Quantification of causation by von-Neumann entropy

Bin Yi$^1$ and Sougato Bose$^1$

$^1$Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London, United Kingdom.

(Dated: January 4, 2022)

Liang information flow is a quantity widely used in classical network theory to quantify causation, and has been applied widely, for example, to finance and climate. The most striking aspect here is to freeze/subtract a certain node of the network to ascertain its causal influence to other nodes of the network. Such an approach is yet to be applied to quantum network dynamics. Here we generalize Liang information flow to the quantum domain using the von-Neumann entropy. Using that we propose to assess the relative importance of various nodes of a network to causally influence a target node. We exemplify the application by using small quantum networks.

Introduction

The significance of information flow lies not only in communication, but also in its logical implication of causation[1–5]. Established in the context of classical physics, the mathematical theory of causality has been widely applied to a variety of disciplines, e.g., climate science[6, 7], network dynamics[8–11], neuroscience[12–17], finance[18, 19], turbulence[20, 21]. Historically, various measures of classical information flow were proposed[5, 7, 22, 23]. Nonetheless, they were proposed axiomatically as an ansatz. The broadly applied concept of transfer entropy[5, 15, 18, 24] fails to account for many one-way causality schemes, sometimes even give qualitatively wrong results[25, 26], and the Granger causality[27] is inapplicable to generic deterministic systems. In light of the limitations, Liang and Kleeman established a universally applicable formalism within the framework of classical dynamical systems[27–32]. The series of work, which starts from 2005[27], puts the notion of information flow and causation on a rigorous footing, as Liang(2016)[30] argued: "Information flow and causality can be derived ab initio" The formalism has been validated with various benchmark cases including Kaplan-Yorke map, Rössler system, baker transformation, Hénon map[30], and successfully applied to many realistic problems: glaciology[33], neuro-science[34], El Niño-Indian Ocean Dipole relation[29], precipitation-soil moisture interaction[35], global climate change[36], etc.

The discussion of causality in quantum physics can be traced back to the paradigmatic Bell experiment[37]. Causal structure places constraints on the correlations that can be generated in any classical hidden variable theories. Quantum physics, under the same causal structure, violates such constraints[38–42]. Motivated by the connection between causality and correlations, various attempts have been made to estimate causal influences in certain quantum environments[43–50]. The quantification of causal effects in quantum regime shed new light on the applications of quantum information processing. In particular, a causality measure, characterizing temporal quantum correlations between the input and output of a quantum channel[51], upper bounds the channel capacity[52]. Furthermore, a information-flux approach was introduced for many-body systems to quantify the influence from a specific element to another, aiming to facilitate the design of quantum processors equipped with large registers[53, 54]. In quantum mechanics, correlation functions of Heisenberg picture evolving operators are often used to ascertain casual influences, but one has to be careful that correlations does not imply causation.

Somewhat counterintuitively, the most straightforward approach to ascertaining causality, for example, one which an experimentalist will naturally employ, namely, to subtract a given component from a network to quantify its influence on other subsystems, remain unexplored. Motivated by that, in this work, we adopt Liang’s methodology to establish a formalism of quantum information flow. As opposed to all the approaches mentioned above in the quantum context, here one detaches or freezes a certain subsystem of a network (sender) in order to ascertain its causal influence on other subsystems (target). The change of a target element’s von-Neumann entropy, which possess various interpretations[55], then defines the information flow from the sender. When the sending and receiving element evolves independently, that is, the two elements has no causal impact on each other, then the information flow measure vanishes.

Quantum Liang information flow: Definition

Consider arbitrary multi-partite system with density state $\rho$, evolving under unitary operator $U(t) = e^{-iHt/\hbar}$. $H$ represents Hamiltonian of the system. Following Liang’s methodology (see appendix A for more details), we decompose the time rate change of von-Neumann entropy of subsystem $A$, $dS_A/dt$, into two parts: $T_{B\rightarrow A}$, the rate of information flow from subsystem B to A, and $dS_{AB}/dt$, the entropic evolution rate of subsystem A with influence from B excluded:

$$
T_{B\rightarrow A} = \frac{dS_A}{dt} - \frac{dS_{AB}}{dt} \quad (1)
$$

$S$ is von-Neumann entropy given by $S = -\text{Tr}(\sigma \log \sigma)$ for arbitrary density state $\sigma$. $S_{AB} = S(\rho_{AB}) = S[\varepsilon(t)_{AB} \rho_A(0)]$, where $\varepsilon(t)_{AB}$ is a density state mapping, denoting the evolution of A with B frozen.
If we consider time evolution as a discrete mapping during interval ∆t, the cumulative information flow is then:

\[ T_{B \rightarrow A} = \int T_{B \rightarrow A} dt = \Delta(S_A - S_{AB}) \tag{2} \]

We will discuss the definition and properties of \( \varepsilon(t)_{AB} \) in the following section. Note that von-Neumann entropy, therefore the information flow formalism, possess various interpretations [55]. Particularly distinct from classical Shannon entropy, von-Neumann entropy quantifies the entanglement within a pure bipartite quantum system. \( S_{AB} \) (or \( S_A \)) can then be interpreted as the entanglement between A and the rest of the universe with (or without) B frozen. The term \( (S_A - S_{AB}) \) that appears in eq.1 is then the difference of these two entanglement measures, in units of ebits. \( T_{B \rightarrow A} \) then quantifies the causal influence of B on A in the sense of how much it causes the entanglement of A with the rest of the universe to change. Similarly, other interpretations of von-Neumann entropy, such as uncertainty of a given state, also applies here.

