The wormhole effect on the path integral of reduced density matrix: Unlock the mystery of energy spectrum and entanglement spectrum

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Based on the path integral formulation of the reduced density matrix, we develop a new algorithm to overcome the exponential growth of computational complexity in reliably extracting low-lying entanglement spectrum from quantum Monte Carlo simulations. We test the method on Heisenberg spin ladder with long entangled boundary between two chains and the results support the Li and Haldane’s conjecture on entanglement spectrum of topological phase. We then explain the conjecture via the wormhole effect in the path integral and show that it can be further generalized for systems beyond gapped topological phases. Our further simulation results on the bilayer antiferromagnetic Heisenberg model with 2d entangled boundary across the (2 + 1)d O(3) quantum phase transition clearly demonstrate the correctness of the wormhole picture. Finally, we state that since the wormhole effect amplifies the bulk energy gap by a factor of $\beta$, the relative strength of that with respect to the edge energy gap will determine the behavior of low-lying entanglement spectrum of the system.

INTRODUCTION

The fruitful dialogue and fusion between quantum informatics and highly entangled condensed matter systems, have been gradually appreciated and recognized in recent years\cite{1,2}. Within this trend, quantum entanglement serves as the quintessential quantity to detect and characterize the informational, field-theoretical and topological properties of many-body quantum states\cite{3–9}. It offers, among many interesting features, the direct connection to the conformal field theory (CFT) and categorical description of the problem at hand\cite{7–24}. More than a decade ago, Li and Haldane proposed that the entanglement spectrum (ES) is an important, maybe more fundamental, measurement in this regard than the entanglement entropy (EE)\cite{25–27}. Since then, low-lying ES has been widely employed as a fingerprint of CFT and topology in the investigation in highly entangled quantum matter\cite{28–45}. Moreover, for topological states (e.g., quantum Hall state), they pointed out a possible deep correspondence between the low-lying ES and the true energy spectra on the edge. This is another famous Haldane’s conjecture, other than the one for the gapped spin-1 chain. Later, Qi, Katsura and Ludwig theoretically demonstrated the general relationship between entanglement spectrum of (2 + 1)d gapped topological states and the spectrum on their (1 + 1)d edges\cite{46}. However, besides such gapped topological phases, how universal the Li and Haldane’s conjecture is remains an interesting and open question to this day.

On the numeric front, most of the ES studies so far have focused on (quasi) 1d systems. Due to the exponentially growth of computation complexity and memory cost, the existing numerical methods such as exact diagonalization (ED) and density matrix renormalization group (DMRG) have obvious limitations for entangling region with long boundaries and higher dimensions. Quantum Monte Carlo (QMC) is a powerful tool for studying large size and higher dimensional open quantum many-body systems\cite{47–49}, as the important sampling scheme can in principle convert the exponential complexity into polynomial\cite{49–50}. But in the first appearance, it looks difficult to obtain ES from QMC, as it can’t obtain the quantum (ground state) wavefunction directly. However, it has been successfully shown that the computation of Rényi EE can be cast into the sampling of the partition function in modified manifold with different boundary condition for the entangling region and the rest of the system\cite{51–57}, and the universal information of many interesting quantum many-body phases and phase transitions in EE have been reliably extracted in QMC simulations\cite{57,17,19,21,58–62}.

This paper is a response to these open questions and recent developments. Here we first develop a protocol to overcome the exponential growth of computational complexity in obtaining the ES via QMC combined with stochastic analytic continuation\cite{4–8,10,11,13,70,71}. Then, we test the method on a Heisenberg ladder with long entangling region between two coupled chains. In the next step, we develop a pedagogical understanding of the conjecture within the path-integral formulation, in which we find a wormhole effect on the imaginary time edges of environment to induce the modes of entanglement Hamiltonian. According to such physical picture, the Haldane’s conjecture should not only be true in the gapped topological phase, but can be further generalized to other systems such as the quantum critical point (QCP). We then compute the ES of antiferromagnetic (AFM) Heisenberg bilayer model across the (2 + 1)d O(3) QCP, where the entangling region is between the two coupled layers, to demonstrate the correct of our wormhole picture. We find that since the wormhole effect amplifies...
the bulk energy gap by a factor of $\beta = \frac{1}{T}$, it is the relative strength of that with respect to the edge energy gap will determine the behavior of low-lying entanglement spectrum of the system.

