The fundamental link between entanglement dynamics and non-equilibrium statistics in isolated quantum systems has been established in theory and confirmed via experiment. However, the understanding of several consequential phenomena, such as the Many-Body Localization (MBL), has been obstructed by the lack of a systematic approach to obtain many-body entanglement dynamics. This paper introduces the Quantum Correlation Transfer Function (QCTF) approach to entanglement dynamics in many-body quantum systems and employs this new framework to demonstrate the mechanism of MBL in disordered spin chains. We show that in the QCTF framework, the entanglement dynamics of two-level constituent particles of a many-body quantum system can be fully characterized directly from the system’s Hamiltonian, which circumvents the bottleneck of calculating the many-body system’s time-evolution. By employing the QCTF-based approach to entanglement dynamics, we demonstrate MBL dynamics in disordered Heisenberg spin chains through the suppressed quasi-periodic spin’s entanglement evolution after a quench from an anti-ferromagnetic phase by showing that in strongly-disordered spin chains with short-range interactions, the quantum correlation between particles is exponentially attenuated with respect to the site-to-site distance. Moreover, we obtain the lowest possible amplitude of the quasi-periodic spin’s entanglement as a function of disorder in the chain. The QCTF analysis of MBL dynamics is verified by exact numerical simulation of the system’s evolution. We also show that QCTF provides a new foundation to study the Eigenstate Thermalization Hypothesis (ETH). The QCTF methodology can be extended in various ways to address general issues regarding non-equilibrium quantum thermodynamics in spin lattices with different geometries.

I. INTRODUCTION

Entanglement is a fundamental property of quantum physics. Despite the long-standing controversy around this phenomenon in the early period of developing quantum mechanics, recent experiments have confirmed the special role of entanglement in quantum statistics by demonstrating thermalization in closed quantum systems [1–3]. These observations support former theoretical speculations on the link between entanglement and statistics in closed quantum systems [4–6], notably the Eigenstate Thermalization Hypothesis (ETH), in which the thermal behavior in an interacting many-body quantum system is attributed to its individual eigenstates [7–9]. Moreover, this novel viewpoint to quantum statistics allows for explaining certain phenomena, impossible to treat in semi-classical theories in which the pivotal role of entanglement is not taken into consideration [9–11]. As a remarkable example, we highlight the absence of thermalization in disordered chains of quantum particles, known as the Many-Body Localization (MBL) phenomenon [12,13]. In spite of the established fundamental link between entanglement and statistics in many-body quantum systems, characterizing the dynamics of entanglement has been obstructed by its inherent complexity due to the exponentially large Hilbert space that often underlie many-body quantum systems. This article targets two important gaps in the literature. First, by introducing a new theoretical framework to characterize entanglement dynamics in many-body quantum systems, and second by employing this new approach to demonstrate the mechanism of MBL. These two objectives will be explained further in this section as background to the paper.

A systematic approach to characterize many-body entanglement dynamics has been built on the work of Holzhey, Larsen, and Wilczek in 1994 [14], and Calabrese and Cardy in 2004 [15], which employs the so-called replica trick on a quantum field with conformal symmetry to obtain the entanglement entropy. This approach is analytically solvable for the continuum limit of 1D spin lattices, corresponding to a 1+1d conformal field theory [16,17], which has lead to proving variants of ETH for this class of systems [18,19]. Nevertheless, systems wherein the conformal symmetry is absent are predominant and of high interest. In the context of conformal field theory several crucial features such as parametric disorder, few-body and edge effects are not possible to treat. These features have been shown to give rise to novel phenomena such as eigenstate phase transitions [20,21], as discussed in the next paragraph. Several aspects of the entanglement behavior in many-body quantum systems have remained unexplored, especially when disorder is present, which is fundamentally important and “notoriously difficult”, as referred to by Ed-
transforming the unitary time-evolution of the system relation dynamics in many-body quantum systems by paper is to employ the QCTF approach to demonstrate system \[44, 45\]. Accordingly, the second objective of this trajectories are highly unstable for an interacting classical is of exceptional interest due to the absence of such be- cles site-to-site distance \[41–43\]. The MBL phenomenon spins attenuate exponentially with respect to the parti- ture (which we prove correct in this paper). In partic- approach, that is contingent on a fundamental conjec- lattices is the quasi-Local Integrals Of Motion (LIOMs) underlying mechanism of MBL has not been theoretically general numerical demonstrations of MBL dynamics, the un- the interacting particles after a quench \[1\]. Despite sev- wherein entanglement develops and saturates between this phenomenon is evident in quench experiments where a quantum system’s behavior, commonly initialized at a non-entangled state, is studied after a sudden change in its Hamilto- nian. In this scenario, strongly-interacting spins in a sufficiently disordered chain (in the MBL phase) cease to entangle, when initially uncorrelated \[40\]. This phe- nomenon is in contrast to quantum thermal behavior, wherein entanglement develops and saturates between the interacting particles after a quench \[1\]. Despite sev- eral numerical demonstrations of MBL dynamics, the un- derlying mechanism of MBL has not been theoretically demonstrated. A proposal to explain the MBL in 1D lattices is the quasi-Local Integrals Of Motion (LIOMs) approach, that is contingent on a fundamental conjecture (which we prove correct in this paper). In partic- ular, in the MBL phase, quantum correlations between spins attenuate exponentially with respect to the particle’s site-to-site distance \[41, 42\]. The MBL phenomenon is of exceptional interest due to the absence of such behavior in the classical analogue where non-ergodic trajectories are highly unstable for an interacting classical system \[44, 45\]. Accordingly, the second objective of this paper is to employ the QCTF approach to demonstrate the mechanism of MBL.

This paper presents a new approach to obtain the correlation dynamics in many-body quantum systems by transforming the unitary time-evolution of the system into a complex-valued function, the QCTF. To this end, a transformation is defined to encode the system’s dynamics into the analytic properties (i.e., poles and zeros) of the QCTF. By virtue of this transformation, the dynamics of correlations in the many-body quantum system, inherently obscured in the system’s state, can be explicitly revealed through closed-contour integrations in the complex space where the QCTF is defined. We show that this technique provides a foundation to study the ETH by quantifying the entanglement of strongly-interacting many-body eigenstates. Although the QCTF formulation is valid for arbitrary quantum states, the subsequent QCTF-based entanglement analysis in this paper will fo- focus on the class of many-body quantum systems consist- ing of constituent particles each having two energy levels, i.e., spin-\(\frac{1}{2}\) lattices, which are of prime current interest. Therefore, following the first objective of the paper, the formulation of QCTF is introduced and then employed to obtain the entanglement dynamics of spin-\(\frac{1}{2}\) particles of generic many-body quantum systems. This frequency-based analysis allows for inferring crucial properties of the system’s correlation dynamics. Importantly, within the QCTF framework, correlation dynamics is obtained directly from the quantum system’s characteristics, which would otherwise require extensive computational effort using time-domain analysis methods, such as numerical iteration based on exact-diagonalization or the Matrix Product State (MPS) formulations. More precisely, in the QCTF framework we exploit the fact that correlations between the particles of a quantum system emerge as a result of the relative evolution of orthogonal ampli- tudes in the system’s wave function. Therefore, by focusing on, and analyzing these relative evolutions, we circumvent the need to calculate the full time-dependence of the many-body quantum system’s state. The novel QCTF approach is further used to demonstrate the mechanism of MBL in the widely used model of disordered Heisenberg spin chains of arbitrarily length. Employing the QCTF leads to the frequency spectrum of the dy- namical entanglement measure in the many-body quan- tump system. Utilizing this feature, we show that at the high-disorder strength limit (i.e., MBL phase), the fre- quency spectrum of the quenched entanglement measure is composed of a few dominant components which corre- spond to the interaction between neighboring sites. Ad- ditionally, we employ the Mellin transformation to prove that the residual amplitudes corresponding to interac- tion with further sites are exponentially attenuated in the site distance. This analysis proves the latter piv- otal conjecture regarding the MBL phenomenon \[41, 43\]. Furthermore, the QCTF-based approach confirms that in the MBL phase the quenched subsystem’s entanglement is quasi-periodic and its amplitude is lower bounded as a function of the disorder strength. We verify the valid- ity of the QCTF formulation with numerical simulation of the MBL dynamics in disordered Heisenberg chains of computationally feasible length.

The reminder of this paper is organized as follows. In Section\[1\] the general principles of the QCTF framework
are presented and the basic form of the QCTF is introduced. Section II utilizes a QCTF-based analysis to reveal the entanglement dynamics of interacting two-level particles of a many-body quantum system. In this section, the particle’s entanglement of the system’s generic many-body eigenstates is characterized in terms of the properties of the corresponding quantum system. Section III presents a detailed analysis of the MBL phase in disordered spin chains. In Subsection III A time-independent perturbation theory is employed to obtain the QCTF formulation of strongly-disordered Heisenberg spin chains. Accordingly, the entanglement evolution of spins is derived and the MBL dynamics is demonstrated. In Subsection III B the Mellin transformation is employed to prove the aforementioned conjecture on exponential decay of correlations in the MBL phase with respect to inter-particle distances. Subsection III C includes numerical verification of the theoretical QCTF analysis of the MBL dynamics. Concluding remarks are given in section IV where we also suggest a path for further development and applications of the QCTF. Note that each figure’s caption contains extensive explanatory material complimentary to the main text. Finally, mathematical derivations and proofs of key results in the main text are given in the Appendix.

