Clustering of conditional mutual information and quantum Markov structure at arbitrary temperatures

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[Motivation and Background]

In the realm of quantum many-body physics, a fundamental challenge lies in uncovering structures that apply universally, regardless of specific system details. One of the simplest ways to characterize this is by examining the correlation function between two observables, which reveals a distinct short-range behavior in non-critical phases [Hastings, PRL (2004)]. Recent advances in quantum information science have introduced various methods for comprehending the complexity of quantum phases of matter from an information-theoretic perspective. Among these, one particularly renowned and elegant concept is the area law of quantum entanglement. While the area law has been a conjecture in high dimensions at absolute zero temperature [Anshu et al., STOC'22, QIP'22], it has been rigorously confirmed to hold true at non-zero temperatures [Wolf et al., PRL (2008), Kuwahara et al., PRX (2021), QIP'21]. The area law has had a profound impact on various areas of research. It has greatly influenced numerical techniques employing the tensor network formalism [Vidal et al., PRL (2003)]. Additionally, it has paved the way for developing efficiency-guaranteed algorithms that compute physical observables [Landau et al., Nat. Phys. (2015), QIP'14]. In more recent developments, the study of bipartite quantum entanglement between distant subsystems has emerged as a promising avenue for universally revealing short-range characteristics, even at thermal critical point [Kuwahara et al., PRX (2022), QIP'22]. So far, quantum long-range entanglement is believed to manifest primarily in the form of tripartite (or higher-order multipartite) correlations at non-zero temperatures.

Over the past two decades, our understanding of quantum phases has evolved, revealing that they cannot be fully characterized solely through bipartite correlation measures. A prominent example of this complexity is found in topologically ordered phases, which exhibit genuinely multipartite correlations [Kato et al., PRA (2016)]. Efforts in the field have been directed towards devising comprehensive information-theoretic measures to capture multipartite correlations in quantum many-body systems. Thus far, one of the most established measures for quantifying tripartite correlations is Conditional Mutual Information (CMI) [Sutter, arXiv:1802.05477]. CMI has found versatile applications, including the definition of topological entanglement entropy [Levin-Wen, PRL (2006), Kitaev-Preskill, PRL (2006)]. Recent studies have uncovered additional uses for CMI, such as characterizing information scrambling [Ding et al., JHEP (2016)], identifying measurement-induced quantum phase transitions [Gullans-Huse, PRX (2020)], and studying entanglement in conformal field theory [Hayden et al., PRD (2013)], among others. In different contexts, researchers have extensively investigated the operational significance of CMI. Particularly, they have rigorously clarified the relationship between CMI and the error of the recovery map [Fawzi-Renner, CMP (2015), QIP'16, Sutter et al., Proc. R. Soc. Lond (2016), QIP'16].

Here, our fundamental question is "*Can we establish a universal theorem on the tripartite correlation based on the CMI?*" To provide context for this query, we draw upon the well-known Hammersley-Clifford theorem within classical many-body systems, which establishes an equivalence between classical Gibbs states and the concept of a Markov network (or Markov random field). This network's characteristics are a finite correlation length of CMI. Then, one might envision a similar relationship in quantum systems in the analogy of classical Gibbs states. Although it breaks down in a strict sense, conjectures have emerged suggesting that a modified form of the theorem could hold approximately, with CMI decaying rapidly as the distance [See Ineq. (2) below]. To date, mathematical proofs have been restricted in two scenarios: i) for 1D Gibbs states at arbitrary temperatures [Kato-Brandõ, CMP (2019), QIP'17], and ii) for high-dimensional Gibbs states above a certain temperature threshold [Kuwahara et al., PRL (2020), QIP'20]. Both of these cases correspond to non-critical thermal phases. However, when temperatures are low, the structure of entanglement becomes exceptionally complex, exhibiting long-range entanglement even at $\mathcal{O}(1)$ temperatures [Hastings, PRL (2011), Anshu et al., STOC'23, QIP'23]. Up to this point, any theoretical efforts have not overcome this challenge, and the clustering of CMI remains an inaccessible problem.

The resolution of this conjecture holds substantial significance in various ways. In the realm of quantum many-body physics, it enables us to impose stricter constraints on the nature of long-range entanglement that persists at non-zero temperatures. Additionally, it assures us that the recovery map for the quantum Gibbs state can be constructed using local quantum channels, even when dealing with low temperatures. From a practical standpoint, the Markov property is one of the foundational assumptions when dealing with unknown probability distributions in classical theory [Hinton, Scholapedia, 2007]. In the quantum domain, the concept of the Markov property plays fundamental roles in various quantum technologies. Some notable applications include quantum Hamiltonian learning [Anshu et al., Nat. Phys. (2021), QIP'21], efficiency-guaranteed quantum Gibbs sampling [Brandão-Kastoryano, CMP (2019), QIP'17, quantum marginal problems [Kim, PRX (2021), QIP'22], and more. The establishment of the quantum version of the Hammersley-Clifford theorem has long been an ambitious goal in the field of quantum information science.

