(x-y) + \frac{1}{2}K_{\alpha\beta}(x-y)$. Since the $\hat{\rho}(x-y)$ is a block difference kernel, which can be viewed as the continuum limit of the block Toeplitz matrix, the analytic expression of the entanglement entropy may be determined by generalizing the (strong) Szego theorem[22,23] in the future.

6. Conclusions and outlook

In summary, we detailly study the cMPO for TFIM. We determine the analytic structure of cMPO for TFIM and show that it has the well-defined operator formalism: $T = \mathrm{e}^{-\frac{1}{2}\hat{H}_\mathrm{F}}$. The Hilbert space structure of $\hat{H}_\mathrm{F}$ at the scaling limit is analyzed especially, which verifies the corresponding field theoretical predictions explicitly. A calculation also shows the ground state entanglement entropy for TFIM's cMPO is finite both at critical and off-critical points, which supports the rationality of using cMPS as an approximated ground state for the cMPO method.[1]

Motivated by the Hamiltonian structure of TFIM's cMPO and the theoretical predictions of CFT, we also design an algorithm to calculate the critical exponents for the general lattice

model through the excitation spectrum of the corresponding cMPO. We use the analytic results of TFIM as the benchmark. Our numerical algorithm may also be used to calculate the excited states for the continuous model on a ring.

Although the solvability of TFIM's cMPO is heavily on the special structure of the two-dimensional Ising model, we tend to believe that the Hamiltonian structure for cMPO is universal to some extent. In fact, in the bethe ansatz techniques for thermodynamics, apart form the traditional Yang–Yang approach,[24] there also exists the quantum transfer matrix approach,[25,26] which may be viewed as the (integrable) cMPO in some sense.

The derivation in this work is based on taking the continuum limit of a certain lattice model. However, it is not difficult to show that the cMPO has a very similar (lattice independent) integral formalism to the cMPS case,

$$\begin{aligned} T \;=\; & \mathrm{Tr}_{\mathrm{aux}}\mathcal{P}\exp\left\{\int_0^L \mathrm{d}x\left[Q(x)\otimes 1+\sum_{i=1}^{d}L_i(x)\otimes\psi_i(x)\right.\right. \\ & +\sum_{i=1}^{d}R_i(x)\otimes\psi_i^{\dagger}(x)+\sum_{i,j=1}^{d}(P_{ij}(x)-1\delta_{ij}) \\ & \left.\left.\otimes\psi_i^{\dagger}(x)\psi_j(x)\right]\right\} \end{aligned} \tag{38}$$

for the corresponding unit cell tensor

$$t_{ij}=\begin{pmatrix}1+\varepsilon Q & \sqrt{\varepsilon}\boldsymbol{L}\\ \sqrt{\varepsilon}\boldsymbol{R} & \boldsymbol{P}\end{pmatrix}_{ij}.$$

It is also possible to construct a series of solvable models sharing the same ground states with the corresponding cMPOs, whose ground states have the cMPS structure. Detailed analysis will appear in the late.

Appendix A: Diagonalization of V

In this section, for the reader's convenience, we review the procedure of the diagonalization of the transfer matrix V in Eq. (7), following the classic paper,[10] where the slight difference is the exchange of V_1 and V_2 in our definition. We map the transfer matrix to the free fermion and then diagonalize it using the Bogoliubov transformation.

For simplicity, we define $1=\beta=N\tau$ and let N be even. We need to diagonalize the following transfer matrix:

$$\begin{aligned} & V(\bar{K}_2,K_1)=V_1^{\frac{1}{2}}V_2V_1^{\frac{1}{2}},\\ & V_1^{\frac{1}{2}}(\bar{K}_2)=\exp(\bar{K}_2\sum_{j=1}^{N}\sigma_j^z),\\ & V_2(K_1)=\exp(K_1\sum_{j=1}^{N}\sigma_j^x\sigma_{j+1}^x). \end{aligned} \tag{A1}$$

The Jordan–Wigner transformation is defined as

$$\sigma_j^z=\mathbf{1}-2c_j^{\dagger}c_j,$$

$$\sigma_j^x=\prod_{k=1}^{j-1}(\mathbf{1}-2c_k^{\dagger}c_k)(c_j+c_j^{\dagger}). \tag{A2}$$

We substitute Eq. (A2) into Eq. (A1),

$$V_1^{\frac{1}{2}}(\bar{K}_2)=\exp\left(-\bar{K}_2\sum_j c_j^{\dagger}c_j\right)\exp\left(\frac{N}{2}\bar{K}_2\right), \tag{A3}$$

$$V_2(K_1)=\exp\left[K_1\sum_j(c_j^{\dagger}-c_j)(c_{j+1}^{\dagger}+c_{j+1})\right]. \tag{A4}$$

If $(-1)^{\hat{N}}=1$, we have APBC, $c_1=-c_{N+1}$; if $(-1)^{\hat{N}}=-1$, we have PBC, $c_1=c_{N+1}$.

Because of the translation invariance, we can use Fourier transformation

$$c_j=\frac{1}{\sqrt{N}}\mathrm{e}^{-\mathrm{i}\pi/4}\sum_k\mathrm{e}^{\mathrm{i}kj}c_k \tag{A5}$$

for APBC, $k=\frac{\pi(2n+1)}{N}=\{\pm\frac{\pi}{N},\pm\frac{3\pi}{N},\ldots,\pm\frac{(N-1)\pi}{N}\}$; for PBC, $k=\frac{\pi(2n)}{N}=\{0,\pm\frac{2\pi}{N},\ldots,\pm\frac{(N-2)\pi}{N},\pi\}$.

The transfer matrix thus has the block diagonal form

$$V=\prod_{0\le k\le\pi}V_k. \tag{A6}$$

For $k\neq 0,\pi$,

$$V_k=\mathrm{e}^{2\bar{K}_2}V_{1k}^{\frac{1}{2}}V_{2k}V_{1k}^{\frac{1}{2}}, \tag{A7}$$

where

$$\begin{aligned} & V_{1k}^{\frac{1}{2}}=\mathrm{e}^{-\bar{K}_2(c_k^{\dagger}c_k+c_{-k}^{\dagger}c_{-k})},\\ & V_{2k}=\mathrm{e}^{2K_1[\sin k(c_{-k}^{\dagger}c_k^{\dagger}+c_kc_{-k})+\cos k(c_k^{\dagger}c_k+c_{-k}^{\dagger}c_{-k})]}. \end{aligned} \tag{A8}$$

For $k=0,\pi$,

$$V_{k=0}=\mathrm{e}^{\bar{K}_2}\exp[-2(\bar{K}_2-K_1)c_0^{\dagger}c_0], \tag{A9}$$

$$V_{k=\pi}=\mathrm{e}^{\bar{K}_2}\exp[-2(\bar{K}_2+K_1)c_{\pi}^{\dagger}c_{\pi}]. \tag{A10}$$

In $k=0$, π sector, it is already diagonal, we need diagonalize sectors $k\neq 0,\pi$. The Fock space of V_k has dimension four. We choose following four basis:

$$\Phi_0=|0\rangle,\ \Phi_k=c_k^{\dagger}|0\rangle,\ \Phi_{-k}=c_{-k}^{\dagger}|0\rangle,\ \Phi_{-k,k}=c_{-k}^{\dagger}c_k^{\dagger}|0\rangle. \tag{A11}$$

The V_{1k} is already diagonal under certain basis,

$$\begin{aligned} & V_{1k}^{\frac{1}{2}}(\Phi_0,\Phi_k,\Phi_{-k},\Phi_{-k,k})\\ & =(\Phi_0,\Phi_k,\Phi_{-k},\Phi_{-k,k})\begin{pmatrix}1 & & & \\ & \mathrm{e}^{-\bar{K}_2} & & \\ & & \mathrm{e}^{-\bar{K}_2} & \\ & & & \mathrm{e}^{-2\bar{K}_2}\end{pmatrix}. \end{aligned} \tag{A12}$$

For V_{2k}, the subspace $\{\Phi_k,\Phi_{-k}\}$ is already diagonal,

$$V_{2k}(\Phi_k,\Phi_{-k})=(\Phi_k,\Phi_{-k})\,\mathrm{e}^{2K_1\cos k}\begin{pmatrix}1 & \\ & 1\end{pmatrix}. \tag{A13}$$

As the result, we only need to diagonalize the subspace $\{\Phi_0, \Phi_{-k,k}\}$. When we restrict in the subspace, the operator $c^\dagger_{-k}c^\dagger_k$ becomes

$$c^\dagger_{-k}c^\dagger_k(\Phi_0, \Phi_{-k,k}) = (\Phi_0, \Phi_{-k,k})\sigma^-. \tag{A14}$$

Similarly, c_kc_{-k}, $c^\dagger_kc_k$, and $c^\dagger_{-k}c_{-k}$ become

$$c_kc_{-k} = \sigma^+, \quad c^\dagger_kc_k = c^\dagger_{-k}c_{-k} = \frac{1}{2}(\mathbf{1}-\sigma^z). \tag{A15}$$

As the result, in this two-dimensional space, we have

$$V_k = \mathrm{e}^{2\bar{K}_2}V^{\frac{1}{2}}_{1k}V_{2k}V^{\frac{1}{2}}_{1k}, \tag{A16}$$

where

$$\begin{aligned} V_{1k}(\bar{K}_2) &= \exp[-\bar{K}_2(\mathbf{1}-\sigma^z)], \\ V_{2k}(K_1) &= \exp[2K_1(\sin k\sigma^x - \cos k\sigma^z - \cos k\mathbf{1})]. \end{aligned} \tag{A17}$$

If we define the spinor $\sigma' \equiv \sin k\sigma^x - \cos k\sigma^z$, we have

$$\begin{aligned} V_{1k}(\bar{K}_2) &= \mathrm{e}^{-\bar{K}_2}(\cosh\bar{K}_2 + \sinh\bar{K}_2\sigma^z), \\ V_{2k}(K_1) &= \mathrm{e}^{2K_1\cos k}(\cosh 2K_1 + \sinh 2K_1\sigma'). \end{aligned} \tag{A18}$$

After some algebra, we find

$$V_k = \mathrm{e}^{2K_1\cos k}[\cosh\varepsilon_k + \sinh\varepsilon_k(\sin 2\phi_k\sigma^x + \cos 2\phi_k\sigma^z)], \tag{A19}$$

where

$$\begin{aligned} &\cosh\varepsilon_k = \cosh 2K_1\cosh 2\bar{K}_2 - \sinh 2K_1\sinh 2\bar{K}_2\cos k, \\ &\sinh\varepsilon_k\sin 2\phi_k = \sinh 2K_1\sin k, \\ &\sinh\varepsilon_k\cos 2\phi_k \\ &= \cosh 2K_1\sinh 2\bar{K}_2 - \sinh 2K_1\cosh 2\bar{K}_2\cos k. \end{aligned} \tag{A20}$$

As the result, under the orthogonal transformation O,

$$O = \begin{pmatrix} \cos\phi_k & -\sin\phi_k \\ \sin\phi_k & \cos\phi_k \end{pmatrix}, \tag{A21}$$

V_k becomes diagonal,

$$V_k = \mathrm{e}^{2K_1\cos k}O\begin{pmatrix} \mathrm{e}^{\varepsilon_k} & \\ & \mathrm{e}^{-\varepsilon_k} \end{pmatrix}O^{\mathrm{T}}. \tag{A22}$$

Alternatively, we can define the Bogoliubov transformation

$$\begin{pmatrix} \eta_k \\ \eta^\dagger_{-k} \end{pmatrix} = O^{\mathrm{T}}\begin{pmatrix} c_k \\ c^\dagger_{-k} \end{pmatrix}, \tag{A23}$$

where we define $\phi_{-k} = -\phi_k$ for negative k.