II. BASIC FORMULATION OF THE QCTF

The evolution of a quantum system in this formulation is described via a complex function, i.e. the QCTF, through what we refer to as chronological and structural frequency components. The chronological frequency component describes the system’s time dependence, while the structural frequencies encode the variation of the system’s state, in an arbitrary basis for the underlying Hilbert space. In this formulation, evolution of correlations between the constituent particles of the many-body quantum system can be obtained by integrating the QCTF along certain closed contours in the structural frequency space. We specify the basic QCTF transformation of the system’s density matrix in Subsection II A with special focus on the important case of pure quantum states in Subsection II B.

A. QCTF transformation of the system’s density matrix

For a generic quantum system with discrete energy levels, the basic QCTF is defined via the following 2-variable transformation of the element-wise Laplace-transform of the density matrix, \( \hat{\rho}(s) = \mathcal{L}\{\rho(t)\} \), as

\[
\mathcal{K}(z_d, z_a, s) = \sum_{l,k=0}^{d-1} \langle l|\hat{\rho}(s)|k\rangle z_d^{-l} z_a^{-k},
\]

where \( d \) is the quantum system’s Hilbert space dimension and \( \{l| \) \( l = 0, \ldots, d-1 \} \) is an arbitrary basis for this space. Here the complex variables \( z_d \) and \( z_a \) are structural frequencies, which are conjugate to the diagonal \( (l-k = \text{const.}) \) and anti-diagonal \( (l+k = \text{const.}) \) arrays of elements in the corresponding density matrix, as illustrated and discussed further in Figure III. The Hermiticity of the density matrix leads to the following symmetry of the QCTF

\[
\mathcal{K}(z_d, z_a, s) = \mathcal{K}^*(1/z_d^*, z_a^*, s^*).
\]

Equation (1) is the dual Laurent series expansions of \( \mathcal{K} \), in both \( z_d \) and \( z_a \) variables, centered at the origins of the spaces. Based on the labeling \( l = 0, \ldots, d-1 \) for the Hilbert space basis, the origin \( z_d = 0 \) is a pole of order (at most) \( d-1 \), while the origin \( z_a = 0 \) is a removable singularity in the \( z_a \) space. Also, for finite \( d \), the function \( \mathcal{K} \) is holomorphic in any punctured neighbourhood of the origin, in both structural spaces.

The QCTF (1) provides an equivalent description for the evolution of a quantum system as its density matrix, \( \rho(t) \). To confirm this statement, given any arbitrary basis set \( \{|l'|\} \) and arbitrary time \( t' > 0 \), the transition amplitude \( \langle l'|\rho(t')|k'\rangle \) can be obtained from the QCTF (1) through the following inverse transformation via close-contour integrations in \( \mathbb{C}^3 \) (refer to Appendix A for the proof)

\[
\langle l'|\rho(t')|k'\rangle = \frac{1}{(2\pi i)^2} \oint_{\partial C_a} ds \oint_{\partial C_d} dz_d \oint_{\partial C_a} dz_a e^{st'} \sum_{l,k} \langle k|\rho(t')|l\rangle z_d^{-(l-k)} z_a^{-(l+k)} \mathcal{K}(z_d, z_a, s),
\]

where \( \partial C_{a(d)} \) is any counter-clock-wise (CCW) closed curve in the \( z_{a(d)} \) planes enclosing the origin, wherein \( \mathcal{K} \) is holomorphic except at \( z_{a(d)} = 0 \), and \( \partial C_s \) is any CCW closed curve enclosing all of the poles of \( \mathcal{K} \) on the imaginary axis of the \( s \) domain. In principle, any generic density matrix can be transformed into its QCTF representation. This property allows for describing the evolution of quantum systems with time-dependent Hamiltonians via the QCTF formulation. The remainder of this paper will consider time-independent Hamiltonians, particularly due to their high importance in various current scenarios of many-body quantum statistical mechanics. In summary, the QCTF fully represents an arbitrary density matrix and in the next sections of this paper we will
exploit this equivalence to reveal quantum statistical features of many-body systems in the QCTF framework.

B. QCTF for pure quantum systems

In this subsection, we will focus on the important case of pure state quantum systems (\( \rho = |\psi\rangle \langle \psi| \)). For this purpose, consider the unitary evolution of the initial state \(|\psi_0\rangle\) under Hamiltonian \( H \). Accordingly, we can define the following 1-parameter QCTF transformation, denoted by \( \mathcal{K} \), of the system’s wave-function in the Laplace domain (\(|\tilde{\psi}(s)\rangle = L\{|\psi(t)\rangle\}) as follows:

\[
\mathcal{K}(z, s) = \sum_{l=0}^{d-1} z^l \langle l | \tilde{\psi}(s) \rangle \\
= \sum_{l=0}^{d-1} z^l \langle l | \mathbf{G}(s) | \psi_0 \rangle ,
\]

(4)

where \( \mathbf{G}(s) = (s + \frac{i}{\hbar} H)^{-1} \) is the resolvent of the system. In this case, the basic QCTF can be directly obtained (refer to Appendix [3] for details) as

\[
\mathcal{K}(z_d, z_a, s) = \tilde{\mathcal{K}}(z_d z_a, s) \star \mathcal{K}^s((z_a/z_d)^s, s^s),
\]

(5)

where operation \( \star \) is defined by the ordinary product operation in the \( z_d \) and \( z_a \) domains and the following convolution operation in the \( s \) domain. If \( F_1(s) \) and \( F_2(s) \) are functions in the Laplace domain, then:

\[
F_1(s) \star F_2(s) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} F_1(\sigma + i\omega) F_2(s - \sigma - i\omega) d\omega ;
\]

(6)

for some real \( \sigma \) in the region of convergence (ROC) of \( F_1(s) \). As an important special case of equation (6), we have:

\[
(s + i\omega_1)^{-1} \star (s + i\omega_2)^{-1} = (s + i(\omega_1 + \omega_2))^{-1}.
\]

More generally, the dynamics of a pure quantum system evolving under the Hamiltonian \( H \) can be represented by an operator function \( \mathcal{H}(H, z_d, z_a, s) \), which includes its dynamical correlation properties, independent of its initial state. To see this, using definition \( \mathcal{K} \), the QCTF transformation can be rewritten as the expectation value of \( \mathcal{H} \) with respect to the arbitrary initial state (\(|\psi_0\rangle\)),

\[
\mathcal{K}(z_d, z_a, s) = \langle \psi_0 | \mathcal{H}(H, z_d, z_a, s) | \psi_0 \rangle ,
\]

(7a)

\[
\mathcal{H} = \mathbf{G}^s(s^s) \left( \sum_{l,k} z_a^{l+k} z_d^{l-k} |k \rangle \langle l | \right) \star \mathbf{G}(s) .
\]

(7b)

The operator \( \mathcal{H} \) includes the dynamical properties of the quantum system, including the evolution of correlation between its constituent particles. This property, which will be discussed in detail in the next section, can be employed to understand how the correlation behavior varies for different initial states of the quantum system.

In the QCTF formulation, the general approach to obtain the many-body quantum system’s properties (e.g., the correlation dynamics between the particles) is to integrate a function of the QCTF around appropriate closed contours in the structural frequency spaces. Equation (3) is an example of this procedure to obtain the system’s density matrix elements. Given the fact that QCTF is an equivalent representation of the system’s density matrix, in principle it is possible to obtain the dynamics of various forms of correlation, such as two-particle correlations, higher-order (multi-particle) correlations and particle’s entanglement (the subject of the next section), by integrating a suitable function of the QCTF.

III. ENTANGLEMENT DYNAMICS IN THE QCTF FORMULATION

In this section, the QCTF approach is employed to characterize the entanglement evolution of two-level particles of a generic (many-body) quantum system which is initialized at a pure state and evolves unitarily. First, we introduce the entanglement measure used in the analysis and then we obtain the time evolution (dynamics) of the measure from the quantum system’s QCTF.

Consider a closed quantum system with discrete energy levels, consisting of a two-level particle (referred to as subsystem \( M \)) that interacts with an accompanying \( d \)-dimensional quantum subsystem \( R \). The bipartite quantum system evolves according to the Hamiltonian \( H \) from the initial state \(|\psi_0\rangle = |\psi(t = 0)\rangle\). If we denote the reduced density matrix of the subsystem \( M \) by \( \rho_M(t) = Tr_R\{|\psi(t)\rangle \langle \psi(t) |\} \), then \( Q_M(t) = det(\rho_M(t)) \) is a time-dependent entanglement measure of subsystem \( M \), which is also monotonically related to the second-order Rényi entanglement entropy through \( S_2(M) = -ln(1 - 2Q_M) \). Equivalently, we will use its Laplace transformation \( \tilde{Q}_M(s) = L\{|Q_M(t)\} \) as the dynamical entanglement measure in the analysis.