**Evolution of subsystem A with B frozen**

Since \( \varepsilon(t)_{AB} \) is a mapping of density states, it can be interpreted as a quantum channel acting on subsystem A [55]: \( \rho_A(0) \xrightarrow{\varepsilon(t)_{AB}} \rho_{AB}(t) \). We further require that \( \varepsilon(t)_{AB} \) corresponds to a physical process, therefore it can be obtained from taking the partial trace of the full system, which evolves unitarily. For tripartite system \( \rho_{ABC} \):

\[ \rho_{AB}(t) = \text{Tr}_{BC}\{U_{ABC}(t)\rho_{ABC}(0)U_{ABC}(t)^\dagger\} \tag{3} \]

for some unitary operator \( U_{ABC} \).

Moreover, we require that the evolution mechanism with some subsystems frozen takes product form between the frozen qubits and the rest of the system:

\[ U_{ABC}(t) = V_{AC} \otimes W_B \tag{4} \]

where \( V_{AC} \) and \( W_B \) are unitary operators acting on subsystems AC and B respectively.

Frozen mechanism of the form Eq.4 guarantees what Liang referred to as the principle of nil causality [30] (See appendix C for proof):

\[ T_{B \rightarrow A} = 0 \text{ if the evolution of } A \text{ is independent of } B, \text{that is, the unitary evolution operator } U_{ABC}(t) \text{ takes separable form } M_A \otimes N_{BC} \otimes O_{AC} \otimes Q_B. \]

Therefore, causal structure is embedded in the information flow formalism. If quantum operations, conducted at 4-dimensional coordinate \( x \) and \( y \), are space-like separated, hence non-causal, then the operations acting at \( x \) does not affect the state located at \( y \) and vice versa. The quantum operations at \( x \) and \( y \) commute and the joint evolution is in product form. Thus the quantum Liang information flow from one coordinate to another vanishes.

Yet, we have not specified \( V_{AC} \) and \( W_B \) in eq.4. We will postpone it until the section after, in which we will show that the information flow in bipartite system is independent of the specification.

### A. Bipartite system

Consider bipartite state \( \rho_{AB} \) under unitary evolution \( U_{AB}(t) \). Consulting with eq.4, \( U_{AB} \) takes the form \( V_A \otimes W_B \) in 2 dimensions. Since von-Neumann entropy is invariant under unitary change of basis, \( \rho_{AB} = V_A \rho_A(0) V_A^\dagger \) and \( \frac{dS_{AB}}{dt} = 0 \). Therefore, the rate of information flow from B to A: \( T_{B \rightarrow A} = \frac{dS_{AB}}{dt} \). Similarly, \( T_{A \rightarrow B} = \frac{dS_{BA}}{dt} \).

If the initial state \( \rho_{AB}(0) \) is pure, that is, the system is closed, by Schmidt decomposition, \( \rho_A \) and \( \rho_B \) share the same set of eigenvalues. Since closed bipartite system is symmetric, \( S_A(t) = S_B(t) \) and \( T_{B \rightarrow A} = T_{A \rightarrow B} \).

In general, if the initial state \( \rho_{AB}(0) \) is mixed, which can arise from entanglement with some external system, then we no longer have the symmetry \( T_{A \rightarrow B} \neq T_{B \rightarrow A} \). Consider CNOT gate with controlled qubit A and target qubit B acts on the initial state \( \rho_{AB}(0) = \frac{1}{2}|0\rangle\langle 0| \otimes |A\rangle|0\rangle \otimes |0\rangle \otimes |B\rangle \otimes |0\rangle \otimes |1\rangle \otimes |1\rangle \otimes |1\rangle \otimes |1\rangle \). The cumulative information flow for this discrete mapping \( T_{B \rightarrow A} = \Delta S_A = 0 \) and \( T_{A \rightarrow B} = \Delta S_B = 1 \text{bit} \). The asymmetric quantum information flow obtained for initially mixed bipartite system parallels its classical counterpart. See appendix B for details.

For multi-partite system \( \rho_{ABCD} \ldots \), the information flow from the rest of a closed system towards a particular unit, say A, is equivalent to the bipartite scenario: \( T_{BCD} \ldots \rightarrow A = \frac{dS_A}{dt}, T_{BCD} \ldots \rightarrow A = \Delta S_A \).

### B. Multipartite system

Information flow within bipartite quantum system is trivial to calculate due to its symmetric structure. In general, evaluation of the information flow from one unit to another requires a method to fix \( V_{AC} \) in eq.4. In this section, we illustrate such an approach with tripartite system \( \rho_{ABC} \).

Consider time evolution operator \( U(t) = \exp[-iHt/h] \).