As the result, V_k has the quadratic form in the second quantization formalism for $k > 0$ ($k \neq 0$ and π),

$$V_k = \mathrm{e}^{2K_1\cos k}\mathrm{e}^{-\varepsilon_k(\eta^\dagger_k\eta_k + \eta^\dagger_{-k}\eta_{-k}-1)}. \tag{A24}$$

To consider the restriction $\sum_k \cos k = 0$ for both even and odd sectors, we finally have

$$V = \exp\left[-\sum_k \varepsilon_k\left(\eta^\dagger_k\eta_k - \frac{1}{2}\right)\right]. \tag{A25}$$

Particularly, in the odd sector, for modes $k = 0$ and π, we define $\eta_0 \equiv c_0$ and $\eta_\pi \equiv c_\pi$.

Appendix B: Spectrum at the continuum limit

We first summarize the above formulas using parameters K and Γ. The following identity proves to be useful:

$$\begin{aligned} \cosh\left[\ln\coth\frac{x}{N}\right] &= \coth\frac{2x}{N}, \\ \sinh\left[\ln\coth\frac{x}{N}\right] &= \frac{1}{\sinh\frac{2x}{N}}. \end{aligned} \tag{B1}$$

To substitute Eq. (B1) into Eq. (A20) with $x = K, \Gamma$, we have

$$\begin{aligned} \cosh\varepsilon_k &= \frac{\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N} - \cos k}{\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}}, \\ \cos 2\phi_k &= \frac{\cosh\frac{2\Gamma}{N} - \cosh\frac{2K}{N}\cos k}{\sqrt{[\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N} - \cos k]^2 - [\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}]^2}}, \\ \sin 2\phi_k &= \frac{\sinh\frac{2K}{N}\sin k}{\sqrt{[\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N} - \cos k]^2 - [\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}]^2}}. \end{aligned} \tag{B2}$$

The corresponding cMPO is

$$\begin{aligned} T = &\lim_{N\to+\infty}\left(\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\right)^{\frac{N}{2}} \\ &\times\exp\left[-\sum_k\varepsilon_k\left(\eta^\dagger_k\eta_k - \frac{1}{2}\right)\right], \end{aligned} \tag{B3}$$

where

$$\begin{pmatrix} \eta_k \\ \eta^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} \cos\phi_k & \sin\phi_k \\ -\sin\phi_k & \cos\phi_k \end{pmatrix}\begin{pmatrix} c_k \\ c^\dagger_{-k} \end{pmatrix}. \tag{B4}$$

B1. Vacuum energy

The vacuum energy $E_0^{\mathrm{NS/R}}$ in the NS and R sectors correspond to the dominant and second-largest eigenvalues Λ_0 and Λ_1 of cMPO, respectively: $\frac{1}{2}E_0^{\mathrm{NS/R}} = -\ln\Lambda_{0/1}$.

We need to calculate the following limit according to Eq. (B3):

$$E_0^{\mathrm{NS/R}} = -\lim_{N\to+\infty}\left[N\ln\left(\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\right) + \sum_{k\in\mathrm{NS/R}}\varepsilon_k\right]. \tag{B5}$$

On the other hand, we already know the final expression of E_0^{NS} in history according to the relationship between dominant eigenvalue and free energy density f,

$$\frac{1}{2}E_0^{\mathrm{NS}} = -\ln\Lambda_0 = \beta f, \tag{B6}$$

where $\beta f = -\frac{1}{\pi}\int_0^\pi \ln[2\cosh(\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta})]\,\mathrm{d}\theta$, which is a well-known result for TFIM.[11] Our calculation should coincide with this classic result.

Before concrete calculation, let us first estimate the large N asymptotic behavior of the summation in Eq. (B5). Using Taylor expansion: $\lim_{x\to 0}\coth x = \frac{1}{x}(1+\frac{1}{3}x^2)+\mathcal{O}(x^3)$ and $\lim_{x\to 0}\frac{1}{\sinh x} = \frac{1}{x}(1-\frac{1}{6}x^2)+\mathcal{O}(x^3)$, we have

$$\cosh\varepsilon_k = \frac{N^2}{4\Gamma K}(1-\cos k)+\left(\frac{\Gamma}{K}+\frac{K}{\Gamma}\right)\times\left(\frac{1}{6}\cos k+\frac{1}{3}\right)+\mathcal{O}\left(\frac{1}{N^2}\right). \tag{B7}$$

According to the formula $\cosh^{-1}x = \ln(x+\sqrt{x^2-1})$ for $x\geq 0$, we have the following estimation of ε_k:

$$\varepsilon_k \sim \ln N \to \sum_k \varepsilon_k \sim N\ln N. \tag{B8}$$

We can also estimate the normalization term

$$N\ln\left(\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\right)\sim -N\ln N. \tag{B9}$$

As the result, we find that the RHS of Eq. (B5) is the summation of two divergent terms, with the same order but opposite signs. According to the discussion about Eq. (B6), the summation should be finite, which indicates that we should combine the two terms to have a finite expression of N, and finally take limit $N\to+\infty$.

Motivated by the exact expression of free energy density, we introduce the auxiliary variable θ through the following integral identity[27] (for example, see Ref. [27], p. 534, 4.224.9):

$$\int_0^\pi \ln(a+b\cos x)\,\mathrm{d}x = \pi\ln\frac{a+\sqrt{a^2-b^2}}{2}. \tag{B10}$$

We choose $a=\cosh\varepsilon_k$, $b=1$. For $\Gamma\geq K$, since $\varepsilon_k = \cosh^{-1}a = \ln(a+\sqrt{a^2-1})$, we have

$$\varepsilon_k = \frac{1}{\pi}\int_0^\pi \ln[2(\cosh\varepsilon_k+\cos\theta)]\,\mathrm{d}\theta. \tag{B11}$$

To substitute it into Eq. (B5), we have

$$E_0^{\mathrm{NS/R}} = -\frac{1}{\pi}\lim_{N\to\infty}\int_0^\pi \ln\left\{2^N\prod_{k\in\mathrm{NS/R}}\left[\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N}+\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\cos\theta-\cos k\right]\right\}\mathrm{d}\theta. \tag{B12}$$

for $\Gamma\geq K$. For $\Gamma<K$, we need an extra correction of the zero mode for E_0^{R}.

According to the following inequality:

$$\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N}+\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\cos\theta \geq \cosh\frac{2(\Gamma-K)}{N}\geq 1, \tag{B13}$$

we can parameterize it as $\cosh x$,

$$\cosh x \equiv \cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N}+\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\cos\theta. \tag{B14}$$

Then Eq. (B12) becomes

$$E_0^{\mathrm{NS/R}} = -\frac{1}{\pi}\lim_{N\to\infty}\int_0^\pi \mathrm{d}\theta\ln\left\{2^N\prod_{k\in\mathrm{NS/R}}[\cosh x-\cos k]\right\}. \tag{B15}$$

The following algebraic identity is important (see Ref. [27], p. 41, 1.395.2):

$$\cosh nx-\cos ny = 2^{n-1}\prod_{k=0}^{n-1}\left[\cosh x-\cos\left(y+\frac{2\pi k}{n}\right)\right]. \tag{B16}$$

For the NS sector, we choose $y=-\frac{N-1}{N}\pi$ and notice $\cos(N-1)\pi=-1$ since N is an even number according to our assumption. We have

$$\cosh Nx+1 = 2^{N-1}\prod_k[\cosh x-\cos k]. \tag{B17}$$

As the result,

$$\frac{1}{2}E_0^{\mathrm{NS}} = -\frac{1}{2\pi}\lim_{N\to\infty}\int_0^\pi \ln[2(\cosh(Nx)+1)]\,\mathrm{d}\theta = -\frac{1}{\pi}\lim_{N\to\infty}\int_0^\pi \ln\left[2\cosh\left(\frac{Nx}{2}\right)\right]\mathrm{d}\theta. \tag{B18}$$

To compare Taylor expansions

$$\cosh x = 1+\frac{2(\Gamma^2+K^2+2\Gamma K\cos\theta)}{N^2}+\mathcal{O}\left(\frac{1}{N^4}\right)$$

and $\cosh x = 1+\frac{1}{2}x^2+\mathcal{O}(x^4)$, we determine x up to the first-order of $1/N$,

$$x = \frac{2\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}}{N}+\mathcal{O}\left(\frac{1}{N^2}\right). \tag{B19}$$

To substitute Eq. (B19) into Eq. (B18) and take the limit $N\to\infty$, we finally have

$$\frac{1}{2}E_0^{\mathrm{NS}} = -\frac{1}{\pi}\int_0^\pi \ln[2\cosh(\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta})]\,\mathrm{d}\theta. \tag{B20}$$

For the R sector, we choose $y=-\frac{(N-2)}{N}\pi$ and notice $\cos Ny=1$, similarly, we have

$$\frac{1}{2}E_0^{\mathrm{R}} = -\frac{1}{\pi}\int_0^\pi \ln[2\sinh(\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta})]\,\mathrm{d}\theta+\frac{1}{2}\left(\left|\ln\frac{\Gamma}{K}\right|-\ln\frac{\Gamma}{K}\right), \tag{B21}$$

where we have an extra correction because of the zero mode.

B2. Excitation spectrum

We denote the vacuum of the NS and R sectors as $|0\rangle_{\mathrm{NS/R}}$, respectively. Since we have $E_0^{\mathrm{NS}} < E_0^{\mathrm{R}}$, the ground state for TFIM's cMPO is $|0\rangle_{\mathrm{NS}}$ with energy E_0^{NS}. To consider the restriction of particle number's parity, the first excitation state is $\eta_0^\dagger|0\rangle_{\mathrm{R}}$ with energy $E_0^{\mathrm{R}}+\varepsilon_0$.

For any excited state, we denote it as

$$|\psi\rangle = \prod_k \eta_k^\dagger |0\rangle_{\mathrm{NS/R}}, \tag{B22}$$

where k is the quantum number of cyclic group Z_N.

Generally, we can choose any

$$k \in \left\{ \pm\frac{\pi}{N}, \pm\frac{3\pi}{N}, \ldots, \pm\frac{(N-1)\pi}{N} \right\}$$

in the NS sector;

$$k \in \left\{ 0, \pm\frac{2\pi}{N}, \ldots, \pm\frac{(N-2)\pi}{N}, \pi \right\}$$

in the R sector. However, we can prove, in the continuum limit, only the small k, which satisfies $k = \lim_{N\to\infty}\frac{2\pi j}{N} = 0$, has a contribution to the free energy. This fact can be easily seen from Eq. (B1), where we have a singular term $\frac{N^2}{4\Gamma K}(1-\cos k)$. For any $k = \lim_{N\to\infty}\frac{2\pi j}{N} \neq 0$, we will have $\varepsilon_k \sim \ln N \to +\infty$, as the result $\mathrm{e}^{-\varepsilon_k} \to 0$, which does not have a contribution to the partition function. To have finite ε_k, we need $\cos k \to 1$, as the result, $k = \frac{2\pi j}{N} \to 0$, where we fix j and let $N \to \infty$. As the result, we establish a one-to-one map between the small k and the discrete quantum number j. We have $j \in Z + \frac{1}{2}$ in the NS sector; $j \in Z$ in the R sector.