The entanglement measure \( \tilde{Q}_M(s) \) can be obtained from the QCTF, which is now defined on an off-diagonal block of the system’s density matrix, \( \tilde{\rho}(s) \). Given any basis for the quantum system which is constructed from the arbitrary basis vectors \{|+, -\}\) for \( M \) and \{|l\}, \( l = 0, ..., d - 1 \}\) (\( d \) can be countably infinite) for \( R \), we define the QCTF on the off-diagonal block \(|+\rangle |\tilde{\rho}(s)\rangle - \rangle\), as follows,

\[
\mathcal{H} = \mathbf{G}^s(s^s) \left( \sum_{l,k} z_a^{l+k} z_d^{l-k} | - \otimes k \rangle \langle + \otimes l | \right) \star \mathbf{G}(s) ,
\]

(8a)

\[
\mathcal{K}(z_d, z_a, s) = \langle \psi_0 | \mathcal{H} | \psi_0 \rangle .
\]

(8b)

Having introduced the suitable form of QCTF for the purpose of this section, in Appendix [3] we prove that
the dynamical entanglement measure \( \tilde{\mathcal{Q}}_M(s) \) can be obtained from the QCTF \( \tilde{\mathcal{M}} \) as follows,

\[
\tilde{\mathcal{Q}}_M(s) = (2\pi i)^{-2} \oint_{\partial C_d} \oint_{\partial C_a} dz_d dz_a \left[ (z_d z_a)^{-1} \mathcal{K}(z_d, z_a, s) * \mathcal{K}^*(1/z_d^*, 1/z_a^*, s^*) \right] - \mathcal{K}_d(z_a, s) * \mathcal{K}_d^*(1/z_a^*, s^*) \bigg|_{z_a=1},
\]

(9)

Here \( \partial C_d(a) \) are closed CCW contours where the integrands are holomorphic except at the origin of the \( z_d(a) \) planes. The first term in \( \tilde{\mathcal{M}} \) corresponds to the Frobenius norm of the off-diagonal sub-matrix \( \langle + | \tilde{\rho}(s) | - \rangle \), while the second term corresponds to the summation of the cross-correlation of its diagonal. These two quantities are identical when the subsystems \( \mathcal{M} \) and \( \mathcal{R} \) are not entangled.

To demonstrate this result, we characterize the static entanglement measure, \( \tilde{\mathcal{Q}}_M \), for the particular case when the many-body quantum system is initialized at one of its eigenstates \( \langle A \rangle \), with energy \( E_A \) (therefore we have \( \mathcal{G}(s) | A \rangle = (s + iE_A)^{-1} | A \rangle \)). To this end, using the arbitrary product basis \( | \pm l \rangle \) for the system, introduced previously in this section, \( | A \rangle \) is expanded as (note that \( | \pm l \rangle \)
and $|\pm\rangle \otimes |l\rangle$ are used interchangeably),
\[
|A\rangle = \sum_{l=0}^{d-1} \left( c^+_l |+l\rangle |+l\rangle + c^-_l |l\rangle |-l\rangle \right)
\]
\[
= |+\rangle \otimes \sum_{l=0}^{d-1} c^+_l |l\rangle + |-\rangle \otimes \sum_{l=0}^{d-1} c^-_l |l\rangle
\]
\[
= \alpha^+ |+\rangle \otimes |A^+\rangle + \alpha^- |-\rangle \otimes |A^-\rangle,
\]
where $\alpha = \sqrt{\sum c^2_l}$ and $|\alpha^+|^2 + |\alpha^-|^2 = 1$. It is convenient to construct a new basis set, $\{\tilde{l}\}$, for the subsystem $R$ such that $|A^+\rangle$ is one of the basis kets; more precisely, we assign $|0\rangle = |A^+\rangle$ (this procedure is always possible, for instance by using the Gram-Schmidt algorithm, starting from $|A^+\rangle$). Note that without loss of generality, it is assumed that $\alpha^+ \neq 0$.

Due to orthogonality of the new basis set, we have $\langle +l | A \rangle = \alpha^+ \delta_{l0}$. The QCTF can be obtained from (SM) as follows,
\[
K(z_d, z_a, s) = s^{-1} \alpha^+ \alpha^- \sum_k \langle z_a/z_d \rangle^k \langle A^- | \tilde{k} \rangle.
\]
Consequently, based on equation (11), the entanglement measure $\tilde{Q}_M(s)$ is
\[
\tilde{Q}_M(s) = \frac{1}{s^{-1} \alpha^+ \alpha^-} \sum_k \langle A^- | \tilde{k} \rangle^2
\]
\[
= \frac{1}{s^{-1} \alpha^+ \alpha^-} \langle A^- | A^+ \rangle^2
\]
\[
= \frac{1}{s^{-1} \alpha^+ \alpha^-} (1 - \langle A^- | A^+ \rangle^2),
\]
where the completeness relation is used in the last step. The chronological frequency dependence $s^{-1}$ corresponds to the unit step function at $t = 0$ in the time domain, which emphasizes the absence of any time-dependence in the entanglement measure. Based on $\tilde{Q}_M(s)$, the subsystem’s entanglement is characterized by the parameters $|\langle A^- | A^+ \rangle|$ and $\alpha^+, \alpha^-$. Note that no assumption is made about the nature of the quantum system or the eigenstate $|A\rangle$, and this equation holds in general.

To demonstrate how this formulation can be employed to study the ETH, now consider a general many-body quantum system consisting of strongly-interacting particles. The term $|\langle A^- | A^+ \rangle|$ in (12) measures the non-locality of $|A\rangle$ at $\mathcal{M}$ (refer to Appendix [12] for details). Therefore in a strongly-interacting quantum system with non-local eigenstates (e.g., eigenstates of translationally-invariant lattices) we expect that $|\langle A^- | A^+ \rangle| \ll 1$. Additionally, since the basis $\{|+, |-\}$ is chosen arbitrarily, for the systems with spin symmetry, e.g., $\text{su}(2)$, variables $|\alpha^+|$ and $|\alpha^-|$ must be non-zero (with a significant concentration around $|\alpha^+| \approx |\alpha^-| \approx 1/\sqrt{2}$, that corresponds to the maximal entanglement, $\tilde{Q}_M(s) \approx s^{-1}$) for almost all of the many-body eigenstates. This property is a general manifestation of the ETH. As a result, by relating the statistics of $|\langle A^- | A^+ \rangle|$ and $\alpha^+ \alpha^-$ to symmetries, the real-space (lattice) dimensionality as well as the range of interactions in the system, a detailed characterization of the entanglement of many-body eigenstates can be achieved.

In summary, this section developed a QCTF-based approach to characterize the entanglement dynamics of the two-level particles in a many-body quantum system. As demonstrated, one form of utilizing this tool is through obtaining the exact QCTF. In the next section, the QCTF is used in a perturbative framework to demonstrate MBL dynamics in a disordered spin chain.

IV. MANY-BODY LOCALIZATION IN DISORDERED HEISENBERG SPIN CHAINS

In this section, the QCTF approach is employed to study MBL dynamics in a disordered chain of strongly-interacting spins. Here we consider the Heisenberg spin chain with nearest-neighbor interactions, initialized at one of the anti-ferromagnetic states, which is the model primarily used in MBL studies [50].

Consider $N$ spin-$1/2$ particles in a one-dimensional lattice with nearest-neighbor spin-spin (exchange) interactions. Additionally, random magnetic fields are introduced at the position of each site, which initiate disorder in the lattice. The Hamiltonian of the closed quantum system is
\[
H = J \sum_{k=1}^{N-1} S_k S_{k+1} + \sum_{k=1}^{N} h_k S^z_k,
\]
where $S_k = \{S^x_k, S^y_k, S^z_k\}$ is the spin operator of the $k$th particle, $J$ is the nearest neighbor coupling strength and the $h_k$’s are random and independent fields drawn from the probability density $P_h(x)$. Based upon prior numerical exploration, it has been conjectured in the limit $N \to \infty$, when $P_h(x)$ is the uniform distribution on the interval $[-W, W]$ then the disordered chain undergoes a MBL transition at a critical disorder strength $W_c$, which separates the thermal and MBL phases [14]. The dynamics of the spin’s entanglement is the feature that distinguishes these two phases when the system is initialized at certain product states. In the thermal phase, each spin’s entanglement converges to a saturation value, while the MBL phase is characterized by suppressed [22], and quasi-periodic (as will be demonstrated in this section) dynamics of the spin’s entanglement.

Numerical studies have located the critical disorder strength of this system to be in interval $3.5 \leq W_c < 4$ [17, 18]. In what follows, the large disorder (MBL) limit is analyzed via the QCTF approach.