We define the evolution of A with B frozen by replacing the interaction terms relevant to B in the Hamiltonian \( H \), with identity operator. For instance, take Hamiltonian of the following form:

\[ H_{ABC} = H_{0A} + H_{0B} + H_{0C} + A \otimes C + B \otimes C \tag{5} \]

where \( H_{0i} \) with \( i = A, B, C \), is the free Hamiltonian. And \( A, B, C \), which describe their interactions, are hermitian operators acting on subsystem A, B, C respectively. The
evolution mechanism with B frozen is then: $U_{ABC} = e^{-iH_{ABC}t/\hbar}$, where

$$H_{ABC} \equiv H_{0A} + H_{0C} + A \otimes C + I_B \quad (6)$$

$U_{ABC}$ is clearly of the product form given in eq4, with $W_B = I$ and $\mathcal{V}_{AC}$ generated by hermitian operator $H_{0A} + H_{0C} + A \otimes C$. This can be implemented by moving B far away from the rest of the system so that the effective coupling strength of interaction between B and other subsystems vanishes. Hence, the operational meaning of $U_{ABC}$ is:

“evolution of the system if subsystem B is removed from the original evolution mechanism.”

The operational meaning of the frozen mechanism guarantees that this definition is basis(observable) independent. Now, we are equipped with the tools needed to evaluate quantum Liang information flow. In the next section, we will elucidate this formalism with applications.

**Application: multi-qubit spin system**

Consider a multi-qubit spin chain, the interaction Hamiltonian between any two interacting qubits i,j is given by[56]:

$$H_{\text{spin,ij}} = \eta_{ij}(\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+) \quad (7)$$

where $\sigma_{\pm}$ can be expressed in terms of Pauli matrices $\{\sigma_{x,y,z}\}$, $\sigma_i = \frac{1}{2}(\sigma_i \pm i \sigma_y)$. $\eta$ is relative coupling strength. The Hamiltonian for 3 interacting qubits, labeled A, B, C, of the form eq5 is given by:

$$\eta_{AC}(\sigma_A^+ \sigma_C^- + \sigma_A^- \sigma_C^+) + \eta_{BC}(\sigma_B^+ \sigma_C^- + \sigma_B^- \sigma_C^+) \quad (8)$$

**Relative coupling strength variation** In this section, we investigate cumulative Information flow $T$ from A, B to C with different coupling strength. We set the initial state of the sending qubits A, B being maximally mixed while the receiving qubits C pure: $\rho(0) = I_A \otimes I_B \otimes |0\rangle\langle 0|_C$. So the sending qubits are competing to propagate uncertainty towards the target qubit. The Hamiltonian with one qubit frozen, say A, is obtained by erasing the hermitian terms involving qubit A in Hamiltonian eq8:

$$H_{ABC} = \lambda \sigma_C^+ \sigma_B^+ + \sigma_C^- \sigma_B^- + I_A \quad (9)$$

The evolution of $\rho_{ABC}$ is defined similarly by removing hermitian terms relevant to qubits A,B altogether. Therefore, $\Delta S_{\text{ABC}}$ vanishes and the joint cumulative information flow from AB to C is: $T_{AB\rightarrow C} = \Delta S_C$.

Set $\eta_{AC} = 1$, $\eta_{BC} = 3$, at time $t \sim 0.49$, the entropy of C reaches its maxima of 1 bit for the first time. This is the maximum uncertainty qubit C can receive, determined by its dimension. For the purpose of illustration, we compare the cumulative information flow from different sending qubits before this capacity is reached. The early time behavior of cumulative information flow $T_{AB\rightarrow C}(t)$, $T_{A\rightarrow C}(t)$, $T_{B\rightarrow C}(t)$ is plotted in figure 1.

![3-qubit spin chain from top to bottom: $T_{AB\rightarrow C}$, $T_{B\rightarrow C}$, $T_{A\rightarrow C}$. Coupling strength: $\eta_{AC} = 1$, $\eta_{BC} = 3$. Initial state: $\rho(0) = I_A \otimes I_B \otimes |0\rangle\langle 0|_C$.](image)

From figure1, we notice that: The cumulative information flow from B to C is greater than that from A to C: $T_{B\rightarrow C} > T_{A\rightarrow C}$. This formalism is consistent with the intuition that the strongly coupled qubit has greater impact towards the target.

**Superadditivity** The direct addition of cumulative information flow from individual qubit A, B is smaller than the joint information flow: $T_{B\rightarrow C} + T_{A\rightarrow C} < T_{AB\rightarrow C}$ in this example. It means that turning off qubit A and B altogether has more impact on qubit C than the direct addition of turning A, B off one at a time. Similar result is obtained for the early time behavior of 5 qubit spin chain (See Appendix D).

**Initial configuration dependence** Note that the information flow formalism also depends on the initial configuration. To see how different initial states affect the information flow, set the coupling constant equal: $\eta_{AC} = \eta_{BC} = 1$. With initial state $\rho_{0(1)} = I_A \otimes (0.9|0\rangle\langle 0| + 0.1|1\rangle\langle 1|)_B \otimes |0\rangle\langle 0|_C$ and $\rho_{0(2)} = I_A \otimes (0.1|0\rangle\langle 0| + 0.9|1\rangle\langle 1|)_B \otimes |0\rangle\langle 0|_C$. In both cases, the initial entropy of qubit B is $\sim 0.47$bit while A is 1 bit. At a first glance, one may be expecting that A is transmitting more uncertainty to C than qubit B. From figure2, we see this is indeed the case for initial state $\rho_{0(1)}$. But when the initial state is switched to $\rho_{0(2)}$, we have $T_{B\rightarrow C} > T_{A\rightarrow C}$. This is because increasing in von-Neumann entropy could result from not only classical uncertainty propagation but also entanglement generation. The qubit interaction given in eq7 entangles $|10\rangle$ and $|01\rangle$ state, while it does not act on $|00\rangle$ and $|11\rangle$ state:

$$(\sigma_+ \sigma_- + \sigma_- \sigma_+) |0\rangle = (\sigma_+ \sigma_- + \sigma_- \sigma_+) |1\rangle = 0$$

$$(\sigma_+ \sigma_- + \sigma_- \sigma_+) |01\rangle = |10\rangle$$

$$(\sigma_+ \sigma_- + \sigma_- \sigma_+) |10\rangle = |01\rangle$$

For initial state $\rho_{0(2)}$, qubit B and C has 90% probability in $|10\rangle_{BC}$ state, the entangling mechanism greatly
3-qubit spin chain with different initial states.

Blue curve: \( T_{A \rightarrow C} \), Orange curve: \( T_{B \rightarrow C} \). Solid curve: Initial state \( \rho_{0(1)} = I_A \otimes (0.9|0\rangle\langle 0| + 0.1|1\rangle\langle 1|)B \otimes |0\rangle \langle 0|C \), Dashed curve: Initial state \( \rho_{0(2)} = I_A \otimes (0.1|0\rangle\langle 0| + 0.9|1\rangle\langle 1|)B \otimes |0\rangle \langle 0|C \). Coupling strength: \( \eta_{AC} = \eta_{BC} = 1 \).

Quantum super-exchange Add constant magnetic field along the z-axis with strength \( B \) at qubit C so that its energy is lifted by an amount \( B \sigma_z \), while qubit A and B remains unaffected. The total Hamiltonian acting on the system then adds up an additional term:

\[
H_{\text{additional}} = I_A \otimes I_B \otimes B \sigma_z(C)
\]

Set coupling strength \( \eta_{AC} = \eta_{BC} = 1 \) and initial state \( \rho(0) = I_A \otimes |0\rangle \langle 0|_B \otimes |I_C \). We wish to compare information flow from A,C to B with various magnetic field strength.

Note that when \( B = 0 \), the dynamics of information flow in the XY model (eq.7), which is not apriori obvious, can be pictured from fig.3(a). Note that the cumulative information flow is initially from C to B and it reaches a high value of 1 bit before it declines and is overtaken by the cumulative information flow from A to B. As the magnetic field strength increases, super-exchange process [57] between A and C becomes progressively dominant. The cumulative information flow from A to C decreases but never vanishes. Thus, we see that information flow from C to B goes down while that from A to B becomes that dictated by an effective weaker super-exchange coupling \( \eta_{AC}/B \) between A and B (\( \sigma_+ \sigma_- + h.c. \))[57].

5-qubit network Consider 5-qubit spin chain, labeled A,B,C,D,E, with E in the center, we wish to investigate information flow towards E. The total Hamiltonian for the 5-qubit spin chain is

\[
H_{\text{spin,tot}} = \sum_i H_{\text{spin,iE}}
\]

with \( i = A, B, C, D \). Set all the coupling strength with E identical: \( \eta_{DE} = \eta_{CE} = \eta_{BE} = \eta_{AE} = 1 \), and initial state of sending qubits A,B,C,D maximally mixed, receiving qubit E pure.

At time \( t \sim 0.69 \), the entropy of E reaches its maximum of 1 bit for the first time, that is, the joint cumulative information flow \( T_{ABCD \rightarrow E} \) has saturated the capacity of the receiving qubit. The cumulative information flow
Cumulative information flow from each sending qubit, which is identical $T_{A\rightarrow E} = T_{B\rightarrow E} = T_{C\rightarrow E} = T_{D\rightarrow E}$, is plotted for the time interval $t \in [0, 0.69]$ in figure 4(a). At $t \sim 0.69$, $T_{E\rightarrow E} \sim 0.011$.

![Cumulative Information Flow](image)

FIG. 4. 5-qubit network (a) Cumulative information flow from any sending qubit towards E with identical coupling strength: $\eta_{DE} = \eta_{CE} = \eta_{BE} = \eta_{AE} = 1$. (b) Cumulative information flow towards the center with additional coupling $\eta_{CD} = 5$. Orange curve: A (or B) to E, Blue curve: C (or D) to E. Interaction diagram given in figure 5.

Now let us add mutual interaction between C, D with relative coupling strength $\eta_{CD} = 5$ and observe how does the information flow towards the center qubit E changes. The total Hamiltonian is now given by:

$$\sum_i H_{spin,iE} + H_{spin,CD}$$

(12)

The interaction pattern is shown in figure 5. With presence of this additional interaction term, the cumulative information flow from each sending qubit to E is plotted in figure 4(b).

Compare figure 4(b) with figure 4(a), the presence of the additional interaction term between C,D greatly reduces the transmitted uncertainty from qubit C (D) to qubit E, while increases that from qubit A (B) to qubit E. After time $t \sim 0.49$, $T_{C\rightarrow E}$ reaches negative value, that is, qubit C (D) is reducing the uncertainty of qubit E. At $t = 0.69$, $T_{A\rightarrow E} = T_{B\rightarrow E} \sim 0.122$bits, $T_{C\rightarrow E} = T_{D\rightarrow E} \sim -0.036$bits.