The energy spectrum of the corresponding operator can be analytically continued from the correlation function in imaginary time. However, the relation between RDM and the modular Hamiltonian, $\rho_A = e^{-\mathcal{H}_A}$, doesn’t contain any information of an effective imaginary time $\beta_A$ of the subsystem. To compute ES, the first task is to construct a "partition function" of $\mathcal{H}_A$ with effective imaginary time $\beta_A$.

The solution comes from the $n$-th order of RDM, $\rho_A^n$, which can be written as $\rho_A^n = e^{-n \mathcal{H}_A}$. In this way, we can readily make use of such effective imaginary time $\beta_A = n$ at $n = 1, 2, 3, \cdots$ points. It’s similar to how the Rényi EE is computed in QMC via the replica partition function \[ Z^{(n)}_A = \text{Tr}[\rho_A^n] = \text{Tr}[e^{-n \mathcal{H}_A}]. \] (2)

As depicted in Fig. 1, $Z^{(n)}_A$ is a partition function in a replicated manifold, where the boundaries of area $A$ of the $n$ replicas are connected in imaginary time and the boundaries of the area $\overline{A}$ are independent (for sites in $\overline{A}$ for each replica, the usual periodical boundary condition of $\beta$ is maintained). It can be seen that the effective $\beta_A = n$ of the subsystem $A$ is in the unit of integer numbers whereas the $\beta = 1/T$ of the total system is in the inverse unit of the physical energy scale of the original system, $J$ of the Heisenberg model, for instance.

As shown in Fig. 1 since the imaginary times $\tau_A$ between two nearest replicas differs by $\delta \tau_A = 1$ (an effective imaginary time evolution operator $e^{-\mathcal{H}_A}$ of subsystem acts between them), we can measure the imaginary time correlation function at integer points, to obtain $G(\tau_A)$ of $\tau_A = 0, 1, 2, \cdots, n$. The correlation function $G(\tau_A) \sim e^{-\Delta \tau_A}$ when $\beta_A \rightarrow \infty$ where $\Delta$ is the lowest energy gap in the ES. When there is large gap, the $G(\tau_A)$ decays very fast and it is very hard to extract the high energy part of spectrum because the distance $\delta \tau_A = 1$ is not small enough. However, since the important information of ES is usually encoded in the low-lying spectra, it can be obtained with controlled accuracy from the long-time imaginary time correlations in QMC simulations, i.e. the more number of replicas $n$, the longer the imaginary time correlation $\tau_A$, and lower "energy" $\omega_{\mathcal{H}_A}$ in ES accessed. With the good quality $G(\tau_A)$ at hand, the stochastic analytic continuation (SAC) scheme \[ \text{SAC} \] can reveal reliable spectral information, $S(\omega_{\mathcal{H}_A}(k))$, as have been widely tested in fermionic and bosonic quantum many-body systems in 1d, 2d and 3d \[ \text{SSE} \], \[ \text{SAC} \]. In the following two examples, we use stochastic series expansion (SSE) QMC for quantum spin systems \[ \text{SSE} \], \[ \text{SAC} \] with SAC to obtain the related ESs. All the imaginary time correlations are computed via spin $S^z$ operators, i.e., $G_k(\tau_A) = \langle S^z_{-k}(\tau_A)S^z_k(0) \rangle$.