Subsection [12] begins the analysis of the MBL phase of [13] by obtaining its perturbative QCTF representa-
tion. We consider the interaction Hamiltonian as the perturbation to the disorder Hamiltonian in (13). Accordingly, using equation (9), we characterize the entanglement dynamics of spins in terms of Probability Density Functions (PDF) for their frequencies and corresponding amplitudes. In Subsection IV.B we prove that the frequency components corresponding to higher order perturbations are exponentially small in amplitude, which indicates the strong convergence of the perturbation series. Lastly, we test our results in Subsection IV.C in two ways. First, we compare the numerically obtained entanglement evolution in a chain of fifteen spins with the predictions from the QCTF formulation. Second, we reconstruct the theoretically derived PDFs from one million simulation samples of spin chains of length six.

A. Perturbative derivation of the entanglement measure

Here we employ time-independent perturbation theory along with the QCTF formulation to analyze the entanglement dynamics of spins in bulk (i.e., far from the edges) of the chain (13). In the MBL phase, the eigenstates of the Hamiltonian (13) are dressed product states from the local eigenstates $|\uparrow, \downarrow\rangle$ of $\sigma_z$. These product states, which are also the eigenstates of the unperturbed (disordered) Hamiltonian, are used as the basis set $\{|l\rangle\}$ of the QCTF transformation. Therefore, the set of direct product states $\{|\uparrow\downarrow, \downarrow\uparrow\rangle_M \otimes \{|l\rangle\}$ spans the system’s Hilbert space. The quantum system is initially in the anti-ferromagnetic state $|\uparrow\downarrow\downarrow\cdots\rangle$. Without loss of generality, we assume that the chosen spin (subsystem $\mathcal{M}$) is initially in state $|\uparrow\rangle$; Let us denote the anti-ferromagnetic state by $|\uparrow\rangle$. Similarly, we label some of the product states as shown in Figure 2. For simplicity, we use the notations $J_k = JS_k S_{k+1}$ and $J = \sum J_k$.

The unperturbed resolvent can now be written as

$$G^0 = (s + \frac{i}{\hbar} E_{0})^{-1} |\uparrow \rangle \langle \uparrow| \big| + (s + \frac{i}{\hbar} E_{1})^{-1} |\downarrow \rangle \langle \downarrow| \big| + (s + \frac{i}{\hbar} E_{-1})^{-1} |\downarrow \rangle \langle \downarrow| \big| + \cdots, \tag{14}$$

where $E_{\pm l}$ are unperturbed energies, which are simply obtained from the $h_k$’s. This unperturbed resolvent has $2^N$ terms corresponding to each of its poles; here we explicitly show three of them. This resolvent does not entangle $\mathcal{M}$ to $\mathcal{R}$, when the system is initially at the anti-ferromagnetic state. In the remainder of this section, we analyze the effect of perturbations to this resolvent on the entanglement dynamics of $\mathcal{M}$. For this purpose, we study the interference of product states due to the perturbation (interaction) Hamiltonian $J$. To this end, we inspect the transition amplitudes between the product states, caused by individual interaction Hamiltonians $J_k$, as shown in Figure 2. We denote the state $|al\rangle$, by $|l\rangle$ in the rest of this section (This is possible because the structure of the interactions prohibits the interference of both $|\uparrow l\rangle$ and $|\downarrow l\rangle$, with the anti-ferromagnetic state $(|\uparrow 0\rangle)$ during the perturbation process, which is achieved by applying a set of ordered perturbation Hamiltonians $\{J_k\}$ consecutively. Importantly, this property implies that the diagonal part of the QCTF, $\mathcal{K}_d$ in (9), vanishes). The interference amplitude between the eigenstates $j$ and $i$ during the perturbation process is denoted by $c_{ij}$. To obtain these amplitudes, the shortest path between these states (in terms of the number of perturbation steps) is considered. Therefore, for the states shown in Figure 2 we can write $c_{ji} = \frac{\langle l(i)\rangle_{E_{-1}} - \langle l(i)\rangle_{E_{1}}}{(E_{-1} - E_{1})}$ for $i < j$, $c_{ij} = c_{ji}^{*}$ for $j < i$ and we set $c_{jj} = 1$. As a result, the $a^{th}$-order perturbed eigenstate $|j^{(a)}\rangle$, $j = -3, \cdots, 3$ has the following expansion,

$$|j^{(a)}\rangle = \sum_{|i-j|\leq a, i=-3, \cdots, 3} c_{ji}|i\rangle. \tag{15}$$

Using (15), the perturbed resolvent can be obtained from (13). Accordingly, using equations (8a, SD), the QCTF is obtained as:

$$\mathcal{K}(z_d, z_o, s) = \sum_{l,k} z_d^{l+k} z_o^{-l-k} \sum_{i,j} c_{i0} c_{j0} c_{ij} c_{j0} c_{i0} c_{j0} (s + \frac{i}{\hbar} (E_i^{(1)} - E_j^{(1)}))^{-1}, \tag{16}$$

where $\sum'$ denotes the summation over $l$’s and $k$’s corresponding to $|\uparrow l = 0, \pm 3\rangle$ and $|\downarrow k = \pm 1, \pm 2\rangle$ respectively. The first order energy corrections will be shown to reasonably describe the MBL phase. Based on this perturbative form of the QCTF, the entanglement measure is obtained using relation (9) as follows:

$$\mathcal{Q}_M(s) = \sum_{l,k} \sum_{i,j,i',j'} c_{i0} c_{j0} c_{i'k} c_{j'k} c_{i0} c_{i'0} c_{j'0} c_{j0} (s + \frac{i}{\hbar} (E_i^{(1)} - E_j^{(1)} - E_i^{(1)} + E_j^{(1)}))^{-1}. \tag{17}$$

Utilizing this equation, the minimum order of perturbation in $\mathcal{Q}$ for a particular set of $l$ and $k$ is equal to $2(|l| + |k|)$, which is always an even number (refer to Appendix E.2 for further explanation). As a result, the most significant (lowest perturbation order) non-zero frequency contributions correspond to $l = 0$ and $k = \pm 1,$
which are the second order contributions to $\tilde{Q}_M(s)$ at frequencies $f = \pm |E_0^{(1)} - E_1^{(1)}|/\hbar$, such that

$$
\tilde{Q}_M^{(2)}(s) = c_{\pm 10}^0 \pm \hbar \left( s + \frac{i}{\hbar} (E_0^{(1)} - E_1^{(1)}) \right)^{-1} + \frac{\sigma^+}{\hbar} \left( s + \frac{i}{\hbar} (E_1^{(1)} - E_0^{(1)}) \right)^{-1},
$$

where $\tilde{Q}_M^{(2n)}(s)$ denotes the contributions of order $2n$ to the entanglement measure. According to this relation, the corresponding amplitudes $(f = \pm |E_0^{(1)} - E_1^{(1)}|/\hbar)$ can be obtained in terms of the probability density functions, denoted by $P_F^{(2)}(f)$ and $P_A^{(2)}(a)$ respectively. If $P_h(x)$ denotes the uniform distribution of $\hbar$'s on the interval $[-W, W]$, we can show that (see Appendix E.2 and E.3 for the proof)

$$
P_F^{(2)}(f) = \begin{cases} 
\frac{h(\frac{1}{W} - \frac{2W}{J})}{h(\frac{1}{W} - \frac{2W}{J})}, & 0 \leq f \leq \frac{h}{2W-J} \\
\frac{h}{h(\frac{J}{2W})}, & \frac{h}{2W-J} < f \leq \frac{h}{2W+J}, \\
0, & \text{otherwise}
\end{cases}
$$

$$
P_A^{(2)}(a) = \frac{W \sqrt{8a - 1}}{8(W^2a)^2}, \quad a \geq \frac{1}{8} \left( \frac{J}{W} \right)^2,
$$

which are shown in Figure 8. According to (20), the second-order frequency amplitude is lower bounded at $a_0 = \frac{1}{8}(\frac{J}{W})^2$. This value provides a lower bound on the entanglement amplitude in the MBL phase to second-order perturbation theory, which is expected to adequately predict the entanglement dynamics, as explained in the next subsection.

Despite the adequacy of second order perturbation theory, it is important to test the (next) fourth order contributions. The fourth-order contributions appear for a collective vector of indices in the summations, in (17); for instance $l = 0(i = -1, i' = 0)$ with $k = 1(j = 1, j' = 0)$ produces $(E_1^{(1)} - E_0^{(1)})/\hbar$. Non-zero frequencies which appear as fourth-order contributions are $\pm |E_1^{(1)} - E_1^{(1)}|/\hbar$, $\pm |E_0^{(1)} - E_0^{(1)} - E_0^{(1)}|/\hbar$, $|E_{\pm 1}^{(1)} - E_0^{(1)}|/\hbar$, $\pm |E_{\pm 1}^{(1)} - E_0^{(1)}|/\hbar$, and $|E_{\pm 1}^{(1)} - E_{\pm 1}^{(1)}|/\hbar$. The latter set of frequencies is identical to the second-order frequency components. Interference to $|\pm 3\rangle$ appears in the sixth-order contributions, for instance $l = 0(i = 0, i' = 0)$ with $k = 3(j = 3, j' = 0)$ produces the frequency $(E_3^{(1)} - E_3^{(1)})/\hbar$.