![Schematic Diagram](image)

FIG. 5. Schematic diagram: A,B couples solely with E, while C,D also interacts with each other.

The uncertainty from qubit C (D) now has two routes to propagate, either towards E or D (C). Also, the relative coupling strength $\eta_{CD}$ is five times stronger than $\eta_{CE}, \eta_{DE}$. The strongly coupled route connecting C and D then diverts the uncertainty propagation away from the original path between C (D) and E, so that $T_{C\rightarrow E}(T_{D\rightarrow E})$ decreases. Qubit A and B now has less competition from qubit C and D to propagate uncertainty towards qubit E. Then, $T_{A\rightarrow E}(T_{B\rightarrow E})$ increases.

Application: Two-qubit system in bosonic bath

Let subsystem A and B indicate two non-interacting qubits with ground and excited states $|0\rangle, |1\rangle$, embedded in a common zero-temperature bosonic reservoir labeled C. The Hamiltonian governing the mechanism is given by $H_{SB} = H_0 + H_{int}$, with:

$$H_0 = \omega_0 \sigma_+^A \sigma_-^A + \omega_0 \sigma_+^B \sigma_-^B + \sum_k \omega_k b_k^\dagger b_k$$

$$H_{int} = \alpha_A \sigma_+^A \sum_k g_k b_k + \alpha_B \sigma_+^B \sum_k g_k b_k + h.c.$$  (13)

where $\sigma_\pm^{A(B)}$ and $\omega_0$ are the inversion operator and transition frequency of qubit A(B). $b_k, b_k^\dagger$ are annihilation and creation operator of the environment C. $\alpha_{A(B)}$ is a dimensionless constant measuring the coupling between each qubit and the reservoir.

For the spin-boson model $H_{SB}$, the Hamiltonian operator with B frozen is given by:

$$\omega_0 \sigma_+^A \sigma_-^A + \sum_k \omega_k b_k^\dagger b_k + \alpha_A \sigma_+^A \sum_k g_k b_k + \alpha_A \sigma_-^A \sum_k g_k^* b_k$$

(14)

It describes a single qubit A embedded in the same bosonic reservoir.

Consider dissipative qubit-environment interaction, which gives rise to amplitude damping channel. At zero temperature, the evolved two-qubit state can be solved.
exactly [58]. In the continuum limit for the environment, the effective spectral density \( J(\omega) \) is introduced and taken to have the Lorentzian form:

\[
J(\omega) = \frac{R^2}{\alpha_T^2 \pi} \frac{\lambda}{(\omega - \omega_0)^2 + \lambda^2}
\]

(15)

where \( \alpha_T = (\alpha_A^2 + \alpha_B^2)^{1/2} \) is a collective coupling parameter. \( \lambda \) defines the spectral width of the coupling and linked to the reservoir correlation time \( \tau_C \) by the relation \( \lambda \approx \frac{1}{\tau_C} \). \( R \propto \alpha_T \) determines the collective coupling strength. Eq15 is the spectral density of a cavity field in presence of cavity losses. The spectrum presents a Lorentzian broadening due to imperfect reflectivity of the cavity mirrors. In the weak couplings and/or good cavity limits, \( R/\lambda << 1 \). In the strong couplings and/or good cavity limits \( R/\lambda >> 1 \).

The evolution of \( \rho_A \) is governed by the Hamiltonian eq13, while \( \rho_{AB} \) evolves according to eq14, after tracing out the environment \( C \) and qubit \( B \). Note that to calculate the latter, the effective coupling strength acting on \( A \) is determined by \( R \frac{\alpha_A}{\alpha_T} \) instead of \( R \). It is not difficult to see that in the limit \( \alpha_B \) or \( \alpha_A \) goes to 0, that is, when one of the qubit decouples from the setup, then \( \rho_A \) and \( \rho_{AB} \) obeys the same equation of motion and \( \rho_A(t) = \rho_{AB}(t) \). Similarly, \( \rho_B(t) = \rho_{BA}(t) \). Therefore, \( T_{B \rightarrow A} = T_{A \rightarrow B} = 0 \). In general, evaluation of the information flow requires explicit calculation of the evolved density state. For this model, it is solved in Ref. [58].

Take initial state \( \rho_{AB}(0) = |\psi_0\rangle \langle \psi_0| \), where \( |\psi_0\rangle = \frac{1}{\sqrt{3}} (|01\rangle + \sqrt{2}|10\rangle) \). Let \( \lambda = 1 \), \( \hbar = 1 \), \( \alpha_A/\alpha_B = 10/1 \) and take strong coupling limit \( R = 10 \), the rate of information flow from \( B \) to \( A \) versus that from \( A \) to \( B \) is plotted in figure 6(a). The cumulative information flow is shown in figure 6(b).

From Fig6(a), we see that the rate of information flow from the weakly coupled qubit (\( B \)) towards the strongly coupled qubit (\( A \)) possess higher peak than that from \( A \) to \( B \). On the other hand, as shown in figure 6(b), the cumulative information flow from \( A \) to \( B \) grows steadily and surpass that from \( B \) to \( A \) as the system approaches equilibrium. Note that the information formalism is generically asymmetric \( T_{B \rightarrow A} \neq T_{A \rightarrow B} \) as opposed to most quantum correlation measures.