We relabel the index k by j for the dispersion relation: $\frac{1}{2}\varepsilon_j \equiv \varepsilon_k$ in Eq. (B7). To determine the dispersion relation in the continuum limit, we expand $1-\cos k = \frac{1}{2}(\frac{2\pi j}{N})^2 + \mathcal{O}(\frac{1}{N^4})$ and substitute it into Eq. (B7),

$$\begin{aligned} &\frac{1}{2}\varepsilon_j = \ln(x_j + \sqrt{x_j^2-1}), \quad j \neq 0, \\ &x_j = \frac{\pi^2 j^2}{2\Gamma K} + \frac{1}{2}\left(\frac{\Gamma}{K} + \frac{K}{\Gamma}\right); \end{aligned} \tag{B23}$$

while for the zero mode, we have

$$\frac{1}{2}\varepsilon_0 = \mathrm{sign}(\Gamma - K)\ln(x_0 + \sqrt{x_0^2-1}) = \ln\frac{\Gamma}{K}. \tag{B24}$$

The quantum number k is like the lattice momentum, with lattice size $\tau = \beta/N$. In the continuum limit, the physical momentum P of the certain eigenstate in Eq. (B22) is

$$P = \lim_{\tau\to 0}\sum_k \frac{k}{\tau} = \sum_j \frac{2\pi j}{\beta}, \tag{B25}$$

while the corresponding excitation energy $\Delta E \equiv E - E_0^{\mathrm{NS}}$ is

$$\Delta E = \begin{cases} \sum_j \varepsilon_j, & j \in Z + \frac{1}{2}, \\ \sum_j \varepsilon_j + E_0^{\mathrm{R}} - E_0^{\mathrm{NS}}, & j \in Z. \end{cases} \tag{B26}$$

In summary, we have proved, in the continuum limit, TFIM's cMPO has the structure $T = \mathrm{e}^{-\frac{1}{2}\hat{H}_{\mathrm{F}}}$.

B3. Torus partition function $Z(L,\beta)$

As an application of Eqs. (15), (16), and (18), we can get an expression of TFIM's partition function $Z(L,\beta)$ on a torus. To see the modular invariance in the following, we need to rescale the coupling $h \to h/2$, $J \to J/2$. As the result, TFIM's Hamiltonian becomes $\hat{H} = -\frac{J}{2}\sum_i \sigma_i^x\sigma_{i+1}^x - \frac{h}{2}\sum_i \sigma_i^z$, and the corresponding cMPO becomes $T = \mathrm{e}^{-\hat{H}_{\mathrm{F}}}$.

In the fermion representation, the cMPO is

$$\begin{aligned} T &= \mathrm{e}^{-E_0^{\mathrm{NS}} - \sum_{n\in\mathrm{NS}}\varepsilon_n\eta_n^\dagger\eta_n}\hat{P} + \mathrm{e}^{-E_0^{\mathrm{R}} - \sum_{n\in\mathrm{R}}\varepsilon_n\eta_n^\dagger\eta_n}(1-\hat{P}) \\ &\equiv T^{\mathrm{NS}} + T^{\mathrm{R}}, \end{aligned} \tag{B27}$$

where $\hat{P} = \frac{1+(-)^{\hat{N}}}{2}$ is the projector that restricts the particle parity to be even (odd) in the NS (R) sector.

We can use the trick $(-)^{\hat{N}} = (-)^{\sum_n \eta_n^\dagger\eta_n}$, then the transfer matrix becomes

$$\begin{aligned} T^{\mathrm{NS}} &= \frac{1}{2}\mathrm{e}^{-E_0^{\mathrm{NS}}}\left[\prod_{n\in\mathrm{NS}}\mathrm{e}^{-\varepsilon_n\eta_n^\dagger\eta_n} + \prod_{n\in\mathrm{NS}}\mathrm{e}^{-\varepsilon_n\eta_n^\dagger\eta_n}(-)^{\eta_n^\dagger\eta_n}\right], \\ T^{\mathrm{R}} &= \frac{1}{2}\mathrm{e}^{-E_0^{\mathrm{R}}}\left[\prod_{n\in\mathrm{R}}\mathrm{e}^{-\varepsilon_n\eta_n^\dagger\eta_n} - \prod_{n\in\mathrm{R}}\mathrm{e}^{-\varepsilon_n\eta_n^\dagger\eta_n}(-)^{\eta_n^\dagger\eta_n}\right]. \end{aligned} \tag{B28}$$

The partition function is

$$Z(L,\beta) = \mathrm{Tr}T^L = Z^{\mathrm{NS}} + Z^{\mathrm{R}}, \tag{B29}$$

where

$$\begin{aligned} Z^{\mathrm{NS}} &= \frac{1}{2}\mathrm{e}^{-LE_0^{\mathrm{NS}}}\left[\prod_{n\in\mathrm{NS}}(1+\mathrm{e}^{-L\varepsilon_n})\right. \\ &\quad \left. + \prod_{n\in\mathrm{NS}}(1-\mathrm{e}^{-L\varepsilon_n})\right], \\ Z^{\mathrm{R}} &= \frac{1}{2}\mathrm{e}^{-LE_0^{\mathrm{R}}}\left[\prod_{n\in\mathrm{R}}(1+\mathrm{e}^{-L\varepsilon_n}) - \prod_{n\in\mathrm{R}}(1-\mathrm{e}^{-L\varepsilon_n})\right] \\ &= \frac{1}{2}\mathrm{e}^{-LE_0^{\mathrm{R}}}\prod_{n\in\mathrm{R}}(1+\mathrm{e}^{-L\varepsilon_n}), \end{aligned} \tag{B30}$$

where, in the second equality, we use $\prod_{n\in\mathrm{R}}(1-\mathrm{e}^{-L\varepsilon_n}) = 0$ since $\varepsilon_0 = 0$ in the R sector.

B4. Modular invariance of the partition function

We define the reduced partition function $\tilde{Z} \equiv \mathrm{e}^{LE_0^{\mathrm{NS}}}Z$ by removing the contribution of the ground state energy, which is a non-universal factor. When the model is at the critical point $h_{\mathrm{c}} = J_{\mathrm{c}} = 1$ in the scaling limit, the partition function $\tilde{Z}(L,\beta)$ has the modular invariance. To see this, we analyze its critical spectrum at the scaling limit. According to the discussion in Section 3, we have: $E_0^{\mathrm{R}} - E_0^{\mathrm{NS}} = \frac{2\pi}{\beta}\frac{1}{8}$ and $\varepsilon_n = \frac{2\pi|n|}{\beta}$. To substitute the above expressions into the definition of $\tilde{Z}$, we find that $\tilde{Z}$ is a function of the ratio $\tau = L/\beta$,

$$\tilde{Z}\left(\tau = \frac{L}{\beta}\right) = \frac{1}{2}\left[\prod_{n\in\mathrm{NS}}(1+\mathrm{e}^{-2\pi|n|\frac{L}{\beta}}) + \prod_{n\in\mathrm{NS}}(1-\mathrm{e}^{-2\pi|n|\frac{L}{\beta}})\right]$$

$$+\frac{1}{2}\mathrm{e}^{-\pi\frac{L}{\beta}}\prod_{n\in\mathrm{R}}(1+\mathrm{e}^{-2\pi|n|\frac{L}{\beta}}). \tag{B31}$$

As the result, we build a functional relation between the partition function $Z(L,\beta)$ and the reduced partition function $\tilde{Z}(\tau)$,

$$Z(L,\beta)=\mathrm{e}^{-LE_0^{\mathrm{NS}}}\tilde{Z}(\tau), \tag{B32}$$

where $\tau=L/\beta$.

On the other hand, we can also calculate the partition function by diagonalizing TFIM's Hamiltonian directly.[11] We will have a similar form

$$\begin{aligned}Z(L,\beta)=&\frac{1}{2}\mathrm{e}^{-\beta E_0^{\mathrm{NS}'}}\left[\prod_{n\in\mathrm{NS}}(1+\mathrm{e}^{-\beta\varepsilon'_n})+\prod_{n\in\mathrm{NS}}(1-\mathrm{e}^{-\beta\varepsilon'_n})\right]\\&+\frac{1}{2}\mathrm{e}^{-\beta E_0^{\mathrm{R}'}}\prod_{n\in\mathrm{R}}(1+\mathrm{e}^{-\beta\varepsilon'_n}),\end{aligned} \tag{B33}$$

where $E_0^{\mathrm{NS}'/\mathrm{R}'}$ are TFIM's vacuum energy and ε'_n are TFIM's excitation spectrum. The momentum index $n\in\mathrm{NS}/\mathrm{R}$ restricts in the first Brillouin zone. At the critical point in the scaling limit, we have $E_0^{\mathrm{R}'}-E_0^{\mathrm{NS}'}=\frac{2\pi}{L}\frac{1}{8}$ and $\varepsilon_n=\frac{2\pi|n|}{L}$. When $L\gg 1$, the restriction of n in the Brillouin zone eliminates. As the result, we find another functional relation between Z and $\tilde{Z}$,

$$Z(L,\beta)=\mathrm{e}^{-\beta E_0^{\mathrm{NS}'}}\tilde{Z}\left(\frac{1}{\tau}\right), \tag{B34}$$

where $\tau=L/\beta$.

We also notice $E_0^{\mathrm{NS}}=\beta e_0$ and $E_0^{\mathrm{NS}'}=Le_0$, where e_0 is the ground state energy density (or free energy density at zero temperature).To compare the above two relations in Eqs. (32) and (34), we find that the reduced partition function has inverse symmetry $\tilde{Z}(\tau)=\tilde{Z}(1/\tau)$.

Since the partition function is on the torus, we also have translational invariance $\tilde{Z}(\tau)=\tilde{Z}(\tau+1)$. The two symmetry operations form generators of the modular group $SL(2,Z)$. Thus we verify the modular invariance for TFIM explicitly.

In the above derivation, β is dimensionless since we have absorbed the dimension of h and J into β. (In fact, we have the following dimension relation: $[a]=[\beta]=[h]^{-1}=[J]^{-1}$, where a is the lattice size. The space and imaginary time have the same dimension in the Euclidean QFT.) As the result, to recover the dimension, the modular parameter should be $\tau=La/\beta=l/\beta$, where $l=\lim_{L\to\infty,a\to 0}La$ is the system size with dimension of length.

Appendix C: Correlation matrix and entanglement entropy

C1. Correlation matrix

We define the Majorana representation for fermion modes,

$$\breve{a}_{2j-1}=c_j+c_j^\dagger,$$

$$\breve{a}_{2j}=-\mathrm{i}(c_j-c_j^\dagger). \tag{C1}$$

The correlation matrix Γ^A is defined to be

$$\langle\breve{a}_j\breve{a}_l\rangle=\delta_{jl}+\mathrm{i}\Gamma^A_{jl}. \tag{C2}$$

To determine Γ^A, we could calculate the following matrix elements: $\langle\breve{a}_{2j-1}\breve{a}_{2l-1}\rangle$, $\langle\breve{a}_{2j-1}\breve{a}_{2l}\rangle$, $\langle\breve{a}_{2j}\breve{a}_{2l-1}\rangle$, and $\langle\breve{a}_{2j}\breve{a}_{2l}\rangle$.