Thus, the spin’s entanglement measure was obtained from the system’s perturbed form of QCTF, which includes the contributing frequency components sorted by their corresponding perturbation order. Here, we can take advantage of this analysis to clarify the main idea of QCTF, which is to obtain the entanglement dynamics directly from the system’s Hamiltonian properties with-
out evaluating the system’s time evolution. Although at first glance, the QCTF \cite{16} transforms the entire off-diagonal block in the system’s density matrix, this transformation as well as the dynamical measure \cite{17} specify the structure of the terms in the density matrix and in the entanglement dynamics, respectively. Each frequency component in \cite{18} specifies the relative phase, and its corresponding amplitude, between the terms in the density matrix that contribute to the entanglement measure. This description is made possible through the $\ast$ operation. For instance, in the second-order entanglement measure \cite{18} the relative frequency components are highly simplified. This procedure allows for avoid-

\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{Illustration of the PDFs for (a) the frequency components and (b) their amplitudes in the lowest (second) order perturbation of the entanglement measure $Q_M^{(2)}(s)$ for a spin in the bulk of the chain. Sub-figure (a) shows the PDF for the second-order frequencies $P_f^{(2)}(f)$ in \cite{19}. These frequencies most significantly contribute to the entanglement measure of the spin $M$. For frequencies close to and smaller than $\frac{J}{W}$ (plotted with a dashed line), the local energy levels are vulnerable to strong mixing with the other energy levels (corresponding to the neighboring sites), which interferes with the perturbative treatment; but, the probability of this subset of frequencies contributing is approximately $J/W$, which is negligibly small in the MBL phase ($J \ll W$). Sub-figure (b) shows the PDF for second order amplitudes, $P_a^{(2)}(a)$. In the MBL phase, small amplitudes (i.e., on the order of $\frac{J}{W}$) are highly probable, with a lower cut-off at $a_0$. As shown in this sub-figure, the most probable amplitude ($a_{\text{max}}$) is located very close to the lower cut-off frequency, when taking into account the slow convergence of this PDF at high amplitudes (i.e., scaling as $a^{-\frac{3}{2}}$, plotted as a red dashed line). The lower cut-off implies the existence of a minimum amplitude in the entanglement measure in the MBL phase.

B. Exponential attenuation of high order perturbation amplitudes

In this subsection, we show that although the number of frequency components in the entanglement measure increases with the order of perturbation, their contribution gets exponentially suppressed. This property, not only validates the convergence of perturbation series \cite{17}, more importantly, it captures the essence of the MBL dynamics, as will be discussed. According to \cite{17} and the definition of the $c_{ij}$'s, the amplitudes of the $n$th-order contributions scale as $J^{2n}(c_{ij}c_{ik}c_{kj}c_{j\ell}c_{\ell\ell})^{-1}$ where indices can be repeated, e.g., $i_2 = i_3$. Here, the scaling property of these random amplitudes is analyzed. This goal can be achieved by finding their PDFs, which is similar to finding $P_A^{(2)}(a)$ for the case of $2n = 2$ in the last subsection. Nevertheless, obtaining the PDFs is not a straightforward way to assess the contribution of the frequency components, because it provides unnecessary detail about their amplitudes. Instead, the critical probability $P^{(2n)} = P\{J^{2n}|(c_{ij}c_{ik}c_{kj}c_{j\ell}c_{\ell\ell})^{-1} > 1\}$ can be studied. This probability is an indicator of the rate of convergence for the multi-variable perturbation series \cite{17}. In the MBL phase, the probability for $|h_i - h_j| < J$ is approximately $J/W$ (refer to Appendix \cite{22} for detail). Although this property does not directly imply that $P^{(2n)}$ scales exponentially in the order number \cite{17} ($\sim (J/W)^{2n}$), by employing the Mellin transformation \cite{19} we show that this property indeed holds.

In our analysis, we use the approximation that the probability densities for terms $|J/(h_i - h_j)| \sim F_A^{(1)}(a)$ are independent, i.e., we ignore the repeated indices. This approximation not only simplifies the analysis enabled by the use of the Mellin transformation, it is also physically relevant, that is, in the $W \gg J$ limit, taking into account the repeated indices decreases the critical probability, therefore, this approximation gives an upper bound for $P^{(2n)}$ (refer to Appendix \cite{23} for more details). Importantly, through this approximation, we are also generalizing the results to initial states beyond the anti-ferromagnetic order. More precisely, as inferred from Figure \ref{fig2} the initial state of the system prescribes how the indices should be repeated, therefore, by considering independent PDFs, we obtain an upper-bound for the critical probability that reflects a wider range of initial states (all of the unperturbed Hamiltonian’s eigenstates).

The critical probability can be written in terms of the...
PDF \( \hat{P}^{(2n)}(x) \) for \( | \frac{h_{i_1}-h_{i_2}}{J} \ldots \frac{h_{i_{2n-1}}-h_{i_{2n}}}{J} | \leq 1 \) as follows,

\[
P^{(2n)} = \mathcal{P}\{ | \frac{h_{i_1}-h_{i_2}}{J} \ldots \frac{h_{i_{2n-1}}-h_{i_{2n}}}{J} | \leq 1 \} = \int_0^1 \hat{P}^{(2n)}(x) dx.
\]

(21)

In Appendix F, we obtain the PDF \( \hat{P}^{(2n)}(x) \) and show that

\[
\ln(P^{(2n)}) \approx 2n \ln \left( \frac{J}{W} \right) + (2n-1) \left( \ln \left( \frac{2n \ln(\frac{2W}{J})}{2n-1} \right) + 1 \right)
\]

(22)

which is approximately linear in \( 2n \) within an acceptable approximation \( \frac{2n}{W} \approx 1 \) for large \( n \). Also, this formula gives the decay rate, which is approximately \( \frac{2n}{W} \ln \frac{2W}{J} \), for spins located further than the immediate neighbouring sites. Thus, the critical probability \( P^{(2n)} \), which is an indicator of the rate of convergence in the multi-variable perturbation series \( (27) \), decays exponentially with the order of perturbation. Therefore, in the MBL phase, the few contributing second-order frequencies are exponentially dominant. Furthermore, the exponential dominance of (non-zero) second-order frequency components supports the absence of DC transport in the MBL phase, which was conjectured to hold \( (27) \).

It is important to note that this analysis is not limited to disordered Heisenberg spin chains. Although generalizing this result to all disordered spin chains is beyond the scope of this paper and requires a detailed analysis, the theoretically demonstrated exponential dominance of low-order collaborating frequencies in the entanglement measure leads to suppressed, and quasi-periodic entanglement dynamics (after a quench to an strongly-interacting Hamiltonian) when the system is initially at one of the eigenstates of its unperturbed (disordered) Hamiltonian. This behavior is the essence of MBL dynamics.

C. Numerical illustration and validation of the QCTF approach to MBL

The theoretical analysis in Subsections IV A and IV B is illustrated and verified here by exact numerical simulations. Figure 4 shows the dynamical entanglement measure in the frequency domain for three spins in a disordered \( (W/J = 10) \) Heisenberg chain of fifteen spins, evolving unitarily according to the Hamiltonian \( (13) \) from an anti-ferromagnetic state. To this end, upon obtaining the entanglement measures, \( Q_M(t) \), which are not shown here for brevity, their corresponding Fourier transforms, \( (\mathcal{F}\{Q_M(t)\}) \), are compared with the predictions of the QCTF approach, given in sub-section IV A. More precisely, the QCTF approach predicts the singularities in \( \tilde{Q}_M(s) \) (for instance, the second-order poles are given in \( (18) \)), shown using black lines in Figure 4. Because the poles are purely imaginary, they coincide with the peaks in the numerically obtained Fourier spectra. The quasi-periodicity of the entanglement measures is confirmed by the observation of a few (one for the edge spin, and two for bulk spins) dominant non-zero frequency components in their corresponding Fourier transformations. The small deviations between the predicted and observed frequencies are due to both the error in the Fourier transformation (due to the finite simulation time) and the (neglected) higher-order perturbations to the energy values. This particular realization of the disordered Heisenberg chain, in addition to demonstrating the effectiveness of the QCTF approach, shows different avenues from which higher order effects can interfere with the second-order approximation of the entanglement dynamics, as discussed in the caption of Figure 4.