**Conclusions:**

In this paper, we have generalized Liang’s methodology to quantify the causal influences in a quantum network. A unique feature of quantum networks is the possibility of entanglement between its components. Thus, there are two ways to increase the entropy of a node: classical uncertainty propagation, as well as the growth of entanglement. The influence of one node on another can thus be interpreted in terms of the induced total uncertainty in bits or the generated entanglement with the rest of the universe in ebits. We have verified the formalism through very simple networks. For example, in simple tripartite systems, the stronger coupled qubits have advantage of inducing uncertainty: Different initial states lead to different information flow depending on the activation of entangling mechanisms; The role of central mediator in the superexchange scheme is pictured; The information flow between two qubits through a common bath could be nontrivial in the sense that the weakly coupled qubit has higher rate of information flow, while in the long run, the strongly coupled qubit has more impact on the weakly coupled one. Another non-trivial result obtained for a 5-qubit network reveals that an additional strong coupling diverts the directions of uncertainty propagation. While for such small networks, one can probably come up with simple intuitive understanding of information flows between nodes, causal influences in general complex quantum networks may be intricate and hidden and a picturization in terms of information flows will certainly aid their understanding. Note that definition of the information flow formalism requires 1. full knowledge of the dynamics and 2. an intervention (frozen mechanism) act upon the system. For its classical counterpart, Liang has showed that when applied to a broad range of real-world problems, the quantification of information flow can be estimated with only local statistics[29–36]. Whether the quantum information flow...
can be estimated without knowing the dynamics apriori or doing the intervention on the system remains a subject for further investigation.

ACKNOWLEDGMENTS

B.Yi would like to thank S.X.Huang for presenting the problem as well as inspiring discussions with X.S.Liang and A.J.Leggett. S.Bose acknowledges the EPSRC grant Nonergodic quantum manipulation EP/R029075/1.