**SPIN-1/2 HEISENBERG LADDER**

As the first example to demonstrate the power of our method, we compute the ES of Heisenberg ladder with
FIG. 2. **ES of Heisenberg ladder.** (a) Heisenberg spin ladder. The red dashed line cut it into two entangled constituents, $A$ and $\bar{A}$. (b) The low-lying ES with $L = 100$, $J' = 1.732$, $J = 1$ and $\beta = 100$, $\beta_A = 200$. The white line is fitting to the data with the dispersion $4.58 \sin(k)$. (c) The low-lying ES with $L = 100$, $J' = 1.732$, $J = -1$ and $\beta = 100$, $\beta_A = 800$. The white line is fitting to the data with the dispersion $7.96 \sin^2(k/2)$.

$L = 100$ and compare with the ED results in small sizes $L = 10, 12, 14$ [27]. The spins on ladder are coupled through the nearest neighbor Heisenberg interactions [24] as shown Fig. 2 (a), with the strength $J$ along the leg and $J'$ on the rung. We first simulate with $J = 1$ and $J' = 1.732$ at $\beta = 100$ and $\beta_A = 200$ (200 replicas).

Our QMC ES in Fig. 2 (b) are consistent with the ED results, but our larger system sizes clearly reveal new features at the thermodynamic limit (TDL). First, with $L = 100$, the finite size gaps at $k = 0$ and $\pi$ are much smaller than the ED results with $L = 14$, e.g. $\Delta(\pi) \sim 0.48$ in ED whereas $\Delta(\pi) \sim 0.1$ in QMC, suggesting the gap closes at TDL. Second, the ES here is expected to bear the low-energy CFT structure, i.e., the ground level of ES, $\xi_0$, will scale as $\xi_0/L = c_0 + d_1/L^2 + O(1/L^3)$ where the $d_1 = \pi c v/6$ according to the CFT predication with the central charge $c = 1$ and $v$ the velocity of ES near the gapless point [24] i.e. the Cloizeaux-Pearson spectrum of the quantum spin chain, $\sqrt{|\sin(k)|}$ [33]. The ED fit at $L = 14$ gave $v \sim 2.36$, however, the fitting of QMC reveals the $v \sim 4.58$, as shown by the fitting line in Fig. 2 (b). This again reflects ES is greatly affected by finite size effect and it is necessary to access larger system sizes for quantitatively correct information.

Furthermore, we simulate the cases with both ferromagnetic (FM) $J = -1$ and antiferromagnetic (AFM) $J' = 1.732$ at $\beta = 100$ and $\beta_A = 800$ on the same ladder to compare with the results in Ref. [27], where the ladder is in the gapped rung singlet phase. Since the ES in TDL is expected to show spectrum of FM spin chain, i.e. quadratic dispersion $\sin^2(k/2)$ close to $k = 0$ [33] [30], we purposely chose $\beta_A = 800$ such that more low-lying ES can be obtained. As shown in Fig. 2 (c), the obtained dispersion of ES indeed resembles that of an edge Hamiltonian of the FM chain. In the ED results with $L = 14$ [27], a linear dispersion is found and it was attributed to the finite size effect. Now that we can access $L = 100$, the ES indeed reveals a quadratic dispersion $7.96 \sin^2(k/2)$ as shown by the white line therein. The results in Fig. 2(b) and (c), clearly demonstrate the correspondence between the ES and the true spectra of the edge Hamiltonian, consistent with the previous ED study, and achieve the TDL readily.
WORMHOLES IN THE PATH INTEGRAL

We find the geometrical manifold of replicas (Fig. 1) provides a very intuitive picture to understand the Haldane's conjecture, in particular, one can use a wormhole effect of the worldline in QMC simulation in space-time to explain the tracing of the environment in the path-integral. As shown in Fig. 3 (a), the gray part is the subsystem A and the white part is the environment $\overline{A}$, when a worldline (black line) goes into one replica, it has many choices for the possible paths. The imaginary time correlations for the worldlines going into bulk will decay to zero as $\beta \to \infty$ for obtaining the ground state. At the same time, the ones go through the imaginary-time-edge of environment will reach the other side through "wormhole" without much attenuation. Thus, tracing $\overline{A}$ actually provides a wormhole-like escapeway to connect both imaginary-time-edges of environment. It automatically guarantees the imaginary time correlations near the connection between replicas is stronger, which contribute to the ES. This picture is proved in our numerics via the correlation function along imaginary time direction in Fig. 3 (b), where the $G_{A,A}(\tau)$ for AFM Heisenberg ladder [the case of Fig. 2 (b)] is shown. It is obvious that there are two time/energy scales: the slow-decaying one is led by the entanglement Hamiltonian, that is the envelope of upper boundary at the $\beta_A = 0, 1, 2, \ldots$ generated by the wormhole effect. The fast-decaying one is led by the original Hamiltonian, which happens in the bulk of one replica between two integer $\beta_A$ points. It goes into the depth of bulk as the "decay" ones in Fig. 3 (a). We note such wormhole effect of the worldline in QMC simulation of ES in the path-integral formulation is for the first time reported.