For the ground state, the fermion correlation in k space is simple,

$$\begin{aligned}&\langle\eta_k\eta_{k'}^\dagger\rangle=\delta_{kk'},\\&\langle\eta_k\eta_{k'}\rangle=\langle\eta_k^\dagger\eta_{k'}\rangle=\langle\eta_k^\dagger\eta_{k'}^\dagger\rangle=0.\end{aligned} \tag{C3}$$

We can use Eq. (C3) to determine the real space correlation. We first calculate $\langle c_jc_l\rangle$,

$$\begin{aligned}\langle c_jc_l\rangle&=\frac{1}{N}\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}}\sum_{kk'}\mathrm{e}^{\mathrm{i}kj+\mathrm{i}k'l}\langle c_kc_{k'}\rangle\\&=\frac{-\mathrm{i}}{N}\sum_{kk'}\mathrm{e}^{\mathrm{i}kj+\mathrm{i}k'l}\langle(\cos\phi_k\eta_k-\sin\phi_k\eta_{-k}^\dagger)\\&\quad\times(\cos\phi_{k'}\eta_{k'}-\sin\phi_{k'}\eta_{-k'}^\dagger)\rangle\\&=\frac{-\mathrm{i}}{N}\sum_{kk'}\mathrm{e}^{\mathrm{i}kj+\mathrm{i}k'l}(-\cos\phi_k\sin\phi_{k'})\langle\eta_k\eta_{-k'}^\dagger\rangle\\&=\frac{-\mathrm{i}}{N}\sum_k\mathrm{e}^{\mathrm{i}k(j-l)}\cos\phi_k\sin\phi_k\\&=\frac{-\mathrm{i}}{2N}\sum_{k>0}\sin2\phi_k(\mathrm{e}^{\mathrm{i}k(j-l)}-\mathrm{e}^{-\mathrm{i}k(j-l)})\\&=\frac{1}{N}\sum_{k>0}\sin k(j-l)\sin2\phi_k,\end{aligned} \tag{C4}$$

then, $\langle c_j^\dagger c_l^\dagger\rangle$ is

$$\begin{aligned}\langle c_j^\dagger c_l^\dagger\rangle&=\langle c_lc_j\rangle^*=-\langle c_jc_l\rangle\\&=-\frac{1}{N}\sum_{k>0}\sin k(j-l)\sin2\phi_k.\end{aligned} \tag{C5}$$

Similarly, we can calculate $\langle c_jc_l^\dagger\rangle$ and $\langle c_j^\dagger c_l\rangle$,

$$\begin{aligned}\langle c_jc_l^\dagger\rangle&=\frac{1}{N}\sum_{kk'}\mathrm{e}^{\mathrm{i}kj-\mathrm{i}k'l}\langle(\cos\phi_k\eta_k-\sin\phi_k\eta_{-k}^\dagger)\\&\quad\times(\cos\phi_{k'}\eta_{k'}^\dagger-\sin\phi_{k'}\eta_{-k'})\rangle\\&=\frac{1}{N}\sum_{kk'}\mathrm{e}^{\mathrm{i}kj-\mathrm{i}k'l}\cos\phi_k\sin\phi_{k'}\langle\eta_k\eta_{k'}^\dagger\\&=\frac{1}{N}\sum_k\mathrm{e}^{\mathrm{i}k(j-l)}(\cos\phi_k)^2\\&=\frac{1}{2N}\left[\sum_k\mathrm{e}^{\mathrm{i}k(j-l)}+\sum_{k>0}\cos2\phi_k(\mathrm{e}^{\mathrm{i}k(j-l)}+\mathrm{e}^{-\mathrm{i}k(j-l)})\right]\\&=\frac{1}{2}\delta_{jl}+\frac{1}{N}\sum_{k>0}\cos k(j-l)\cos2\phi_k,\end{aligned} \tag{C6}$$

$$\begin{aligned}\langle c_j^\dagger c_l\rangle&=\delta_{jl}-\langle c_lc_j^\dagger\rangle\\&=\frac{1}{2}\delta_{jl}-\frac{1}{N}\sum_{k>0}\cos k(j-l)\cos2\phi_k.\end{aligned} \tag{C7}$$

We can determine all the matrix elements of Γ^A by substituting the above formulas into Eq. (C1),

$$\begin{aligned}
\langle \breve{a}_{2j-1}\breve{a}_{2l-1}\rangle &= \langle (c_j + c_j^\dagger)(c_l + c_l^\dagger)\rangle = \delta_{jl},\\
\langle \breve{a}_{2j}\breve{a}_{2l}\rangle &= \delta_{jl},\\
\langle \breve{a}_{2j-1}\breve{a}_{2l}\rangle &= \mathrm{i}\frac{2}{N}\sum_{k>0}\cos k(j-l)\cos 2\phi_k\\
&\quad -\sin k(j-l)\sin 2\phi_k\\
&= \mathrm{i}\frac{2}{N}\sum_{k>0}\cos[2\phi_k + k(j-l)] \equiv \mathrm{i}g(j-l),\\
\langle \breve{a}_{2j}\breve{a}_{2l-1}\rangle &= -\mathrm{i}g(l-j),
\end{aligned} \tag{C8}$$

where we define

$$g(l) = \frac{2}{N}\sum_{k>0}\cos(2\phi_k + kl). \tag{C9}$$

Because of the block structure of Γ^A, we define the two-by-two matrix Π_l according to Eq. (C8),

$$\begin{pmatrix} \langle \breve{a}_{2j-1}\breve{a}_{2l-1}\rangle & \langle \breve{a}_{2j-1}\breve{a}_{2l}\rangle \\ \langle \breve{a}_{2j}\breve{a}_{2l-1}\rangle & \langle \breve{a}_{2j}\breve{a}_{2l}\rangle \end{pmatrix} = \delta_{jl} + \mathrm{i}\Pi_{j-l}, \tag{C10}$$

where

$$\Pi_l \equiv \begin{pmatrix} 0 & g(l) \\ -g(-l) & 0 \end{pmatrix}. \tag{C11}$$

As the result, Γ^A becomes

$$\begin{aligned}
\Gamma^A_{j\alpha,k\beta} &= [\Pi_{j-k}]_{\alpha\beta}\\
&= g(j-k)\otimes\sigma^+_{\alpha\beta} - g(k-j)\otimes\sigma^-_{\alpha\beta},
\end{aligned} \tag{C12}$$

which is a block Toeplitz matrix.

When we consider the subsystem of the first M fermion modes, we can find a rotation $V \in O(2M)$ to rotate the subsystem into the Schur form

$$\Gamma^B_M = V\Gamma^A_M V^{\mathrm{T}} = \oplus_{l=1}^M \begin{pmatrix} 0 & v_l \\ -v_l & 0 \end{pmatrix},$$

$$\breve{b}_m = \sum_{n=1}^{2M} V_{mn}\breve{a}_n, \tag{C13}$$

which corresponds to decoupling the M fermion modes into the product state

$$\rho_M = \otimes_{l=1}^M \rho_l, \tag{C14}$$

where ρ_l has eigenvalue $\frac{1\pm v_l}{2}$.

Since each ρ_l contributes a binary entropy $s_l = -\frac{1+v_l}{2}\ln\frac{1+v_l}{2} - \frac{1-v_l}{2}\ln\frac{1-v_l}{2}$, the entanglement entropy of the subsystem is the summation of binary entropy of M modes: $S_M = \sum_{l=1}^M s_l$. If we define the matrix $\hat{\rho} = \frac{1}{2}(1 + \mathrm{i}\Gamma^A)$, the entanglement entropy can be written as $S_M = -\mathrm{Tr}[\hat{\rho}\ln\hat{\rho}]$.

C2. Integral representation of $g(l)$

In this subsection, we give an integral representation of the elements of the correlation matrix Γ^A: $g(l)$.

We have proved in the last section, $g(l)$ is

$$g(l) = \frac{2}{N}\sum_{k>0}\cos kl\cos 2\phi_k - \sin kl\sin 2\phi_k \equiv \frac{2}{N}\sum_{k>0} g_k(l), \tag{C15}$$

where ϕ_k is the Bogoliubov phase defined in Eq. (B2).

We notice both the denominators of $\cos 2\phi_k$ and $\sin 2\phi_k$ have the structure $1/\sqrt{a^2-b^2}$. Similar to Eq. (B11), we can also introduce the auxiliary variable θ. We use the following integral identity (see Ref. [27], p. 393, 3.613.1.):

$$\frac{1}{\sqrt{1-a^2}} = \frac{1}{\pi}\int_0^\pi \frac{\mathrm{d}\theta}{1+a\cos\theta} \tag{C16}$$

and choose $a = \frac{\sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}}{\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N}-\cos k}$. We have

$$\begin{aligned}
g_k(l) &= \cos kl\cos 2\phi_k - \sin kl\sin 2\phi_k = \frac{\cos kl(\cosh\frac{2\Gamma}{N} - \cosh\frac{2K}{N}\cos k) - \sin kl\sinh\frac{2K}{N}\sin k}{\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N} - \cos k}\frac{1}{\sqrt{1-a^2}}\\
&= \frac{1}{\pi}\int_0^\pi \mathrm{d}\theta \frac{1}{[\cosh\frac{2\Gamma}{N}\cosh\frac{2K}{N} + \sinh\frac{2\Gamma}{N}\sinh\frac{2K}{N}\cos\theta] - \cos k}\\
&\quad\times\left[\cosh\frac{2\Gamma}{N}\cos kl - \frac{1}{2}\left(\cosh\frac{2K}{N} + \sinh\frac{2K}{N}\right)\cos k(l-1) - \frac{1}{2}\left(\cosh\frac{2K}{N} - \sinh\frac{2K}{N}\right)\cos k(l+1)\right]\\
&= \frac{1}{\pi}\int_0^\pi \mathrm{d}\theta\left[\cosh\frac{2\Gamma}{N}\cos kl - \frac{1}{2}\left(\cosh\frac{2K}{N} + \sinh\frac{2K}{N}\right)\cos k(l-1)\right.\\
&\quad\left. - \frac{1}{2}\left(\cosh\frac{2K}{N} - \sinh\frac{2K}{N}\right)\cos k(l+1)\right]\Big/(\cosh x - \cos k),
\end{aligned} \tag{C17}$$

where, in the last equality, we use the notation $\cosh x$ defined in Eq. (B14) again.

To substitute Eq. (C17) into Eq. (C15), we have

$$g(l) = \frac{2}{N}\frac{1}{\pi}\int_0^\pi \mathrm{d}\theta\left[\cosh\frac{2\Gamma}{N}I_l - \frac{1}{2}\left(\cosh\frac{2K}{N} + \sinh\frac{2K}{N}\right)I_{l-1} - \frac{1}{2}\left(\cosh\frac{2K}{N} - \sinh\frac{2K}{N}\right)I_{l+1}\right], \tag{C18}$$

where we define $I_l = \sum_{k>0}\frac{\cos kl}{\cosh x - \cos k}$ for $l \in Z$.

C3. Calculate I_l

As shown in the last subsection, in the integral representation of $g(l)$ in Eq. (C18), we define the function I_l, labeled by integer l, by a complex summation of positive k modes. In this sub-section, we prove that I_l can be simplified to be a simple function of l.

Since I_l is an even function of l: $I_l = I_{-l} \equiv I_{|l|}$, we only need to consider the case $l \geq 0$.

In the following, let us derive a recursion formula of I_l. We divide I_l into two parts A_l and B_l,

$$\begin{aligned} I_l &= \sum_k \frac{\cos k(l+1)}{\cosh x - \cos k} \\ &= \sum_k \frac{1}{\cosh x - \cos k}[\cos kl \cos k - \sin kl \sin k] \\ &\equiv A_l - B_l. \end{aligned} \tag{C19}$$

After some algebra, we find

$$\begin{aligned} A_l &= \sum_k \cos kl \left[\frac{\cosh x}{\cosh x - \cos k} - 1\right] \\ &= \cosh x I_l - \sum_{k>0} \cos kl = \cosh x I_l - \frac{N}{2}\delta_{l,0}, \end{aligned} \tag{C20}$$

$$\begin{aligned} B_l &= \sum_k \frac{\sin k}{\cosh x - \cos k}[\sin k(l-1)\cos k + \cos k(l-1)\sin k] \\ &= \sum_k \sin k \sin k(l-1)\left[\frac{\cosh x}{\cosh x - \cos k} - 1\right] \\ &\quad + \sum_k \cos k(l-1)\frac{1-\cos^2 k}{\cosh x - \cos k} \\ &= \sum_k \frac{\cos k(l-2) - \cos kl}{2}\frac{\cosh x}{\cosh x - \cos k} - \sum_k \sin k(l-1)\sin k \\ &\quad + \sum_k \cos k(l-1)\left[\cos k - \frac{\sinh^2 x}{\cosh x - \cos k} + \cosh x\right] \\ &= \frac{\cosh x}{2} I_{l-2} - \frac{\cosh x}{2} I_l - \sinh^2 x I_{l-1} \\ &\quad - \sum_{k>0} \cos kl + \cosh x \sum_{k>0} \cos k(l-1) \\ &= \frac{\cosh x}{2} I_{l-2} - \frac{\cosh x}{2} I_l - \sinh^2 x I_{l-1} \\ &\quad - \frac{N}{2}\delta_{l,0} + \frac{N\cosh x}{2}\delta_{l,1}, \end{aligned} \tag{C21}$$

where we use $\sum_k \cos kl = \frac{N}{2}\delta_{l,0}$.