[1] K. Hlaváčková-Schindler, M. Palaš, M. Vejmelka, and J. Bhattacharya, Physics Reports 441, 1 (2007).
[2] J. Pearl et al., Cambridge, UK: Cambridge University Press 19 (2000).
[3] P. Spirtes, C. N. Glymour, R. Scheines, and D. Heckerman, Causation, prediction, and search (MIT press, 2000).
[4] B. P. Bezrucho and D. A. Smirnov, Extracting knowledge from time series: An introduction to nonlinear empirical modeling (Springer Science & Business Media, 2010).
[5] T. Schreiber, Physical review letters 85, 461 (2000).
[6] W. Wang, B. T. Anderson, R. K. Kaufmann, and R. B. Myrinen, Journal of Climate 17, 4752 (2004).
[7] J. Runge, J. Heitzig, N. Marwan, and J. Kurths, Physical Review E 86, 061121 (2012).
[8] R. Sun, IEEE Transactions on Neural Networks 5, 604 (1994).
[9] N. Ay and D. Polani, Advances in complex systems 11, 17 (2008).
[10] L. Sommerlade, M. Eichler, M. Jachan, K. Henschel, J. Timmer, and B. Schelter, Physical Review E 80, 051128 (2009).
[11] M. Timme and J. Casadiego, Journal of Physics A: Mathematical and Theoretical 47, 343001 (2014).
[12] E. Pereda, R. Q. Quiroga, and J. Bhattacharya, Progress in neurobiology 77, 1 (2005).
[13] K. J. Friston, L. Harrison, and W. Penny, Neuroimage 19, 1273 (2003).
[14] B. Schelter, M. Winterhalder, M. Eichler, M. Peifer, B. Hellwig, B. Guschlbauer, C. H. Lücking, R. Dahlhaus, and J. Timmer, Journal of neuroscience methods 152, 210 (2006).
[15] M. Staniek and K. Lehnertz, Physical review letters 100, 158101 (2008).
[16] R. G. Andrzejak and T. Kreuz, EPL (Europhysics Letters) 96, 50012 (2011).
[17] J. Wu, X. Liu, and J. Feng, Journal of Neuroscience Methods 167, 367 (2008).
[18] R. Marschinski and H. Kantz, The European Physical Journal B-Condensed Matter and Complex Systems 30, 275 (2002).
[19] S. S. Lee, The Review of Financial Studies 25, 439 (2012).
[20] G. Tissot, A. Lozano-Durán, L. Cordier, J. Jiménez, and B. R. Noack, in Journal of Physics: Conference Series, Vol. 506 (IOP Publishing, 2014) p. 012006.
[21] M. Materassi, G. Consolini, N. Smith, and R. De Marco, Entropy 16, 1272 (2014).
[22] J. A. Vastano and H. L. Swinney, Physical Review Letters 60, 1773 (1988).
[23] J. Sun and E. M. Bollt, Physica D: Nonlinear Phenomena 207, 49 (2014).
[24] F. Duan, F. Yang, T. Chen, and S. L. Shah, IEEE transactions on control systems technology 21, 2052 (2013).
[25] D. W. Hahs and S. D. Pethel, Physical review letters 107, 128701 (2011).
[26] D. A. Smirnov, Physical Review E 87, 042917 (2013).
[27] X. San Liang and R. Kleeman, Physical review letters 95, 244101 (2005).
[28] X. San Liang, Physical Review E 78, 031113 (2008).
[29] X. San Liang, Physical Review E 80, 052150 (2014).
[30] X. San Liang, Physical Review E 94, 052201 (2016).
[31] X. S. Liang, arXiv preprint arXiv:2104.09290 (2021).
[32] S. S. Liang, Entropy 23, 670 (2021).
[33] S. Vaninis, Q. Dalai, and H. Goosse, Geophysical Research Letters 46, 12125 (2019).
[34] D. T. Hristopolus, A. Babul, S. Babul, L. R. Brucar, and N. Virji-Babul, Frontiers in human neuroscience 13, 419 (2019).
[35] D. F. T. Hagan, G. Wang, X. San Liang, and H. A. Dolman, Journal of Climate 32, 7521 (2019).
[36] A. Stips, D. Macias, C. Coughlan, E. Garcia-Gorriz, and X. San Liang, Scientific reports 6, 1 (2016).
[37] J. S. Bell, Physics Physique Fizika 1, 195 (1964).
[38] J. S. Freedman and J. F. Clauser, Physical Review Letters 28, 938 (1972).
[39] A. Aspect, P. Grangier, and G. Roger, Physical review letters 49, 91 (1982).
[40] B. G. Christensen, K. T. McCusker, J. B. Altepeter, B. Calkins, T. Gerrits, A. E. Lita, A. Miller, L. K. Shalm, Y. Zhang, S. W. Nam, et al., Physical review letters 111, 130406 (2013).
[41] M. A. Rowe, D. Kielpinski, V. Meyer, C. A. Sackett, W. M. Itano, C. Monroe, and D. J. Wineland, Nature 409, 791 (2001).
[42] M. Giustina, A. Mech, S. Ramelow, B. Wittmann, J. Kofler, J. Beyer, A. Lita, B. Calkins, T. Gerrits, S. W. Nam, et al., Nature 497, 227 (2013).
[43] M. Gachechiladze, N. Miklin, and R. Chaves, Physical Review Letters 125, 230401 (2020).
[44] J. Henson, R. Lal, and M. F. Pusey, New Journal of Physics 16, 113043 (2014).
[45] R. Chaves, C. Majenz, and D. Gross, Nature communications 6, 1 (2015).
[46] F. Costa and S. Shrapnel, New Journal of Physics 18, 063032 (2016).
[47] T. Fritz, Communications in Mathematical Physics 341, 391 (2016).
[48] J. Barrett, R. Lorenz, and O. Oreshkov, arXiv preprint arXiv:1906.10726 (2019).
[49] E. Wolfe, A. Pozas-Kerstjens, M. Grinberg, D. Rossel, A. Acín, and M. Navascués, Physical Review X 11, 021043 (2021).
[50] J. Åberg, R. Nery, C. Duarte, and R. Chaves, Physical Review Letters 125, 110505 (2020).
[51] J. F. Fitzsimons, J. A. Jones, and V. Vedral, Scientific reports 5, 1 (2015).
Liang and Kleeman identified that the entropy change of subsystem 1 given by eqA4 can be decomposed into two parts: the evolution due to $X_1$ alone, with effect from subsystem 2 excluded, denoted as $\frac{dS_{1\rightarrow 2(\text{classical})}}{dt}$. Another part is the influence from $X_2$. Through heuristic reasoning based on the interpretation of eqA3, Liang and Kleeman argue that if subsystem 1 evolves on its own, the entropy change of subsystem 1 would depend only on $\partial F_1/\partial x_1$:

$$\frac{dS_{1\rightarrow 2(\text{classical})}}{dt} = E(\nabla \cdot F) = \int_{\Omega} \rho \frac{\partial F_1}{\partial x_1} dx_1 dx_2 \quad (A5)$$

Later on, Liang(2016[30]) proved that the above result eqA5 can be derived by treating $x_2$ as a fixed parameter at time $t$, rather than a variate.

The rate of information flow from $X_2$ to $X_1$ is then:

$$T_{2\rightarrow 1} = \frac{dS_{1\rightarrow 2(\text{classical})}}{dt} - \frac{dS_{2\rightarrow 1(\text{classical})}}{dt} = -\int_{\Omega} \rho \frac{F_1}{\rho_1} \frac{\partial \rho_1}{\partial x_1} + \frac{\partial F_1}{\partial x_1} dx_1 dx_2 \quad (A6)$$

This formula verifies what Liang refers to as the principle of nil causality:

If $F_1$ is independent of $x_2$, then the information flow from 2 to 1 vanishes: $T_{2\rightarrow 1} = 0$.

If $T_{2\rightarrow 1}$ is negative (positive), the interpretation is that system 2 is making system 1 more (less) certain. Note that the information flow formalism eqA6 is asymmetric, that is $T_{2\rightarrow 1} \neq T_{1\rightarrow 2}$. When the information flow from 2 to 1 vanishes, that from 1 to 2 maybe non-zero. The asymmetry feature distinguishes the information flow formalism with classical correlation measures.