To test our results in more depth, we numerically iterate the unitary evolution of \( 10^5 \) random realizations of the disordered Heisenberg spin chain \( (13) \) with \( J = 1 \) and \( W = 10, 15 \) and \( 20 \) from an anti-ferromagnetic state. Followed by evaluating the system’s state, we obtain the density matrix for spins at the edge and in the bulk (with at least two sites away from the edges) of chains with six spins. As discussed in the previous subsection and demonstrated in Figure 4, the second-order frequency components correspond to interactions with immediate neighbours, which also make up the major part of the spin’s entanglement dynamics. Therefore, by considering smaller chains here, the statistics of the second-order frequencies is not affected and access to a higher number of simulation samples \( (10^6) \) is made computationally feasible. Eventually, we reconstruct the PDFs \( P^{(2)}_E(f) \) and \( P^{(2)}_A(a) \) through extracting the peaks in the Fourier transformation (at the locations predicted by our analysis) of the entanglement measure, as shown in Figure 5. The numerical results confirm the QCTF theoretical predictions at all of the disorder strengths, with higher precision at stronger disorders, as expected. Due to the difference in first-order energy corrections for an edge spin compared with a spin in the bulk of the chain, the PDFs of the second-order frequencies are slightly different, particularly at the high-frequency corner of the PDFs (refer to Appendix E for more detail). This phenomenon is captured in the numerical simulation, as shown in the insets in Figure 5(a), which affirms the effectiveness of the QCTF perturbative analysis. The deviation between the numerical and theoretical PDFs, which results from higher order contributions, fades away as the disorder strength increases, as shown in Figure 5(b).
V. CONCLUSION

The new description of quantum many-body dynamics through QCTF provides an equivalent representation as the wave-function or the density matrix formalisms.
while explicitly revealing the correlation dynamics in the system. This new formalism allows for obtaining the entanglement dynamics in a quantum system directly from the system’s Hamiltonian features, therefore it circumvents the bottleneck of evaluation of many-body system’s evolution. As a result, a measure for the entanglement dynamics of two-energy level particles of a many-body quantum system was obtained through integrating the QCTF along specific closed contours. The QCTF treatment was shown to be capable of efficiently characterizing the entanglement of highly-correlated many-body eigenstates, which provides a theoretical framework for further studying the Eigenstate Thermalization Hypothesis (ETH).

In addition to the general QCTF formulation presented in this paper, a primary application focus was on the MBL dynamics in the disordered Heisenberg spin chains, for which the spin’s entanglement dynamics were characterized in terms of probability density functions for amplitudes and corresponding frequency components of the entanglement measure. The QCTF method allowed for implementing time-independent perturbation theory to directly obtain the particle’s entanglement, while bypassing the evaluation of system’s time evolution. This capability enabled us to prove a critical conjecture regarding the MBL phase that the entanglement’s dynamics is dominated by local interactions and the effect of further sites decays exponentially [41–43]. Accordingly, we showed that entanglement’s evolution of a spin in the chain’s bulk is quasi-periodic in time. This finding supports the absence of DC transport in the MBL phase, which was also conjectured to hold in strongly-interacting chains [12, 37], and had been shown to exist in weakly-interacting spin chains [51]. Furthermore, in this analysis we obtained the minimum possible amplitude for the dominant frequency components of the subsystem’s entanglement, which implies a lower bound on the quasi-periodic entanglement amplitude in the MBL phase. The QCTF analysis can be applied to different probability distributions for the disordered field, which we denoted by $P_h(x)$, e.g., a Gaussian field, which shows one aspect of the generality of the QCTF formulation.

Although the principles and the basic form of QCTF are defined in general, that includes treating mixed quantum states, the application of QCTF in the paper was focused on entanglement dynamics of pure state quantum systems. This special focus was motivated by recent experimental observations and theoretical arguments on quantum thermalization and MBL in isolated pure state quantum systems. The QCTF approach was employed in two different ways: exact, when quantifying the static entanglement of many-body eigenstates in Section III and perturbative, in the MBL analysis in Section IV. Although employing the general QCTF formulation is not limited to these two means of utilization, other ways that QCTF can be employed will be a subject for future research. Additionally, there are several directions for future research building on the QCTF formalism. One application is to consider the MBL phenomenon in different spin-$\frac{1}{2}$ lattice geometries, e.g., 2D spin networks or the effect of long-range interactions on the MBL dynamics. Another direction is to extend the entanglement analysis to mixed quantum states and to systems where the particles each have a higher number of energy levels. Furthermore, based on the equivalence of the QCTF and density matrix descriptions, other classes of quantum phenomena, such as high-order correlations [22] and multi-partite entanglement [51] can be studied by linking the Hilbert space basis vectors to the real space (lattice) coordinates. Additionally, the QCTF framework should be considered to address quantum systems with time-depandent Hamiltonians, including the important class of controlled quantum systems. In this regard, the QCTF approach has the prospect of providing a new theoretical framework to control entanglement dynamics in many-body quantum systems, which is of significant importance to potentially many applications including quantum information science. In summary, we hope that the QCTF provides a means to analyze any-body quantum statistical mechanics, that yields new insights of fundamental and practical significance.

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APPENDIX

The Appendices contain detailed proofs and derivations of several items stated in the main text.

Appendix A: Derivation of equation (3)

Using equation (1), we can rewrite the R.H.S of equation (3) as follows

\[
\frac{1}{(2\pi i)^3} \oint_{\partial C_1} ds \oint_{\partial C_d} dz_d \oint_{\partial C_a} dz_a e^{\epsilon t} \sum_{l,k} \sum_{l',k'} \langle k|k' \rangle \langle l'|l \rangle z_d^{(l''-k'')-(l-k)-1} z_a^{(l''+k'')-(l+k)-1} \langle l''|\rho(s)|k'' \rangle.
\] (A1)
Note that the three integrals are independent and can be evaluated interchangeably. We consider the \( z_d \) and \( z_a \) integrals first. Using the fact that the integrand is holomorphic inside the closed contours \( \partial C_d \) and \( \partial C_a \), except at the origin, by employing Cauchy’s residue theorem the value of these two integrations are equal to the residue of the integrand at the origin (\( z_d = 0, z_a = 0 \)) times \((2\pi i)^2\). Also note that since \( \langle l'|\tilde{\rho}(s)|k'' \rangle \) has no \( z_d, z_a \) dependence, the residue of the integrand in the \( C^2 \) space is equal to the coefficient of \((z_a z_d)^{-1}\) in the summation, which corresponds to the terms with \( k'' = k, l'' = l \). Therefore, after evaluating the structural integrations, equation (A2) is

\[
\mathcal{K} = \frac{1}{2\pi i} \oint_{\partial C_a} dse^{st} \sum_{l,k} \langle l'|l \rangle \langle l|\tilde{\rho}(s)|k \rangle \langle k|k' \rangle = \langle l'|\tilde{\rho}(s)|k' \rangle = \langle l'|\rho(t')|k' \rangle, \tag{A2}
\]

where we have used the definition of the inverse Laplace transform, and the linearity of the transform.

**Appendix B: Derivation of equation (5)**

Here, we show that the QCTF in (5) can be interpreted as a transformation of the system’s density matrix using one chronological frequency, \( s \), and two structural frequencies, \( z_a \) and \( z_d \). Using (4) and the definition of operation \( \ast \), we can rewrite (5) as

\[
\mathcal{K}(z_d, z_a, s) \ast \mathcal{K}^\ast ((z_a/z_d)^\ast, s^\ast) = \sum_{l,k=0}^{d-1} \langle l|G(s)|\psi_0 \rangle \ast \langle \psi_0|G^\dagger(s^\ast)|k \rangle z_d^{l-k} z_a^{l+k}. \tag{B1}
\]

We define \( \tilde{c}_l(s) = \langle l|G(s)|\psi_0 \rangle = \mathcal{L}\{\langle l|\psi(t) \rangle \} = \mathcal{L}\{c_l(t)\} \). Then using definition (6) results in:

\[
\tilde{c}_l(s) \ast \tilde{c}_k(s^\ast) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \tilde{c}_l(\sigma + i\omega) \tilde{c}_k(\sigma - i\omega) (s - \sigma - i\omega)^{l+k} = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \omega \tilde{c}_l(t_1) \tilde{c}_k(t_2) e^{-\omega(s-t_2 - \sigma(t_1-t_2)) - i\omega(t_1-t_2)}
\]

\[
\quad = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \tilde{c}_l(t_1) \tilde{c}_k(t_2) e^{-s t_2 - \sigma(t_1 - t_2) - i\omega(t_1-t_2)}
\]

\[
\quad = \int_{-\infty}^{\infty} d\sigma \tilde{c}_l(t) \tilde{c}_k(t) e^{-st} = \langle l|\tilde{\rho}(s)|k \rangle. \tag{B2}
\]

Therefore, substituting \( \langle l|G(s)|\psi_0 \rangle \ast \langle \psi_0|G^\dagger(s^\ast)|k \rangle \) in (B1) with \( \langle l|\tilde{\rho}(s)|k \rangle \) gives:

\[
\mathcal{K}(z_d, z_a, s) = \sum_{l,k=0}^{d-1} \langle l|\tilde{\rho}(s)|k \rangle z_d^{l-k} z_a^{l+k}. \tag{B3}
\]