To substitute Eqs. (C20) and (C21) into Eq. (C19), we have a recursion formula of I_l (with an extra term $\delta_{l,1}$),

$$I_{l+1} = \frac{3\cosh x}{2} I_l + \sinh^2 x I_{l-1} - \frac{\cosh x}{2} I_{l-2} - \frac{N\cosh x}{2}\delta_{l,1}. \tag{C22}$$

When we consider $l \geq 0$, Eq. (C22) is reduced to be a simple recursion series,

$$I_{l+3} = \frac{3\cosh x}{2} I_{l+2} + \sinh^2 x I_{l+1} - \frac{\cosh x}{2} I_l, \quad l \geq 0. \tag{C23}$$

If we denote the eigen-solution to be $I_l(k) = \mathrm{e}^{\mathrm{i}kl} \equiv \alpha^l$, we will find three eigenvalues: $\alpha_1 = -\frac{\cosh x}{2}$, $\alpha_2 = \mathrm{e}^{-x}$, and $\alpha_3 = \mathrm{e}^{x}$. Then the general solution is

$$I_l = \sum_{j=1}^{3} a_j \alpha_j^l, \tag{C24}$$

where the coefficients a_i can be determined through the initial condition: I_0, I_1, and I_2.

To calculate I_0, we need the following identity (see Ref. [27], p. 40, 1.382.1):

$$\sum_{n=0}^{\frac{N}{2}-1} \frac{1}{\frac{\sin^2\frac{\pi(2n+1)}{2N}}{\sinh x} + \frac{1}{2}\tanh\frac{x}{2}} = N\tanh\frac{Nx}{2}, \tag{C25}$$

we have

$$\begin{aligned} I_0 &= \sum_{k>0} \frac{1}{\cosh x - \cos k} = \sum_k \frac{1}{2\sin^2\frac{k}{2} + 2\sinh^2\frac{x}{2}} \\ &= \frac{1}{2\sinh x}\sum_k \frac{1}{\frac{\sin^2\frac{k}{2}}{\sinh x} + \frac{1}{2}\tanh\frac{x}{2}} \\ &= \frac{N\tanh\frac{Nx}{2}}{2\sinh x}. \end{aligned} \tag{C26}$$

The I_1 is easy to calculate based on the result of I_0,

$$I_1 = \sum_k \left[\frac{\cosh x}{\cosh x - \cos k} - 1\right] = \cosh x I_0 - \frac{N}{2}. \tag{C27}$$

We can get I_2 using the recursion formula Eq. (C22) and property $I_1 = I_{-1}$,

$$\begin{aligned} I_2 &= \frac{3\cosh x}{2} I_1 + \sinh^2 x I_0 - \frac{\cosh x}{2} I_{-1} - \frac{N\cosh x}{2} \\ &= \sinh^2 x I_0 + \cosh x I_1 - \frac{N\cosh x}{2}. \end{aligned} \tag{C28}$$

To substitute the above three initial conditions in Eqs. (C26)–(C28) into the general solution in Eq. (C24), we can determine the three coefficients: $a_1 = 0$, $a_2 = \frac{N}{4\sinh x}(\tanh\frac{Nx}{2} + 1)$, and $a_3 = \frac{N}{4\sinh x}(\tanh\frac{Nx}{2} - 1)$. Since I_l is an even function of l, we finally have

$$I_l = \frac{N}{2\sinh x}\left[\tanh\left(\frac{Nx}{2}\right)\cosh(xl) - \sinh(x|l|)\right]. \tag{C29}$$

C4. The 1/N expansion of $g(l)$

For the moment, we have found a relatively simple expression of $g(l)$ in Eqs. (C18) and (C29) with trotter step N. In this subsection, we try to find the form of $g(l)$ in the continuum limit $N \to \infty$. We need to expand $g(l)$ up to the first order of $1/N$.

To substitute the expression of I_l into $g(l)$, we have

$$\begin{aligned} g(l) &= \frac{1}{\pi}\int_0^\pi \mathrm{d}\theta \varphi(\theta, l), \\ \varphi(\theta, l) &= \frac{1}{\sinh x}\left[\cosh\frac{2\Gamma}{N}\tilde{I}_l - \frac{1}{2}\left(\cosh\frac{2K}{N} + \sinh\frac{2K}{N}\right)\tilde{I}_{l-1}\right. \end{aligned}$$

$$-\frac{1}{2}\left(\cosh\frac{2K}{N}-\sinh\frac{2K}{N}\right)\tilde{I}_{l+1}\Bigg], \tag{C30}$$

where we define $\tilde{I}_l=\frac{2\sinh x}{N}I_l$ for convenience.

In the continuum limit, we can define the continuous coordinate as $r=\lim_{N\to\infty}\frac{l}{N}$, and then we have

$$xl=(Nx)(\frac{l}{N})\equiv(Nx)r. \tag{C31}$$

Instead of l, we can view $\tilde{I}_l$ as the function of r.

In the expression of $\varphi(\theta,l)$, we have $\tilde{I}_l$, $\tilde{I}_{l-1}$, and $\tilde{I}_{l+1}$ three terms, with the difference $\delta r=\pm\frac{1}{N}$ near r. For $r\neq 0$, we expand $\tilde{I}(r+\delta r)$ near r,

$$\begin{aligned}
&\tilde{I}(r+\delta r)=\tilde{I}(r)+\tilde{I}'(r)\delta r+\frac{1}{2}\tilde{I}''(r)(\delta r)^2+\mathcal{O}((\delta r)^3),\\
&\tilde{I}(r)=\tanh\left(\frac{Nx}{2}\right)\cosh(Nxr)-\sinh(Nx|r|),\\
&\tilde{I}'(r)=Nx[\tanh\left(\frac{Nx}{2}\right)\sinh(Nxr)-\mathrm{sign}(r)\cosh(Nxr)],\\
&\tilde{I}''(r)=(Nx)^2\left[\tanh\left(\frac{Nx}{2}\right)\cosh(Nxr)-\mathrm{sign}(r)\sinh(Nxr)\right].
\end{aligned} \tag{C32}$$

To substitute the formulas in Eq. (C32) for $\tilde{I}_{l+1}\equiv\tilde{I}(r+\frac{1}{N})$ and $\tilde{I}_{l-1}\equiv\tilde{I}(r-\frac{1}{N})$ into the expression of $\varphi(\theta,l)$ in Eq. (C30), we have

$$\begin{aligned}
\varphi(\theta,l)=&\frac{1}{\sinh x}\Bigg[\left(\cos\frac{2\Gamma}{N}-\cosh\frac{2K}{N}\right)\tilde{I}(r)\\
&+\frac{1}{N}\sinh\frac{2K}{N}\tilde{I}'(r)-\frac{1}{2N^2}\cosh\frac{2K}{N}\tilde{I}''(r)+\mathcal{O}\left(\frac{1}{N^3}\right)\Bigg]\\
=&\frac{1}{\sinh x}\Bigg[\left(\cos\frac{2\Gamma}{N}-\cosh\frac{2K}{N}\right)\\
&\times\left(\tanh\left(\frac{Nx}{2}\right)\cosh(Nxr)-\sinh(Nx|r|)\right)\\
&+x\sinh\frac{2K}{N}\left(\tanh\left(\frac{Nx}{2}\right)\sinh(Nxr)\right.\\
&\left.-\mathrm{sign}(r)\cosh(Nxr)\right)\\
&-\frac{x^2}{2}\left(\tanh\left(\frac{Nx}{2}\right)\cosh(Nxr)\right.\\
&\left.-\mathrm{sign}(r)\sinh(Nxr)\right)+\mathcal{O}\left(\frac{1}{N^3}\right)\Bigg].
\end{aligned} \tag{C33}$$

To simplify Eq. (C33), we need the following Taylor expansion formulas:

$$\begin{aligned}
&Nx=2\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}+\mathcal{O}\left(\frac{1}{N^2}\right)\equiv 2\kappa(\theta)+\mathcal{O}\left(\frac{1}{N^2}\right),\\
&\tanh\frac{Nx}{2}=\tanh\kappa+\mathcal{O}\left(\frac{1}{N^2}\right),\\
&\cosh(Nxr)=\cosh(2\kappa r)+\mathcal{O}\left(\frac{r}{N}\right),\\
&\sinh(Nx|r|)=\sinh(2\kappa|r|)+\mathcal{O}\left(\frac{r}{N}\right),\\
&\sinh x=\frac{2\kappa}{N}+\mathcal{O}\left(\frac{1}{N^3}\right).
\end{aligned} \tag{C34}$$

To substitute them into Eq. (C33), for $l\neq 0$, we have

$$\begin{aligned}
\varphi(\theta,l)=&\frac{1}{\sinh x}\Bigg[\frac{2(\Gamma^2-K^2)}{N^2}(\tanh\kappa\cosh 2\kappa r-\sinh 2\kappa|r|)+\frac{4\Gamma K}{N^2}(\tanh\kappa\sinh 2\kappa r-\mathrm{sign}(r)\cosh 2\kappa r)\\
&-\frac{2\kappa^2}{N^2}(\tanh\kappa\cosh 2\kappa r-\mathrm{sign}(r)\sinh 2\kappa r)+\mathcal{O}\left(\frac{1}{N^3}\right)\Bigg]\\
=&\frac{\frac{\Gamma^2-K^2-\kappa^2}{\kappa}\sinh\kappa(1-2|r|)-\mathrm{sign}(r)2K\cosh\kappa(1-2|r|)}{N\cosh\kappa}+\mathcal{O}\left(\frac{1}{N^2}\right)\equiv\frac{1}{N}f(\theta,r)+\mathcal{O}\left(\frac{1}{N^2}\right).
\end{aligned} \tag{C35}$$

However, we must take care of the case $l=0$ ($r=0$) because $\tilde{I}(r)$ is not differentiable at $r=0$. (Notice $\sinh(Nx|r|)$ is not differentiable at $r=0$.) We should discuss it separately.