With such a picture, it is easy to understand the working of Haldane’s conjecture [25], i.e. the entanglement spectrum of $A$ is similar with the energy spectra of a closed system $A$ without coupling to $\overline{A}$. Fig. 3 (c) is an example of the evolution of worldline in such a closed system and Fig. 3 (d) is that of a replicated system such as that in Fig. 1. For the replicated system, we can measure the physical observables at the integer $\beta_A$ points to extract the information of $\mathcal{H}_A$. What we see at these time points of replica should be the same as in a closed system $A$ controlled by $\mathcal{H}_A$ at the same imaginary times. The replicated system is evolved by $H$ and all the worldlines cannot go to the environment at the replica-connections, which means the rule of worldline evolution we see at the integer $\beta_A$ is similar to that in a closed $A$ system of $H$. As shown in Fig. 3 (d), the real worldline (solid line) means it is at the $\tau_A = 0, 1, 2, \ldots$ we can measure, i.e., the connected part of two nearest replicas, and the virtual process goes in/out of one replica are denoted as the dashed line. Furthermore, because $\mathcal{H}_A$ is independent on imaginary time, the rule of worldline evolution should be same in any time. Thus, $\mathcal{H}_A$ is likely to be the similar as $H$ of real closed $A$ system. And if $H$ has edge states, $\mathcal{H}_A$ will also has edge states, hence the Li and Haldane’s conjecture.

The above argument can be applied to the case where every sites of subsystem $A$ is coupled with environment $\overline{A}$, such as the ladder case, and extend the previous spatial-cut explanation of the Haldane’s conjecture where the subsystem and environment are coupled only on boundary [46]. To further verify our wormhole picture, we simulate a coupled bilayer system, in which one layer is the subsystem $A$ and the other is the environment $\overline{A}$. According to our picture, the ES should be similar to the energy Hamiltonian of a closed one layer system. The results are shown below.

**FIG. 4. ES of Heisenberg bilayer across (2+1) O(3) transition.** (a) Antiferromagnetic Heisenberg bilayer. The red dashed line cut it into two entangled constituent layers, $A$ and $\overline{A}$. (b) The low-lying ES of in the Néel phase with $L = 50$, $J' = 1.732$, $J = 1$ and $\beta = 100$, $\beta_A = 32$. (c) The low-lying ES at the quantum critical point with $L = 50$, $J' = 2.522$, $J = 1$ and $\beta = 100$, $\beta_A = 32$. (d) The low-lying ES in the dimerized phase with $L = 50$, $J' = 3$, $J = 1$ and $\beta = 100$, $\beta_A = 32$. We show the obtained ES along the high-symmetry path $(0, 0) - (\pi, 0) - (\pi, \pi) - (0, 0)$. The white line is fitting to the data with the dispersion $7.5\sqrt{1 - \frac{1}{3}(\cos(\mathbf{k}_x) + \cos(\mathbf{k}_y))^2}$, the linear spin wave for antiferromagnetic Heisenberg model on square lattice.