It should be pointed out that the evaluation of eqA6 requires full knowledge of the dynamics. In 2014[29], Liang showed that $T_{2\rightarrow 1}$ can be estimated with local statistics. The maximum-likelihood estimator of eqA6 is shown to be a combination of some sample covariances, which greatly facilitates the implementation of the causality analysis.

This formalism has been widely applied to realistic schemes[29, 33–36]. Among them, we will briefly mention its application to a network consisting of Stuart-Landau oscillators[31], a typical model for many biological phenomena[59]. The magnitude of Liang information flow quantifies the influence of individual components to produce the collective behavior of the whole system. The direct addition of individual contributions does not equal the cumulative information flow, demonstrating its collective property. Moreover, the node with greatest information flow is verified to be the most crucial as its suppression leads to shut down of the entire network. Surprisingly, such a node may be sparsely connected, rather
than a center of network. The information-flow based causality analysis successfully explains why small defects at local node could severely damage structural integrity.

Appendix B: closed bivariate system

The classical model considered in eqA1 is dissipative. System 1 and 2 exchanges energy with the environment through external force \( F \). If system 1 and 2 is closed, the divergence of force \( \nabla \cdot F = 0 \). As a result, eqA3, eqA5 becomes:

\[
\frac{dS}{dt} = 0
\]

Therefore, excluding B or not has no impact on von-Neumann entropy, \( \rho \). By the unitary invariance of von-Neumann entropy, \( \frac{dS_A}{dt} = \frac{dS_{AB}}{dt} = 0 \), thus \( T_{B \rightarrow A} = 0 \).

\[
T_{2 \rightarrow 1} = \frac{dS_{(classical)}}{dt} \tag{B1}
\]

EqB1 is completely in agreement with the quantum formalism obtained for initially mixed bipartite system.

Appendix C: the principle of nil causality

If \( U_{ABC}(t) \) follows eq4, then the statement of causality is satisfied, that is, \( T_{B \rightarrow A} = 0 \) when A evolves independent of B.

Proof. If \( U_{ABC} = M_A \otimes N_{BC} \), the evolution of A is solely determined by unitary operator \( M_A \). Excluding B from the joint evolution of subsystem BC, denoted \( N_{BC} \), has no effect on A. Therefore, \( \rho_A(t) = \rho_{AB}(t) = M_A \rho_A(0) M_A^\dagger \). By the unitary invariance of von-Neumann entropy, \( \frac{dS_A}{dt} = \frac{dS_{AB}}{dt} = 0 \), thus \( T_{B \rightarrow A} = 0 \).

If \( U_{ABC}(t) = \mathcal{O}_{AC} \otimes \mathcal{Q}_B \), it is already of the form given in eq4. Therefore, excluding B or not has no impact on the joint evolution of system AC. That is,

\[
\rho_A(t) = Tr_{BC} \{ U_{ABC}(t) \rho_{ABC}(0) U_{ABC}^\dagger(t) \} = Tr_C [ \mathcal{O}_{AC} \rho_{AC}(0) \mathcal{O}_{AC}^\dagger ] = Tr_{BC} \{ U_{ABC}(t) \rho_{ABC}(0) U_{ABC}^\dagger(t) \} = \rho_{AB}(t)
\]

Therefore, \( T_{B \rightarrow A} = \frac{dS_A}{dt} - \frac{dS_{AB}}{dt} = 0 \).

Whether the converse proof also holds remains an open question.

Appendix D: 5 qubit system

To check if stronger coupled sending qubit delivers more information towards the receiving qubit, we set \( \eta_{DE} = 1 \), \( \eta_{CE} = 2 \), \( \eta_{BE} = 3 \), \( \eta_{AE} = 4 \) and let the initial state of the sending qubits A,B,C,D being maximally mixed and the receiving qubit E pure, so that \( \rho_0 = I_A/2 \otimes I_B/2 \otimes I_C/2 \otimes I_D/2 \otimes \langle 0 \rangle_0 \).

Calculation of information flow from the \( k \)th qubit to E, where \( k \) runs through the sending qubits, requires the evolution mechanism with the \( k \)th qubit frozen:

\[
H_{spin,k} = \sum_{j \neq k} H_{spin,jE} \tag{D1}
\]

The joint information flow from A,B,C,D to E is simply the change of \( S_E \):

\[
T_{A,B,C,D \rightarrow E} = \Delta S_E \tag{D2}
\]

At time \( t \sim 0.26 \), the entropy of E reaches its maxima \( S_E = 1 \) bit for the first time. The Information flow from each sending qubit to E, as defined in eq2, is plotted in figure 7, before the capacity is reached.

The stronger coupled qubit delivers more information to E at all time during \( t \in [0, 0.26] \):

\[
T_{A \rightarrow E} > T_{B \rightarrow E} > T_{C \rightarrow E} > T_{D \rightarrow E} \tag{D3}
\]

At \( t = 0.26 \), \( T_{A \rightarrow E} \sim 0.0731 \) bits, \( T_{B \rightarrow E} \sim 0.0132 \) bits, \( T_{C \rightarrow E} \sim 0.0022 \) bits, \( T_{D \rightarrow E} \sim 0.0001 \) bits.

![FIG. 7. Individual Information flow towards qubit E from top to bottom: A,B,C,D.](image-url)