When $r=0$, since

$$\tilde{I}_0=\tanh\frac{Nx}{2},\quad \tilde{I}_1=\tilde{I}_{-1}=\tanh\frac{Nx}{2}\cosh x-\sinh x, \tag{C36}$$

we have

$$\varphi(\theta,l=0)=\frac{1}{\sinh x}\left[\cosh\frac{2\Gamma}{N}\tilde{I}_0-\cosh\frac{2K}{N}\tilde{I}_1\right]=\frac{1}{\sinh x}\left[\frac{2\kappa}{N}+\frac{2(\Gamma^2-K^2-\kappa^2)\tanh\kappa}{N^2}+\mathcal{O}\left(\frac{1}{N^3}\right)\right]=1+\frac{1}{N}f(\theta,0)+\mathcal{O}\left(\frac{1}{N^2}\right). \tag{C37}$$

In summary, up to the first order of $1/N$, we have

$$g(l)=\delta_{l,0}+\frac{1}{N}\frac{1}{\pi}\int_0^\pi \mathrm{d}\theta f\left(\theta,\frac{l}{N}\right), \tag{C38}$$

$$f(\theta,x)=\frac{\frac{\Gamma^2-K^2-\kappa^2(\theta)}{\kappa(\theta)}\sinh[\kappa(\theta)(1-2|x|)]-\mathrm{sign}(x)2K\cosh[\kappa(\theta)(1-2|x|)]}{\cosh\kappa(\theta)}, \tag{C39}$$

where we use the definition

$$\kappa(\theta)=\sqrt{\Gamma^2+K^2+2\Gamma K\cos\theta}$$

and $\mathrm{sign}(x)$ is the sign function: $\mathrm{sign}(x)=\begin{cases}1 & x>0,\\ 0 & x=0,\\ -1 & x<0.\end{cases}$

C5. Derive integral equation

With the preparation of the above subsections, we can finally derive the integral equation of the correlation matrix in the continuum limit. We consider the subsystem with ratio $\Lambda=\beta'/\beta\in[0,1]$. The continuum limit can be realized as follows. We assume under certain trotter step τ, the total system has N fermion modes and subsystem M fermion modes, which satisfies

$$\Lambda=\lim_{N\to\infty}\frac{M}{N}. \tag{C40}$$

The corresponding correlation matrix Γ_M^A is real anti-symmetric and thus $\mathrm{i}\Gamma_M^A$ is Hermitian. According to Eq. (C12), the eigen-equation for $\mathrm{i}\Gamma_M^A$ is

$$\begin{aligned}\mathrm{i}\Gamma_M^A\chi=\lambda\chi\to&\sum_{k=1,\beta}^{M}\mathrm{i}[g(j-k)\sigma^+_{\alpha\beta}-g(k-j)\sigma^-_{\alpha\beta}]\chi_{k\beta}\\&=\lambda\chi_{j\alpha},\end{aligned} \tag{C41}$$

where we denote the corresponding eigenvector as $\chi_j=(\chi_{j1},\chi_{j2})$, $j=1,2,\ldots,M$.

In the continuum limit, since $\chi(x)=\chi_j/\sqrt{\tau}$, we have

$$\begin{aligned}&\mathrm{i}\sum_y\frac{1}{N}\left[\int_0^\pi\mathrm{d}\theta f(\theta,x-y)\sigma^+_{\alpha\beta}-\int_0^\pi\mathrm{d}\theta f(\theta,y-x)\sigma^-_{\alpha\beta}\right]\chi_\beta(y)\\&+\mathrm{i}(\sigma^+_{\alpha\beta}-\sigma^-_{\alpha\beta})\chi_\beta(x)=\lambda\chi_\alpha(x),\end{aligned} \tag{C42}$$

where we use Eq. (C38).

To transform the above summation into an integral, we instead of the summation $\sum_y\frac{1}{N}$ with $\int_0^\Lambda\mathrm{d}y$,

$$\int_0^\Lambda\mathrm{d}y\boldsymbol{K}(x-y)\chi(y)-\sigma^y\chi(x)=\lambda\chi(x), \tag{C43}$$

where the kernel is

$$\boldsymbol{K}(x-y)=\begin{pmatrix}0 & \frac{\mathrm{i}}{\pi}\int_0^\pi\mathrm{d}\theta f(\theta,x-y)\\ -\frac{\mathrm{i}}{\pi}\int_0^\pi\mathrm{d}\theta f(\theta,y-x) & 0\end{pmatrix}$$

and $f(\theta,x)$ has been defined in Eq. (C39).

As the result, the eigen-equation of the correlation matrix becomes an integral equation in the continuum limit. The corresponding entanglement entropy is given by Eq. (36), as described in the main text.

Appendix D: Ground state correlation at the continuum limit

The ground state of TFIM's cMPO is a fermion Gaussian state, which is completely captured by its two-point correlation functions: $\langle\psi(x)\psi(y)\rangle$, $\langle\psi^\dagger(x)\psi(y)\rangle$, $\langle\psi^\dagger(x)\psi^\dagger(y)\rangle$ and $\langle\psi(x)\psi^\dagger(y)\rangle$.

We can find the explicit form of correlation functions at the continuum limit. Since we have anti-periodic boundary condition for the ground state in the fermion representation, we can label the two points as x and y with $x,y\in[0,\beta)$. Using the relation $\psi(x)=c_j/\sqrt{\tau}$, where $\tau=\beta/N$, we have

$$\begin{aligned}&\langle\psi(x)\psi(y)\rangle\\&=\frac{N}{\beta}\langle c_jc_l\rangle=\frac{N}{4\beta}\langle(\breve{a}_{2j-1}+\mathrm{i}\breve{a}_{2j})(\breve{a}_{2l-1}+\mathrm{i}\breve{a}_{2l}\rangle\\&=\frac{N}{4\beta}[-g(j-l)+g(l-j)]\\&=-\frac{1}{4\pi\beta}\int_0^\pi\mathrm{d}\theta\left[f\left(\theta,\frac{x-y}{\beta}\right)-f\left(\theta,\frac{y-x}{\beta}\right)\right],\end{aligned} \tag{D1}$$

where, in the second equality, we use the transform relation Eq. (C1) between the fermion and Majorana representation; while in the last equality, we use the $1/N$ expansion of $g(l)$ in Eq. (C38).

To substitute the definition of $f(\theta,x)$ into the above equation, we finally have

$$\langle\psi(x)\psi(y)\rangle=\mathrm{sign}(x-y)\frac{J}{\pi}\int_0^\pi\mathrm{d}\theta\frac{\cosh[(\beta-2|x-y|)\sqrt{h^2+J^2+2hJ\cos\theta}]}{\cosh[\beta\sqrt{h^2+J^2+2hJ\cos\theta}]}, \tag{D2}$$

where $x,y\in[0,\beta)$ (as the result, $-\beta<x-y<\beta$).

Similarly, we have

$$\langle\psi^\dagger(x)\psi(y)\rangle=\frac{J}{\pi}\int_0^\pi\mathrm{d}\theta\frac{J+h\cos\theta}{\sqrt{h^2+J^2+2hJ\cos\theta}}\frac{\sinh[(\beta-2|x-y|)\sqrt{h^2+J^2+2hJ\cos\theta}]}{\cosh[\beta\sqrt{h^2+J^2+2hJ\cos\theta}]}. \tag{D3}$$

We can calculate $\langle\psi^\dagger(x)\psi^\dagger(y)\rangle$ and $\langle\psi(x)\psi^\dagger(y)\rangle$ following the same routine. However, using the commutation relations, we can easily find $\langle\psi^\dagger(x)\psi^\dagger(y)\rangle = -\langle\psi(x)\psi(y)\rangle$ and $\langle\psi(x)\psi^\dagger(y)\rangle = \delta(x-y) - \langle\psi^\dagger(x)\psi(y)\rangle$.

Appendix E: Exact cMPS representation at $h = 0$

E1. Exact cMPS

At $h = 0$, TFIM reduces to the classical 1D Ising model

$$\hat{H} = -J\sum_j \sigma_j^z\sigma_{j+1}^z \tag{E1}$$

and the corresponding cMPS's unit cell becomes

$$t_{ij} = \begin{pmatrix} \mathbf{1} & \sqrt{\tau J}\sigma^z \\ \sqrt{\tau J}\sigma^z & \mathbf{0} \end{pmatrix}_{ij}. \tag{E2}$$

In this section, we prove that the dominant eigenvector has the following exact cMPS representation with bond dimension two:

$$\varphi_i^{\alpha\beta} = \begin{pmatrix} \mathbf{1} \\ \sqrt{\tau J}\sigma^z \end{pmatrix}_i, \tag{E3}$$

where $Q = \mathbf{0}$ and $R = \sqrt{J}\sigma^z$.

For convenience, we set $J = 1$. By exchanging the physical index $\{\alpha,\beta\}$ and the virtual index $\{i,j\}$ in Eq. (E2), the cMPO's unit cell has a diagonal form

$$\tilde{t}_{\alpha\beta} = \begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix}_{\alpha\beta}, \tag{E4}$$

where $A \equiv \begin{pmatrix} 1 & \sqrt{\tau} \\ \sqrt{\tau} & 0 \end{pmatrix}$ and $D \equiv \begin{pmatrix} 1 & -\sqrt{\tau} \\ -\sqrt{\tau} & 0 \end{pmatrix}$.

Then the cMPO reads

$$T = \mathrm{Tr}\left[\prod \tilde{t}\right] = \lim_{\tau\to 0}[\otimes_{j=1}^N A + \otimes_{j=1}^N D], \tag{E5}$$

where $N\tau = \beta$.

If we denote the dominant eigenvector of matrice A and D as $|\lambda_+\rangle$ and $|\eta_+\rangle$. We argue that the exact dominant eigenstate of T has the following form:

$$|\Phi\rangle = \lim_{\tau\to 0}[\otimes_{j=1}^N|\lambda_+\rangle + \otimes_{j=1}^N|\eta_+\rangle]. \tag{E6}$$

To prove this, we solve the eigen-problem for A and D up to the first order of τ. We have

$$\begin{aligned} A &= U\Lambda U^\dagger, \\ D &= V\Lambda V^\dagger, \end{aligned} \tag{E7}$$

where

$$\begin{aligned} U &\equiv (|\lambda_+\rangle, |\lambda_-\rangle) = \begin{pmatrix} 1-\frac{\tau}{2} & -\sqrt{\tau} \\ \sqrt{\tau} & 1-\frac{\tau}{2} \end{pmatrix} + \mathcal{O}(\tau^2), \\ V &\equiv (|\eta_+\rangle, |\eta_-\rangle) = \begin{pmatrix} 1-\frac{\tau}{2} & \sqrt{\tau} \\ -\sqrt{\tau} & 1-\frac{\tau}{2} \end{pmatrix} + \mathcal{O}(\tau^2), \\ \Lambda &= \begin{pmatrix} 1+\tau & \\ & -\tau \end{pmatrix} + \mathcal{O}(\tau^2). \end{aligned} \tag{E8}$$

We find, up to the first order of τ, A and D have the same eigenvalues: $\{1+\tau, -\tau\}$. We can also determine the transformation rule between two eigenstates $|\lambda_+\rangle$ and $\eta_+\rangle$ from Eq. (E8):

$$\begin{aligned} |\eta_+\rangle &= (1-2\tau)|\lambda_+\rangle - 2\sqrt{\tau}|\lambda_-\rangle + \mathcal{O}(\tau^2), \\ |\lambda_+\rangle &= (1-2\tau)|\eta_+\rangle + 2\sqrt{\tau}|\eta_-\rangle + \mathcal{O}(\tau^2). \end{aligned} \tag{E9}$$

We first prove that Eq. (E6) is an eigenstate of T, then we prove that it corresponds to the dominant eigenvalue.

The $T|\Phi\rangle$ has the following form:

$$\begin{aligned} T|\Phi\rangle = \lim_{\tau\to 0} &\otimes_{j=1}^N A|\lambda_+\rangle + \otimes_{j=1}^N A|\eta_+\rangle \\ &+ \otimes_{j=1}^N D|\lambda_+\rangle + \otimes_{j=1}^N D|\eta_+\rangle. \end{aligned} \tag{E10}$$

Since $A|\lambda_+\rangle = (1+\tau)|\lambda_+\rangle + \mathcal{O}(\tau^2)$, $D|\eta_+\rangle = (1+\tau)|\eta_+\rangle + \mathcal{O}(\tau^2)$, $A|\eta_+\rangle = (1+\tau)(1-2\tau)|\lambda_+\rangle + \mathcal{O}(\tau^{\frac{3}{2}})$, and $D|\lambda_+\rangle = (1+\tau)(1-2\tau)|\eta_+\rangle + \mathcal{O}(\tau^{\frac{3}{2}})$, where we use Eq. (E9), we have

$$\begin{aligned} T|\Phi\rangle &= \lim_{\tau\to 0}(1+\tau)^N[1+(1-2\tau)^N] \\ &\quad \times [\otimes_{j=1}^N|\lambda_+\rangle + \otimes_{j=1}^N|\eta_+\rangle] \\ &= \mathrm{e}^\beta(1+\mathrm{e}^{-2\beta})\lim_{\tau\to 0}[\otimes_{j=1}^N|\lambda_+\rangle + \otimes_{j=1}^N|\eta_+\rangle] \\ &= 2\cosh\beta|\Phi\rangle. \end{aligned} \tag{E11}$$

As the result, we find $|\Phi\rangle$ is an eigenstate of T with eigenvalue $2\cosh\beta$.