**ANTIFERROMAGNETIC HEISENBERG BILAYER**

An AFM Heisenberg model on bilayer square lattice [15] as shown Fig. 4 (a), where $J$ and $J'$ are the intra- and inter-layer couplings, are studied. We compute the ES with the bottom layer as $A$ and the top layer as $\overline{A}$. The $(2 + 1)$d O(3) QCP, separating the Néel phase and inter-layer dimer product state, is found to locate at $J'/J = 2.522(1)$ from high-precision QMC simulations [19, 22, 91, 92]. The EE of antiferromagnetic Heisenberg bilayer has been studied in Ref. [33], but the ES is still lacking. We simulate three cases to demon-
strate our prediction: $J' / J = 1.732$ in the Néel phase [Fig. 4(b)], $J' / J = 2.522$ at the critical point [Fig. 4(c)], $J' / J = 3$ in the dimerized phase [Fig. 4(d)] at $\beta = 100$ and $\beta_A = 32$ with size $L = 50$.

All the three cases strongly support our understanding: the ESs have two gapless modes with a strong one at $\pi, \pi$ and a weak one at $(0,0)$, closely resembling those the Goldstone modes in square antiferromagnetic Heisenberg model [11, 13, 92]. We therefore fit all the three ESs in Fig. 4(b), (c) and (d) with the similar linear spin wave [95, 96] dispersions. As far as we are aware of, these results serve as the first measurement of ES in 2d entangling region, also consistent with our wormhole picture of worldline in QMC simulation of ES.

**ENTANGLEMENT INDUCES LONG RANGE INTERACTION**

Although the entanglement Hamiltonian is almost same as the virtual edge Hamiltonian, there is some high order terms which might not be irrelevant. In the analytical study on 1d solvable models [43], it was found that $H_A$ contains long range interactions beyond the the edge Hamiltonian of $H$ which only has local terms. In the 2d case, our results in Fig. 4 suggests similar results.

When the bilayer is deep inside the dimerized phase ($J' / J \gg 2.522$), it is known that the $\rho_A = e^{-\mathcal{H}_A}$ (the RDM of one layer) corresponds to a close system in disordered phase, because all the spins are in the dimerized state and the correlations between spins in one layer are short-ranged. This implies, in our context, a 2d system described by $H_A$ at an effective temperature $1 / \beta_A = 1$ is disordered. Then, as the effective temperature $1 / \beta_A$ is reduced in the QMC simulation, i.e., increasing the number of replicas. From Fig. 4(d) ($J' / J = 3$), the $\rho_A = e^{-n\mathcal{H}_A}$ shows a clear Goldstone mode which represents a ordered Néel phase, at the effective temperature $1 / \beta_A = 1 / n = 1 / 32$. This suggests that there is an effective thermal phase transition of $H_A$, from disorder to ordered phase. However, Mermin-Wagner theorem [97, 98] told us that, it is impossible for a 2d system to spontaneously break a continuous symmetry at finite temperature. The only possibility is that there are long-range interactions in the $H_A$ of our system, as in the 1d cases [44], such that the Mermin-Wagner theorem is circumvented.

**AMPLIFICATION OF BULK ENERGY GAP IN ES**

Our wormhole picture of the path-integral in replicated manifold for ES is very general. One only needs to compare the energy costs in different paths along the imaginary time. As the summation of weights in path integral is $e^{-\int D(\mathcal{L}) \Delta(\mathcal{L})}$, where the $\mathcal{L}$ is the path and $\Delta(\mathcal{L})$ is the gap of this path. In a rough mean field estimation, the cost can be treated as $\mathcal{L} \times \Delta(\mathcal{L})$. The $\mathcal{L}$ is the (imaginary time) path length and $\Delta(\mathcal{L})$ is the mean gap along this path. The wormhole effect gives the ratio of the cost between the bulk and entangled edge as $\beta \Delta_b : \Delta_e$, where $\beta$ is the estimated length of imaginary time in subsystem bulk and that for the entangled edge will be 1. Therefore, the energy gap of bulk is amplified by a factor of $\beta$ in the ES and it makes the low-lying ES always close to the edge energy mode at $\beta \rightarrow \infty$ limit, not only in the topological state cases (gapped bulk and gapless edge), but also both bulk and edge have finite gaps. We therefore conject that if the $\beta$ is finite, the entangled edge are gapped and subsystem bulk is gapless, the low-lying ES will be more like the energy spectra of bulk. Moreover, if both bulk and edge are gapped, the $\beta$ will lead to a competition of both gaps and induce a transition of the ES at finite temperature. We note the similar dynamical behaviours (amplification of bulk gap) has also been observed in 1d system when it can be described by CFT [99]. However, our result is beyond CFT and dimension, and is more general and fundamental.