**Appendix C: Proof of equation (9)**

We start from the system’s state in the time domain, \( |\psi(t)\rangle \), and expand it in the product basis vectors of each subsystem, \( \{|+\rangle, |-\rangle\} \), and \( \{|l\rangle, l = 0, \ldots, d-1\} \), as follows

\[
|\psi(t)\rangle = \sum_{a \in \{+,-\}} \sum_{l=0,...,d-1} c_{al}(t)|a \otimes l\rangle; \tag{C1}
\]

\[
c_{al}(t) = \langle a \otimes l|\psi(t)\rangle.
\]

Based on this expansion, we may construct the matrix \( M_{2 \times d} \) such that its first and second rows consist of \( \{c_{+l}(t)\} \) and \( \{c_{-l}(t)\} \) respectively (the time dependence in c’s are not shown below for simplicity):

\[
M(t) \doteq \begin{pmatrix} c_{+0} & c_{+1} & \cdots & c_{+l} & \cdots & c_{d-1} \\ c_{-0} & c_{-1} & \cdots & c_{-l} & \cdots & c_{-d-1} \end{pmatrix}. \tag{C2}
\]

If subsystem \( M \) is not entangled to subsystem \( R \) at \( t = t' \), then \( |\psi(t')\rangle \) is a product state and the rows of \( M(t') \) are linearly dependent, i.e. \( \text{rank}(M(t')) = 1 \). This condition on the rank of \( M \) is necessary and sufficient for the subsystem \( M \) to not be entangled to subsystem \( R \). Thus, if \( \text{rank}(M) = 2 \) these subsystems are entangled. To construct a smooth indicator of entanglement, consider the following square sub-matrices \( M_{ij}^{(2 \times 2)} \), formed from the \( i \)th and \( j \)th columns of \( M \),

\[
M_{ij}^{(2 \times 2)} = \begin{pmatrix} c_{+i} & c_{+j} \\ c_{-i} & c_{-j} \end{pmatrix}, \tag{C3}
\]
and use them to define the entanglement measure $Q_M(t)$ as follows:

$$Q_M(t) = \sum_{0 \leq i < j \leq d-1} |\det (M^{ij}(t))|^2.$$  \hfill (C4)

More generally, $Q_M(t') = 0$ is a necessary and sufficient condition for the subsystem $M$ not to be entangled at $t'$.

Expanding the summations in $Q(M)$ will result in

$$Q_M(t) = \sum_{0 \leq i < j \leq d-1} \det (M^{ij}) \left( \det (M^{ij}) \right)^*$$  \hfill (C5a)

$$= \sum_{0 \leq i < j \leq d-1} (c_{ij}c_{-j} - c_{ij}c_{-i})(c^*_{ij}c^*_{-j} - c^*_{ij}c^*_{-i})$$  \hfill (C5b)

$$= \sum_{0 \leq i \neq j \leq d-1} |c_{ij}|^2 |c_{-j}|^2 - \sum_{0 \leq i \neq j \leq d-1} c_{ij}c_{-j}c_{ij}c_{-i}$$  \hfill (C5c)

$$= \left( \sum_{0 \leq i \leq d-1} |c_{ij}|^2 \right) \left( \sum_{0 \leq i \leq d-1} |c_{-i}|^2 \right)$$

which is the determinant of the time dependent reduced density matrix of subsystem $M$.

As the second step, here we prove that the R.H.S of equation (C5) is the Laplace transform of $Q_M(t)$. We start from the first term in (C5). Before proceeding, we introduce the notation $\hat{c}_{ij}(s) = \mathcal{L}\{c_{ij}(t)\} = (a \otimes l)\mathcal{G}(s)|\psi_0\rangle$. Therefore, by using the definition of $\hat{K}(z_d,z_a)$ in (C9), the first term in (C5) and the fact that the $\star$ operation is associative and commutative, we have

$$\mathcal{L}\{\sum_{l,k} |c_{ij}|^2 \sum_{l,k} (c^*_{ij}c^*_{-i}) \sum_{l,k} |c_{-i}|^2 \} = \det (\rho_M(t)),$$

upon employing Cauchy’s residue theorem, based on the definition of the closed contours $\partial C_d$ and $\partial C_a$, then the value of the double integral is equal to $(2\pi i)^2$ times the residue of the integrand at the origin of the structural space $(z_d, z_a)$, which is the coefficient of $z_d^{-1}z_a^{-1}$ in the double summation. Therefore, the only remaining terms after the double integration must satisfy the following set

$$\sum_{l,k} \hat{c}_{+l}(s) \star \hat{c}^*_{+l}(s^*) \star \hat{c}_{-k}(s^*) \star \hat{c}^*_{-k}(s^*) = \mathcal{L}\{\sum_{l,k} |c_{ij}|^2 |c_{-i}|^2\},$$  \hfill (C8)

of conditions:

$$\begin{cases}
    l + k - l' - k' - 1 = -1 \\
    l - k + l' - l' - 1 = -1
\end{cases} \iff \begin{cases}
    l = l' \\
    k = k'
\end{cases}.$$  \hfill (C7)

Consequently, the first term in (C5) is:

$$\mathcal{L}\{\sum_{l,k} |c_{ij}|^2 |c_{-i}|^2\},$$

which is the Laplace-dual of (C5a). In the last step, we operated with $\star$ similar to our calculation in equation (12). Based on this equality, by showing that the second term in (C5) corresponds to (C5b), the proof is accomplished. To this end, we first consider $\hat{K}_d(z_a, s)$. Based on the definitions (8b) and (9) we have:

$$\hat{K}_d(z_a, s) = (2\pi i)^{-1} \sum_{l,k} \mathbf{d} z_d \hat{c}_{+l}(s) \star \hat{c}^*_{-k}(s^*) z_d^{l+k} z_{-k}^{-1-k}.$$  \hfill (C9)

Applying the Cauchy’s residue theorem, the integral is equal to $(2\pi i)$ times the residue of the integrand at the
origin of the $z_d$ space, which is the coefficient of $z_d^{-1}$ in its Maclaurin expansion. Therefore, it is easy to see that for this integrand, only the terms with $l = k$ remain after the integration and we have

$$K_d(z_a, s) = \sum_l \tilde{c}_{l+1}(s) \ast \tilde{c}_{l-1}(s^*) z_a^2l. \quad (C10)$$

which is the Laplace-dual of the second term in (C5c). Therefore, using the linearity of the Laplace transformation, the R.H.S of (9) is equal to the Laplace transformation of $Q_M(t)$, which proves the assertion (9).

### Appendix D: Locality/non-locality of the eigenstate $|A\rangle$

Here we demonstrate how $|A^+A^-\rangle$ is a measure of non-locality of the eigenstate $|A\rangle$ at the location of subsystem $\mathcal{M}$. By expanding $|A^-\rangle$ in the new set of basis kets ($\{|\tilde{l}\rangle\}$), (10) can be rewritten as

$$|A\rangle = (\alpha^+ |+\rangle + \alpha^- \langle A^+ |A^- \rangle |-) \otimes |A^+\rangle + \alpha^- |-\rangle \otimes \sum_{\tilde{l} \neq 0} \langle \tilde{l} |A^-\rangle |\tilde{l}\rangle. \quad (D1)$$

Therefore, if $|\langle A^- |A^+ \rangle | \approx 1$ then $|A\rangle \approx (\alpha^+ |+\rangle + \alpha^- e^{i\phi} \langle A^+ |A^- \rangle |-) \otimes |A^+\rangle$ is very similar to a product state (i.e., it has local character). On the other hand, $|\langle A^- |A^+ \rangle | \approx 0$ implies that $|A\rangle \approx \alpha^+ |+\rangle \otimes |A^+\rangle + \alpha^- |-\rangle \otimes \sum_{\tilde{l} \neq 0} \langle \tilde{l} |A^-\rangle |\tilde{l}\rangle$, which is strictly non-local at the position of $\mathcal{M}$.

### Appendix E: Mathematical details of section IV

#### 1. Minimum perturbation order in $\{E_{\pm}^{(1)}(x)\}$

For specific values of $l$ and $k$ in the outer summation in (17), we first consider the inner summation over $i$, for which there is a term of the form $c_{i+1}^* c_i$. Due to (15), the order of perturbation for such a term is $|i| + |i - l|$, which has its smallest value equal to $|l|$, when $0 \leq i \leq l$ or $l \leq i \leq 0$. The same argument holds for each of the other indices $j$, $j'$ and $j''$; therefore, for a particular set of $l$ and $k$, the smallest order of perturbation is $2(|l| + |k|).

Consequently, the second term in (10) is

$$E_{\pm 0} - E_{\pm 1} = E_{0}^{(1)}(x) - E_{\pm 1}^{(1)}(x) \approx P_{h}(x) \ast P_{h}(x) - E_{\pm 1}^{(1)}(x), \quad (E1)$$

where $\ast$ is the convolution operator. To be clear, the states $|\uparrow \rangle$ and $|\downarrow \rangle$ describe the same orientation of spins in the chain, except for the two of the spins, which are flipped. Consequently, the difference on the L.H.S of this equation is equal to the subtraction $h_r - h_{r+1}$, where $r$ is the index of the particular spin considered in the chain. Finally, the PDF of the term $(h_r - h_{r+1})$ is obtained from the convoluted form on the R.H.S. Note that the expectation values in the middle term correspond to the first order energy corrections, which are equal to $\langle J \rangle_0 - \langle J \rangle_\pm = -J$.