To compare it with the exact free energy density of the 1D Ising model, which is $\beta f = -\ln(2\cosh\beta)$, we find that $|\Phi\rangle$ is the dominant eigenvector.

The $|\Phi\rangle$ in Eq. (E6) is a cMPS because we can rewrite it as

$$|\Phi\rangle = \mathrm{Tr}\left[\prod_i^N \tilde{\varphi}_{\alpha\beta}^i\right], \tag{E12}$$

where $\tilde{\varphi}_{\alpha\beta}^i = \begin{pmatrix} |\lambda_+\rangle & \mathbf{0} \\ \mathbf{0} & |\eta_+\rangle \end{pmatrix}_{\alpha\beta}$.

To exchange the physical index $\{\alpha,\beta\}$ and the virtual index $\{i\}$ again, we find that the cMPS's unit cell is

$$\varphi'^{\alpha\beta}_i = \begin{pmatrix} \mathbf{1}-\frac{\tau J}{2}\mathbf{1} \\ \sqrt{\tau J}\sigma^z \end{pmatrix}_i \tag{E13}$$

which is equivalent to Eq. (E3). In fact, the state in Eq. (E13) is different from the state in Eq. (E3) by a normalization factor $\mathrm{e}^{\frac{\beta J}{2}}$: $|\Phi'\rangle = \mathrm{e}^{\frac{\beta J}{2}}|\Phi\rangle$ if we denote the state in Eq. (E3) as $|\Phi'\rangle$.

We complete our proof.

E2. Entanglement entropy

The entanglement entropy for the general cMPS can be calculated by Schmidt decomposition.[28]

For the Ising cMPS in Eq. (E6), the corresponding normalized state is

$$\varphi_i^{\alpha\beta} = \begin{pmatrix} \mathbf{1} - \tau a \mathbf{1} \\ \sqrt{\tau}\sigma^z \end{pmatrix}_i, \tag{E14}$$

where the normalized factor is $a = \frac{1}{2\beta}\ln(4\cosh\beta)$.

If we denote the subsystem as A, whose size is β', and denote the rest as B, whose size is $\beta - \beta'$, we find that the state in Eq. (E14) is already Schmidt decomposed $|\Phi\rangle = \sum_{(\alpha\beta)} s_{(\alpha\beta)} |\Phi^A_{(\alpha\beta)}\rangle |\Phi^B_{(\alpha\beta)}\rangle$, where $s_{(\alpha\beta)} = \sqrt{\Lambda^A_{(\alpha\beta)}\Lambda^B_{(\alpha\beta)}}$. We have $\Lambda^A = \mathrm{e}^{-2a\beta'}(\mathrm{e}^{\beta'}, \mathrm{e}^{-\beta'}, \mathrm{e}^{-\beta'}, \mathrm{e}^{\beta'})$ and $\Lambda^B = \mathrm{e}^{-2a(\beta-\beta')}(\mathrm{e}^{\beta-\beta'}, \mathrm{e}^{-\beta+\beta'}, \mathrm{e}^{-\beta+\beta'}, \mathrm{e}^{\beta-\beta'})$. Then, the entanglement entropy is $S = -\sum_{(\alpha\beta)} s^2_{(\alpha\beta)} \ln s^2_{(\alpha\beta)}$. The concrete calculation shows

$$S = \ln 2 + \delta S(\beta), \tag{E15}$$

where

$$\begin{aligned} \delta S(\beta) = &-\mathrm{e}^{-2\beta}\left[\frac{2\ln 2}{(1+\mathrm{e}^{-2\beta})^2} - \mathrm{e}^{2\beta}\ln(1+\mathrm{e}^{-2\beta})\right] \\ &+ \beta\,\mathrm{e}^{-4\beta} \times \frac{\mathrm{e}^{2\beta}}{2(\cosh\beta)^2} - \mathrm{e}^{-4\beta} \\ &\times \frac{\mathrm{e}^{4\beta}\ln(1+\mathrm{e}^{-2\beta})}{2(\cosh\beta)^2}. \end{aligned} \tag{E16}$$

We find that the entanglement entropy S is independent of the subsystem's size β'. When $\beta \to \infty$, S tends to be $\ln 2$ with an exponential small correction $\delta S(\beta) < 0$. Up to the sub-leading order, we have

$$S = \ln 2 - \mathrm{e}^{-2\beta}(2\ln 2 - 1) + \mathcal{O}(\beta\,\mathrm{e}^{-4\beta}). \tag{E17}$$

Appendix F: Calculation details of cMPS

F1. Explicit form of ρ_k and N_k

For a general model, we denote the optimized ground state as

$$\begin{pmatrix} \mathbf{1} + \tau Q \\ \sqrt{\tau} R \end{pmatrix}. \tag{F1}$$

To distinguish notations of cMPS and cMPO, we denote cMPO's unit cell with subscript o,

$$t_{\mathrm{o}} = \begin{pmatrix} \mathbf{1} + \tau(h\sigma^z + f) & \sqrt{\tau J}\sigma^x \\ \sqrt{\tau J}\sigma^x & \mathbf{0} \end{pmatrix} \equiv \begin{pmatrix} \mathbf{1} + \tau Q_{\mathrm{o}} & \sqrt{\tau} L_{\mathrm{o}} \\ \sqrt{\tau} R_{\mathrm{o}} & 0 \end{pmatrix}, \tag{F2}$$

where, in the first equality, we use the TFIM as an example. As explained in the main text, since we rescale the cMPO T to be $\mathrm{e}^{\beta f} T$, we need to replace Q_{o} by $Q_{\mathrm{o}} + f$ for cMPO's unit cell, where f is the free energy density.

We first calculate the N_k,

$$\begin{aligned} \frac{1}{\beta}\langle\phi_k|\phi_k\rangle = &\,\mathrm{Tr}[(W\otimes\bar{W})\,\mathrm{e}^{\beta\hat{T}}] + \mathrm{Tr}[(\mathbf{1}\otimes\bar{V} + R\otimes\bar{W}) \\ &\times \int_0^\beta \mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}k\tau}\,\mathrm{e}^{\tau\hat{T}}(V\otimes\mathbf{1} + W\otimes\bar{R})\,\mathrm{e}^{(\beta-\tau)\hat{T}}] \\ = &\,\delta_{k,0}\sum_n \langle l_n|W\otimes\bar{W}|r_n\rangle\,\mathrm{e}^{\beta\Lambda_n} \\ &+ \sum_{n,m}\langle l_n|\mathbf{1}\otimes\bar{V} + R\otimes\bar{W}|r_m\rangle \\ &\times \langle l_m|V\otimes\mathbf{1} + W\otimes\bar{R}|r_n\rangle \int_0^\beta \mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}k\tau}\,\mathrm{e}^{\tau\Lambda_m}\,\mathrm{e}^{(\beta-\tau)\Lambda_n} \\ = &\sum_n \langle l_n|W\otimes\bar{W}|r_n\rangle\,\mathrm{e}^{\beta\Lambda_n} \\ &+ \sum_{n,m}\langle l_n|\mathbf{1}\otimes\bar{V} + R\otimes\bar{W}|r_m\rangle \\ &\times \langle l_m|V\otimes\mathbf{1} + W\otimes\bar{R}|r_n\rangle \frac{\mathrm{e}^{\beta\Lambda_m} - \mathrm{e}^{\beta\Lambda_n}}{\Lambda_m - \Lambda_n + \mathrm{i}k} \\ \equiv &\,\frac{1}{\beta}(V^\dagger, W^\dagger) N_k \begin{pmatrix} V \\ W \end{pmatrix}, \end{aligned} \tag{F3}$$

where $\hat{T} = \mathbf{1}\otimes\bar{Q} + Q\otimes\mathbf{1} + R\otimes\bar{R}$ is the transfer matrix of cMPS's overlap $\langle\Phi|\Phi\rangle$. We diagonalize it to be $\hat{T} = U\Lambda U^{-1}$ and express it using Dirac's bra-ket notation as

$$\hat{T}|r_n\rangle = \Lambda_n|r_n\rangle, \quad \langle l_n|\hat{T} = \Lambda_n\langle l_n|, \tag{F4}$$

where $U = (|r_1\rangle, |r_2\rangle, \ldots)$ and $U^{-1} = \begin{pmatrix} \langle l_1| \\ \langle l_2| \\ \vdots \end{pmatrix}$.

Since the denominator of $\frac{\mathrm{e}^{\beta\Lambda_m} - \mathrm{e}^{\beta\Lambda_n}}{\Lambda_m - \Lambda_n + \mathrm{i}k}$ will cause numerical instability when $\Lambda_m = \Lambda_n$ and $k = 0$, we should take the limit $k \to 0$ by hand,

$$\begin{aligned} &\frac{\mathrm{e}^{\beta\Lambda_m} - \mathrm{e}^{\beta\Lambda_n}}{\Lambda_m - \Lambda_n + \mathrm{i}k} \\ &= \begin{cases} \frac{\mathrm{e}^{\beta\Lambda_m} - \mathrm{e}^{\beta\Lambda_n}}{\Lambda_m - \Lambda_n + \mathrm{i}k}, & k \neq 0, \\ \delta_{\Lambda_m,\Lambda_n}\beta\,\mathrm{e}^{\beta\Lambda_n} + (1 - \delta_{\Lambda_m,\Lambda_n})\frac{\mathrm{e}^{\beta\Lambda_m} - \mathrm{e}^{\beta\Lambda_n}}{\Lambda_m - \Lambda_n + \mathrm{i}k}, & k = 0. \end{cases} \end{aligned} \tag{F5}$$

Similarly, for the ρ_k, we have

$$\begin{aligned} &\frac{1}{\beta}\langle\phi_k|T|\phi_k\rangle \\ &= \sum_{n,m}\langle l_n|\mathbf{1}\otimes\mathbf{1}_{\mathrm{o}}\otimes\bar{V} + \mathbf{1}\otimes L_{\mathrm{o}}\otimes\bar{W}|r_m\rangle \\ &\quad\times \langle l_m|V\otimes\mathbf{1}_{\mathrm{o}}\otimes\mathbf{1} + W\otimes R_{\mathrm{o}}\otimes\mathbf{1}|r_n\rangle \frac{\mathrm{e}^{\beta\Omega_m} - \mathrm{e}^{\beta\Omega_n}}{\Omega_m - \Omega_n + \mathrm{i}k} \\ &\equiv \frac{1}{\beta}(V^\dagger, W^\dagger)\rho_k \begin{pmatrix} V \\ W \end{pmatrix}, \end{aligned} \tag{F6}$$

where we denote the corresponding transfer matrix of the overlap $\langle\Phi|T|\Phi\rangle$ as $\hat{G}$,

$$\begin{aligned} \hat{G} = &\,Q\otimes\mathbf{1}_{\mathrm{o}}\otimes\mathbf{1} + \mathbf{1}\otimes Q_{\mathrm{o}}\otimes\mathbf{1} \\ &+ \mathbf{1}\otimes\mathbf{1}_{\mathrm{o}}\otimes\bar{Q} + R\otimes R_{\mathrm{o}}\otimes\mathbf{1} + \mathbf{1}\otimes\mathbf{1}_{\mathrm{o}}\otimes\bar{R}, \end{aligned} \tag{F7}$$

and we can diagonalize it as

$$\hat{G}|r_n\rangle = \Omega_n|r_n\rangle, \quad \langle l_n|\hat{G} = \Omega_n\langle l_n|. \tag{F8}$$

F2. Gauge fix condition

Both the cMPS and its tangent space state have gauge freedom. We can fix the gauge using the canonical form.[18]

In our calculation, we use the left canonical form.