In the present work, we report an unconditional proof of the conjecture regarding the decay of Conditional Mutual Information (CMI) at arbitrary temperatures and in arbitrary finite dimensions. At this stage, it's important to note that our result does not provide a complete resolution of the quantum version of the Hammersley-Clifford theorem (as depicted in the theorem below). Nevertheless, it furnishes strong evidence that the Markov property generally holds, even at extremely low temperatures.

[**Setup and Main results**]

We consider a quantum system on a D-dimensional lattice, with Λ representing all the locations. For any three sets A, B, and C within Λ, we start by defining the conditional mutual information $\mathcal{I}_\rho(A:C|B)$ between A and C, conditioned on B for a density matrix ρ: $\mathcal{I}_\rho(A:C|B) := S_\rho(AB) + S_\rho(BC) - S_\rho(ABC) - S_\rho(B)$, where $S_\rho(L)$ ($\forall L \subseteq \Lambda$) is defined as the Von-Neumann entropy for ρ on the subsystem L. We then define the Hamiltonian as follows:

$$H = \sum_{Z\subseteq\Lambda} h_Z, \qquad \sum_{Z:Z\ni\{i,i'\}} \|h_Z\| \le \bar{J}_{d_{i,i'}} := \bar{J}_0 e^{-\mu d_{i,i'}} \quad \text{for} \quad \forall i,i' \in \Lambda, \tag{1}$$

where the operator h_Z is an interaction term that acts on $Z \subseteq \Lambda$ and the latter condition implies that the interaction is short-range (i.e., exponentially decaying). Finally, the quantum Gibbs state is defined as $\rho_\beta := e^{-\beta H}/Z_\beta$, where $Z_\beta := \mathrm{tr}\left(e^{-\beta H}\right)$.

The conjecture regarding the decay of Conditional Mutual Information (CMI) is now presented as follows: For an arbitrary quantum Gibbs state ρ_β, the CMI $\mathcal{I}_{\rho_\beta}(A:C|B)$, where $\Lambda = A \sqcup B \sqcup C$, rapidly decays with the distance between A and C:

$$[\textbf{Conjecture}] \quad \mathcal{I}_{\rho_\beta}(A:C|B) \le \mathcal{G}_{\mathcal{I}}(R), \quad R = d_{A,C}, \tag{2}$$

where $\mathcal{G}_{\mathcal{I}}(R)$ is a super-polynomially decaying function which depends on β, $\{A,B,C\}$ and the system details. It's important to note that the condition $\Lambda = A \sqcup B \sqcup C$ is crucial. If $A \sqcup B \sqcup C \subset \Lambda$, even for commuting Hamiltonians, there exists a counterexample of (2) at low temperatures [Castelnovo et al., PRB (2008)]. The central achievement of this work lies in the unconditional proof of the conjecture, which is summarized in the following theorem (Theorems 4 and 5 in the technical manuscript):

Main Theorem. Let us adopt the Θ notation to mean $\Theta(x) = cx$ with c a positive constant that only depends on the fundamental parameters (see Table I in the technical manuscript). Then, for an arbitrary quantum Gibbs state, the conditional mutual information is upper-bounded in the form of (2) with the following expression for $\mathcal{G}_{\mathcal{I}}(R)$:

$$\mathcal{G}_{\mathcal{I}}(R) = \begin{cases} \exp\left[-\dfrac{R}{\Theta(\beta)} + \Theta(\beta)\log(\beta R)\right] & \text{for} \quad D=1, \\ \mathcal{D}_{AC}\exp\left[-\dfrac{R}{\Theta\left[\beta^{D+1}\log(R)\right]} + \Theta(1)\log(\beta|AC|)\right] & \text{for} \quad D\ge 2, \end{cases} \tag{3}$$

where $\mathcal{D}_{AC}$ denotes the Hilbert space dimension on the subset $A \sqcup C$. Several key points to note:

- The result implies the (almost) exponential decay of the conditional mutual information at arbitrary temperatures, where the correlation length only increases polynomially as $\mathcal{O}(\beta)$ and $\mathcal{O}(\beta^{D+1})$ for $D=1$ and $D \geq 2$, respectively. The different scaling for β between 1D and high dimensions arises from the use of different analytical techniques for high-dimensional cases. For 1D, this result significantly improves upon the original one by Kato and Brandão, which yielded $\mathcal{G}_{\mathcal{I}}(R) = e^{-\Theta(1)\sqrt{R/e^{\Theta(\beta)}}}$.
- For $D \geq 2$, we have achieved the exponential decay of the CMI at arbitrary temperatures. However, the current bound is insufficient to prove the global Markov property due to the growth of the coefficient $\mathcal{D}_{AC}$, which increases as $e^{\Theta(|A|+|C|)}$. In essence, if we compare two large subregions (with sizes on the order of $|\Lambda|$), the influence of $\mathcal{D}_{AC}$ dominates over the decay factor $e^{-\mathcal{O}(R/\log(R))}$.
- As for the practical applications of this theorem, it allows us to address the clustering of genuine bipartite entanglement. Unlike previous results [Kuwahara et al., PRX (2022), QIP'22], this theorem can handle the so-called "bound entanglement", which is not classified within the PPT class. The CMI serves as an upper bound for bipartite entanglement in the form of squashed entanglement, and squashed entanglement satisfies faithfulness [Brandã et al., CMP (2011), QIP'11]. This aspect enables us to prove the entanglement clustering for genuine bipartite entanglement, including entanglement formation and relative entanglement.

[**Techniques**]

Analyzing the effective Hamiltonian on subsystems poses the most significant challenge in our work, which is also known as the "entanglement Hamiltonian [Kokail et al., Nat. Phys. (2021)]" or "Hamiltonian of mean force [Talkner-Hänggi, RMP (2020)]." The conditional mutual information is written by $\mathcal{I}_\rho(A:C|B) = \mathrm{tr}\left[\rho H_\rho(A:C|B)\right]$ with $H_\rho(A:C|B) = -\log(\rho_{AB}) - \log(\rho_{BC}) + \log(\rho_{ABC}) + \log(\rho_B)$, where ρ_L ($\forall L \subset \Lambda$) is the reduced density matrix on the subset L. For quantum Gibbs states ρ_β, if the effective term $\log(\rho_{\beta,L}) - H_L$ (H_L: the subsystem Hamiltonian) is approximately determined mainly by the surface region of L, we can prove the clustering of the CMI, with the decay rate characterized by the approximation error. At high temperatures, we can rely on the cluster expansion method, but this expansion is known to diverge at low temperatures. Our primary technical contribution is the development of a theoretical framework to analyze the effective Hamiltonian. The analysis of the effective Hamiltonian consists of roughly three steps: **(i)** reduction of the partial trace to the product of exponential operators (Sec. IV in the technical manuscript), **(ii)** connection of the exponentials to obtain the effective Hamiltonian (Sec. V), and **(iii)** analysis of the quasi-locality (Sec. VI and Sec. VII).

In step (i), we aim to approximate the effective Hamiltonian $\log(\rho_{\beta,L})$ by the form of $\log(\rho_{\beta,L}) \approx \log\left(e^{\tau V}e^{-\beta H}e^{\tau V}\right)$ with an appropriate choice of V, where the approximation error depends on τ. In the present work, we establish two formalisms to determine the operator V. The former is based on the quantum belief propagation (Sec. IV A), and the latter is based on the partial-trace projection [(S.151) in Sec. IV B]. In step (ii), we prove a lemma that expresses $\log\left(e^{\tau V}e^{-\beta H}e^{\tau V}\right)$ in terms of the time-evolution with an appropriate filter function (Lemma 17 and Corollary 18). This lemma allows us to estimate the quasi-locality of the effective Hamiltonian by using the Lieb-Robinson bound. In step (iii), we encounter an analysis of the infinite exponential tower like $e^{e^{e^{\cdot^{\cdot^{\cdot}}}}}$ in connecting the exponential operators. It makes the locality analyses highly complicated since the upper bound can easily diverge to infinity. To overcome the difficulty, we first estimate the quasi-locality around a target subregion L for the effective interaction terms (Subtheorem 1). However, at this stage, quasi-locality itself does not imply that such terms originated only from the surface region of L. Thus, we second aim to prove that its origin certainly lies in the surface region by utilizing the proved quasi-locality (Theorem 2). After the analyses of the effective Hamiltonian, one can prove the exponential clustering theorem for the CMI.

Our technique's advantage is that it allows us to access the structures of the effective Hamiltonian. This feature is beneficial for applying our method to Hamiltonian learning and improving sample complexity [Anshu et al., Electronic notes, 2021]. Furthermore, our approach has the potential to extend to more general classes of the effective Hamiltonian problem, such as the Negativity Hamiltonian at non-zero temperatures [Murciano, PRL (2022)] and the entanglement Hamiltonian at zero temperatures.