**CONCLUSION**

Overall, we develop a practical scheme to extract the low-lying ES from QMC simulation. Combined with the unifying picture of wormhole effect in path-integral formulation, our method makes the ES measurement possible for high dimension quantum many-body systems with large entangling region. Our method is not only limited to QMC for spins, as the existed pioneering works in computing the ES for interacting fermion systems [11, 43], but can also be extended to other numerical approaches for highly entangled quantum matter, such as the finite temperature tensor-network algorithm [103, 102].

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Hamiltonian of ladder and bilayer systems

For the quantum Monte Carlo (QMC) simulations in this paper, we use the stochastic series expansion (SSE) algorithm\[1,2,3\] to deal with the Heisenberg ladder [Fig. 2 (a) in main text] and antiferromagnetic (AFM) Heisenberg bilayer model [Fig. 4 (a) in main text].

The Hamiltonian of the spin-1/2 ladder is

\[ H = J \sum_{<ij>} (S_{A,i}S_{A,j} + S_{\overline{A},i}S_{\overline{A},j}) + J' \sum_{i} S_{A,i}S_{\overline{A},i} \] (3)

Here, \( S_{A,i} \) and \( S_{\overline{A},i} \) are spin-1/2 operators at site \( i \) of \( A \) and \( \overline{A} \). \( <i,j> \) denotes a pair of nearest-neighbor sites on the spin chain of \( L \) sites with periodic boundary conditions. \( J \) is the coupling strength intra-chain and \( J' \) is coupling inter-chains.

Similarly, we can define the spin-1/2 Hamiltonian on a bilayer lattice via the same equation. Where \( S_{A,i} \) and \( S_{\overline{A},i} \) are spin-1/2 operators at site \( i \) of \( A \) and \( \overline{A} \) as Fig. 4 (a) in main text. \( (i,j) \) denotes a pair of nearest-neighbor sites on the square lattice of \( L \times L \) sites with periodic boundary conditions. \( J \) is the coupling strength intra-layer and \( J' \) is coupling inter-layers.

Stochastic analytical continuation

We employ a stochastic analytical continuation (SAC) \[4,5,6,7,8\] method to obtain the spectral function \( S(\omega) \) from the imaginary time correlation \( G(\tau) \) measured from QMC, which is generally believed a numerically unstable problem.

The spectral function \( S(\omega) \) is connected to the imaginary time Green’s function \( G(\tau) \) through:

\[ G(\tau) = \int_{-\infty}^{\infty} d\omega S(\omega)K(\tau, \omega) \] (4)

here \( K(\tau, \omega) \) is the kernel function depending on the temperature and the statistics of the particles. We restrict ourselves to the case of spin systems and with only positive frequencies in the spectral, where \( K(\tau, \omega) = (e^{-\tau \omega} + e^{-(\beta - \tau) \omega})/\pi \). Then, we have

\[ G(\tau) = \int_{0}^{\infty} d\omega \frac{e^{-\tau \omega} + e^{-(\beta - \tau) \omega}}{1 + e^{-\beta \omega}} B(\omega) \] (5)

here \( B(\omega) = S(\omega)(1 + e^{-\beta \omega}) \) is the renormalized spectral function.

In fact, \( G(\tau) \) for a set of imaginary time \( \tau_i \) is obtained by QMC with the statistical errors. The renormalized spectral function can be set into large number of equal-amplitude \( \delta \)-functions

\[ B(\omega) = \sum_{i=0}^{N_\omega} a_i \delta(\omega - \omega_i) \] (6)
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