First, we shift a constant to make the dominant eigenvalue of the transfer matrix of cMPS to be 0,

$$\langle l|\hat{T}=0, \quad \hat{T}|r\rangle=0. \tag{F9}$$

To rewrite the above equation in matrix form, we have

$$lQ+Q^{\dagger}l+R^{\dagger}lR=0, \quad Qr+rQ^{\dagger}+RrR^{\dagger}=0. \tag{F10}$$

Doing an additional invertible linear transformation, we can realize the left canonical form: $l=\mathbf{1}$ and $r=\Lambda^2$, where Λ^2 is a positive diagonal matrix satisfying by $\mathrm{Tr}[\Lambda^2]=1$. We denote the cMPS in the left canonical form as $(Q_{\mathrm{L}},R_{\mathrm{L}})$. Equation (F10) becomes

$$Q_{\mathrm{L}}+Q_{\mathrm{L}}^{\dagger}+R_{\mathrm{L}}R_{\mathrm{L}}^{\dagger}=0, \quad Q_{\mathrm{L}}\Lambda^2+\Lambda^2Q_{\mathrm{L}}^{\dagger}+R_{\mathrm{L}}\Lambda^2R_{\mathrm{L}}^{\dagger}=0. \tag{F11}$$

As a tangent vector of cMPS, the variational excited state $|\phi_k\rangle$ is gauge-invariant under the following reparameterization:

$$V\leftarrow V+[Q_{\mathrm{L}},X], \quad W\leftarrow W+[R_{\mathrm{L}},X], \tag{F12}$$

where X is an arbitrary matrix. We can use the following gauge fix condition to eliminate the D^2 gauge freedom:

$$V=-R_{\mathrm{L}}^{\dagger}W. \tag{F13}$$

Therefore, the N_k is nonsingular.

F3. Jordan–Wigner string

We want to calculate the expectation values of cMPS with the Jordan–Wigner strings:

$$\langle \mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle,$$

$$\langle \mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi^{\dagger}(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle.$$

We evaluate the expectation value in the meaning of normal order. We should distinguish the cases $x<y$ and $x>y$. For example, we could rewrite

$$\langle \mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle$$

as

$$\begin{aligned}&\langle \mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle\\ &=\theta(x-y)\langle \mathrm{e}^{\mathrm{i}\pi\int_y^x\rho(x')\mathrm{d}x'}\psi(x)\psi(y)\rangle\\ &\quad+\theta(y-x)\langle\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_x^y\rho(x')\mathrm{d}x'}\psi(y)\rangle.\end{aligned} \tag{F14}$$

To derive the formulas of expectation values in a simple way, we can view the cMPS as the limit of a (discrete) MPS.[4] We consider a discretized lattice with lattice parameter ε. Then the cMPS can be approximated as the following MPS up to the first order:

$$\begin{aligned}|\Phi\rangle&=\sum_{s_i=0}^{1}\mathrm{Tr}[A^{s_1}\cdots A^{s_N}](a_1^{\dagger})^{s_1}\cdots(a_N^{\dagger})^{s_N}|0\rangle,\\ A^s&=\begin{pmatrix}\mathbf{1}+\varepsilon Q\\ \sqrt{\varepsilon}R\end{pmatrix}_s,\end{aligned} \tag{F15}$$

where a_i is the boson mode living on the site i and has the following relation with the field operator at the continuum limit: $\psi(x)=\lim_{\varepsilon\to0}a_i/\sqrt{\varepsilon}$.

Correspondingly, the Jordan–Wigner string becomes $\mathrm{e}^{\mathrm{i}\pi\sum_j n_j}$, where $n_i=a_i^{\dagger}a_i$. Thus, for $x<y$, we have

$$\begin{aligned}&\langle\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_x^y\rho(x')\mathrm{d}x'}\psi(y)\rangle\\ &=\left\langle\frac{a_j}{\sqrt{\varepsilon}}\,\mathrm{e}^{\mathrm{i}\pi\sum_{j\le k<l}n_i}\frac{a_l}{\sqrt{\varepsilon}}\right\rangle\\ &=\left\langle\left(\frac{a_j}{\sqrt{\varepsilon}}\,\mathrm{e}^{\mathrm{i}\pi n_j}\right)\left(\prod_{k=i+1}^{l-1}\mathrm{e}^{\mathrm{i}\pi n_k}\right)\frac{a_l}{\sqrt{\varepsilon}}\right\rangle.\end{aligned} \tag{F16}$$

We consider the local vacuum state $|\varphi\rangle\equiv(1+\varepsilon Q)\otimes|0\rangle+\sqrt{\varepsilon}R\otimes a^{\dagger}|0\rangle$. Since $\frac{a}{\sqrt{\varepsilon}}\mathrm{e}^{\mathrm{i}\pi n}|\varphi\rangle=-R\otimes|0\rangle$ and $\langle\varphi|\mathrm{e}^{\mathrm{i}\pi n}|\varphi\rangle=1\otimes1+\varepsilon[Q\otimes1+1\otimes\bar{Q}-R\otimes\bar{R}]\equiv\mathrm{e}^{\varepsilon\hat{T}_{\mathrm{str}}}$, up to the first order of ε, we have

$$\begin{aligned}&\langle\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_x^y\rho(x')\mathrm{d}x'}\psi(y)\rangle\\ &=-\mathrm{Tr}[\mathrm{e}^{(\beta+x-y)\hat{T}}(R\otimes1)\,\mathrm{e}^{(y-x)\hat{T}_{\mathrm{str}}}(R\otimes1)],\end{aligned} \tag{F17}$$

where $\hat{T}$ is the transfer matrix of cMPS and $\hat{T}_{\mathrm{str}}$ is the modified transfer matrix because of the Jordan–Wigner string.

Similarly, for $x>y$, we have

$$\begin{aligned}&\langle\mathrm{e}^{\mathrm{i}\pi\int_y^x\rho(x')\mathrm{d}x'}\psi(x)\psi(y)\rangle\\ &=\left\langle\left(\mathrm{e}^{\mathrm{i}\pi n_j}\frac{a_j}{\sqrt{\varepsilon}}\right)\left(\prod_{k=i+1}^{l-1}\mathrm{e}^{\mathrm{i}\pi n_k}\right)\frac{a_l}{\sqrt{\varepsilon}}\right\rangle\\ &=\mathrm{Tr}[\mathrm{e}^{(\beta-x+y)\hat{T}}(R\otimes1)\,\mathrm{e}^{(x-y)\hat{T}_{\mathrm{str}}}(R\otimes1)],\end{aligned} \tag{F18}$$

where, in the last equality, we use $\mathrm{e}^{\mathrm{i}\pi n}\frac{a}{\sqrt{\varepsilon}}|\varphi\rangle=R\otimes|0\rangle$.

In summary, we have

$$\begin{aligned}&\langle\mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle\\ &=\theta(x-y)\mathrm{Tr}[\mathrm{e}^{(\beta-x+y)\hat{T}}(R\otimes1)\,\mathrm{e}^{(x-y)\hat{T}_{\mathrm{str}}}(R\otimes1)]\\ &\quad-\theta(y-x)\mathrm{Tr}[\mathrm{e}^{(\beta+x-y)\hat{T}}(R\otimes1)\,\mathrm{e}^{(y-x)\hat{T}_{\mathrm{str}}}(R\otimes1)].\end{aligned} \tag{F19}$$

Following a similar routine, we can also calculate $\langle\mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi^{\dagger}(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle$,

$$\begin{aligned}&\langle\mathrm{e}^{\mathrm{i}\pi\int_0^x\rho(x')\mathrm{d}x'}\psi^{\dagger}(x)\,\mathrm{e}^{\mathrm{i}\pi\int_0^y\rho(x')\mathrm{d}x'}\psi(y)\rangle\\ &=\theta(x-y)\mathrm{Tr}[\mathrm{e}^{(\beta-x+y)\hat{T}}(R\otimes1)\,\mathrm{e}^{(x-y)\hat{T}_{\mathrm{str}}}(1\otimes\bar{R})]\\ &\quad+\theta(y-x)\mathrm{Tr}[\mathrm{e}^{(\beta+x-y)\hat{T}}(1\otimes\bar{R})\,\mathrm{e}^{(y-x)\hat{T}_{\mathrm{str}}}(R\otimes1)].\end{aligned} \tag{F20}$$

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References

[1] Tang W, Tu H H and Wang L 2020 *Phys. Rev. Lett.* **125** 170604
[2] Cardy J L 1986 *Nucl. Phys. B* **270** 186
[3] Wang X and Xiang T 1997 *Phys. Rev. B* **56** 5061
[4] Verstraete F and Cirac J I 2010 *Phys. Rev. Lett.* **104** 190405
[5] Draxler D, Haegeman J, Osborne T J, Stojevic V, Vanderstraeten L and Verstraete F 2013 *Phys. Rev. Lett.* **111** 020402
[6] Vidal G, Latorre J I, Rico E and Kitaev A 2003 *Phys. Rev. Lett.* **90** 227902
[7] Latorre J I, Rico E and Vidal G 2004 *Quantum Informa-tion and Computation*
[8] Rams M M, Zauner V, Bal M, Haegeman J and Verstraete F 2015 *Phys. Rev. B* **92** 235105
[9] Pirvu B, Murg V, Cirac J I and Verstraete F 2010 *New Journal of Physics* **12** 025012
[10] Schultz T D, Mattis D C and Lieb E H 1964 *Rev. Mod. Phys.* **36** 856
[11] Pfeuty P 1970 *Annals of Physics* **57** 79
[12] Zuber J B and Itzykson C 1977 *Phys. Rev. D* **15** 2875
[13] Di Francesco P, Mathieu P and Sénéchal D 1997 *Conformal field theory Graduate texts in contemporary physics* (New York, NY: Springer)
[14] Boyanovsky D 1989 *Phys. Rev. B* **39** 6744
[15] Blöte H W J, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742
[16] Milsted A and Vidal G 2017 *Phys. Rev. B* **96** 245105
[17] Zou Y, Milsted A and Vidal G 2020 *Phys. Rev. Lett.* **124** 040604
[18] Haegeman J, Cirac J I, Osborne T J and Verstraete F 2013 *Phys. Rev. B* **88** 085118
[19] Haldane F D M 1981 *Phys. Rev. Lett.* **47** 1840
[20] Fisher M P A and Glazman L I 1996 *Transport in a onedimensional luttinger liquid*
[21] Calabrese P and Cardy J 2004 *Journal of Statistical Mechanics: Theory and Experiment* **2004** P06002
[22] McCoy B and Wu T T 1973 *The Two-Dimensional Ising Model*
[23] Its A, Jin B and Korepin V E 2006 arXiv: Quantum Physics
[24] Yang C N and Yang C P 1969 *J. Math. Phys.* **10** 1115
[25] Koma T 1989 *Progress of Theoretical Physics* **81** 783
[26] Destri C and de Vega H J 1992 *Phys. Rev. Lett.* **69** 2313
[27] Gradshteyn I S, Ryzhik I M, Zwillinger D and Moll V 2014 *Table of integrals, series, and products*; 8th ed. (Amsterdam: Academic Press)
[28] Tang W, Xie X, Wang L and Tu H H 2021 *Phys. Rev. D* **104** 114513