For the uniform distribution form of $P_h(x)$ on the interval $[-W, W]$, we have $P_h(x) \ast P_h(-x) = \frac{1}{4W^2}; |x| \leq 2W$, which is shown in Figure IV(a). Therefore, the PDF for the first order energy differences $E_{0}^{(1)}(x) - E_{\pm 1}^{(1)}(x)$ is obtained by shifting $P_h(x) \ast P_h(-x)$ by $J$, which is shown in Figure IV(b). Finally, the PDF of the second-order frequencies $f = \pm |E_{0}^{(1)}(x) - E_{\pm 1}^{(1)}(x)|/\hbar \sim P^{f(2)}_F(x)$, is obtained by adding the value of $P^{f(1)}_F-E_{\pm 1}^{(1)}(x)$ for positive energies to the reflected (about the vertical axis) values for negative energies (due to the absolute value), which is shown by a dashed blue line in Figure IV(b), followed by scaling the horizontal and vertical axes by $1/\hbar$ and $\hbar$ respectively, which is shown in Figure IV(c).

The proof concerns a spin in the bulk of the chain. In the case of edge spins, we have $\langle J \rangle_0 - \langle J \rangle_\pm = -J/2$, therefore the resulting PDF, $P^{f(2)}_F(x)$, must be slightly different, which can be obtained by substituting $J$ by $J/2$ in the derivations and plots.
shows the area corresponding to this equation respectively. Sub-figure (a) shows the PDF for $E_{0} - E_{1} \sim P_{b}(x) \ast P_{b}(-x)$. The PDF for the corrected energy difference $E_{0}^{(1)} - E_{1}^{(1)}$ is obtained by shifting $P_{b}(x) \ast P_{b}(-x) \delta J$ due to equation $[23]$. The dashed line shows the reflected (about the vertical axis) probability densities for negative energies. Sub-figure (c) shows the PDF for the second-order frequencies in the entanglement measure $f_{E_{2}}$. Here, we prove that equation $(2)$ is the PDF of the amplitudes $2|c_{\pm 10}|^{2} \sim P_{A}^{(2)}(a)$. To this end, we start by finding the Cumulative Density Function (CDF) $R_{A}(a) = \int_{-\infty}^{a} P_{A}^{(2)}(a')da'$:

$$R_{A}(a) = \mathbb{P}\left\{ 2|c_{\pm 10}|^{2} \leq a \right\} = \mathbb{P}\left\{ \frac{|\langle \pm 1|J|0\rangle|}{E_{\pm 1} - E_{0}} \leq a \right\} = \mathbb{P}\left\{ |E_{\pm 1} - E_{0}| \geq \frac{J}{\sqrt{2a}} \right\}.$$  

Here, we use the Mellin transformation to show that the critical probability $P^{(2n)}$ scales exponentially in the order number ($\sim (J/W)^{2n}$). To this end, according to $[24]$ we directly obtain the PDF $P^{(2n)}$ from the PDF of the single terms. Before proceeding to the proof, note that the dependence of terms through repeated indices manifests itself strongly in the region where it is accompanied by a decreased critical probability. Also, the critical probability is agnostic to the repeated indices in the region where the terms have a large critical probability. Therefore, by neglecting the repeated indices, we obtain an upper bound on the critical probability.

In the Mellin space, the transformed PDF for the product term, $(M(P^{(2n)}))$ is equal to the product of the transformed PDFs of single fractions $[49]$, which (based on the derivations in section $[22]$) is given by

$$\frac{h_{i} - h_{i+1}}{J} \sim \tilde{P}^{(1)}(x) = \frac{1}{W} - \frac{Jx}{2W^{2}}; \quad 0 \leq x \leq \frac{2W}{J}.$$  

FIG. 6. Illustration of the probability density functions in $[22]$. Each sub-figure corresponds to a step in the proof of equation $[19]$. Sub-figure (a) shows the PDF for $E_{0} - E_{1} \sim P_{b}(x) \ast P_{b}(-x)$. The PDF for the corrected energy difference $E_{0}^{(1)} - E_{1}^{(1)}$ is obtained by shifting $P_{b}(x) \ast P_{b}(-x) \delta J$ due to equation $[23]$. The dashed line shows the reflected (about the vertical axis) probability densities for negative energies. Sub-figure (c) shows the PDF for the second-order frequencies in the entanglement measure $f_{E_{2}}$. Here, we prove that equation $(2)$ is the PDF of the amplitudes $2|c_{\pm 10}|^{2} \sim P_{A}^{(2)}(a)$. To this end, we start by finding the Cumulative Density Function (CDF) $R_{A}(a) = \int_{-\infty}^{a} P_{A}^{(2)}(a')da'$:

$$R_{A}(a) = \mathbb{P}\left\{ 2|c_{\pm 10}|^{2} \leq a \right\} = \mathbb{P}\left\{ \frac{|\langle \pm 1|J|0\rangle|}{E_{\pm 1} - E_{0}} \leq a \right\} = \mathbb{P}\left\{ |E_{\pm 1} - E_{0}| \geq \frac{J}{\sqrt{2a}} \right\}.$$  

Now we can obtain the PDF $P_{A}^{(2)}(a)$ by differentiating $R_{A}(a)$:

$$P_{A}^{(2)}(a) = \frac{d}{da}R_{A}(a) = \frac{W\sqrt{8a} - 1}{8(\frac{J}{W})^{2}}; \quad a \geq \frac{1}{8}(\frac{J}{W})^{2}.$$  

**Appendix F: Exponential decay of $P^{(2n)}$**

Here we use the Mellin transformation to show that the critical probability $P^{(2n)}$ scales exponentially in the order number ($\sim (J/W)^{2n}$). To this end, according to $[24]$ we directly obtain the PDF $P^{(2n)}$ from the PDF of the single terms. Before proceeding to the proof, note that the dependence of terms through repeated indices manifests itself strongly in the region where it is accompanied by a decreased critical probability. Also, the critical probability is agnostic to the repeated indices in the region where the terms have a large critical probability. Therefore, by neglecting the repeated indices, we obtain an upper bound on the critical probability.
Accordingly, its Mellin transformation is

\[ \Phi(z) = \mathcal{M}\{\hat{P}(^{(1)}(x))\} = \int_0^\infty x^{z-1} \hat{P}(^{(1)}(x))dx \]

\[ = \frac{J}{W} \left(\frac{2W}{J}\right)^z \frac{1}{z} - \frac{J/W}{z+1}, \]

Based on this transformation, \( \hat{P}^{(2n)}(x) \) can be obtained as follows

\[ \hat{P}^{(2n)}(x) = \mathcal{M}^{-1}\{ (\Phi(z))^{2n} \} \]

\[ = \left(\frac{J}{W}\right)^{2n} \mathcal{M}^{-1}\{ ((\frac{2W}{J})^{2n})^z \sum_{k=0}^{2n} \binom{2n}{k} x^{k-2n}(\frac{J/W}{z+1})^k \} \]

\[ = \left(\frac{J}{W}\right)^{2n} \left( \ln \left( \frac{2W}{J} x^{n-1} \right) \right)^{2n-1} \]

\[ + \sum_{k=1}^{2n} \frac{(-1)^k (\frac{J}{W})^{2n+k}}{(2n-k)k!} \left( \frac{2W}{J} x^{n-1} \right)^k \frac{M_{k-n,n-k}}{\Gamma(2n)} \left( \ln \left( \frac{2W}{J} x^{n-1} \right) \right)^{2n-1} \]

\[ \approx \left(\frac{J}{W}\right)^{2n} \frac{\ln \left( \frac{2W}{J} x^{n-1} \right)}{\Gamma(2n)} \]

where \( M_{\nu,\mu}(.) \) is the Whittaker function [52]. Therefore, we described the PDF of interest as an inverse Mellin transformation on the R.H.S. Now, using [21], the critical probability can be obtained

\[ P^{(2n)} = \int_0^1 \hat{P}^{(2n)}(x)dx = \left(\frac{J}{W}\right)^{2n} \frac{1}{\Gamma(2n)} \left[ x^{2n-1} \sum_{l=0}^{2n-1} \frac{(2n-1)!}{l!} \left( \ln \left( \frac{2W}{J} x^{n-1} \right) \right)^l \right]_0^1 \approx \left(\frac{J}{W}\right)^{2n} \frac{(2n \ln(\frac{2W}{J}))^{2n-1}}{(2n-1)!}. \]

Thus, using the Stirling’s approximation, \( \ln ((2n-1)!) \approx (2n-1)(\ln(2n-1) - 1) \), we have

\[ \ln \left( P^{(2n)} \right) \approx 2n \ln \left( \frac{J}{W} \right) + (2n-1)(\ln \left( \frac{2n \ln(\frac{2W}{J})}{2n-1} \right) + 1). \]

\[ \text{(F5)} \]

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