

論文の内容の要旨

Theoretical study on volume law of Rényi
entanglement entropy in quantum many-body systems
(量子多体系におけるレニー・エンタングルメントエントロ
ピーの体積則に関する理論的研究)

中川裕也

Quantum entanglement, which represents non-local correlations that cannot be explained by classical mechanics, has played a central role in quantum information science. Recently, it has also become an important tool to study quantum many-body systems: by calculating entanglement measures in a many-body wave function (pure state), one can tell various properties of a system. The most famous and celebrated measures are the von Neumann entanglement entropy (vN-EE) and the n -th Rényi entanglement entropy (n REE) that amount entanglement between a subregion A and its complement B . While the vN-EE and the n REE (the EEs) in quantum many-body systems were featured on the theoretical side at first, state-of-the-art techniques can now measure them experimentally in ultracold atoms, trapped ions, superconducting qubits, and nuclear spins of molecules, which fuels further growing interest among both theorists and experimentalists.

On the other hand, recent studies on the foundation of quantum statistical mechanics and thermodynamics have revealed that thermal equilibrium can be fully described by pure quantum states as far as local observables are concerned, while the conventional description of it is based on mixed-state ensembles. The thermodynamic entropy and free energy, in that case, can be read off from the EEs of small subsystems. They scale with the size of the subsystem, which is called the volume law of entanglement. When the size of the subsystem increases, however, the correspondence between thermal and entanglement entropies breaks down and there appears a quantum correction to the simple volume-law scaling. Explicating the scaling of the EEs with the subsystem size is hence of great importance in connecting quantum physics to thermodynamics as well as analyzing recent experiments in various quantum systems.

In this thesis, we study the volume law of entanglement for pure quantum states representing thermal equilibrium, which we call as thermal pure states. Specifically, we

investigate a functional form of the n REE S_n as a function of the subsystem volume ℓ . We review two central notions for the topic of this thesis, quantum entanglement and pure state thermodynamics, in Chapter 1. Then we present analytical and numerical results on the volume law of entanglement in the following chapters.

In Chapter 2, an analytical formula of the volume law scaling of the n REE is derived by employing the canonical Thermal Pure Quantum (cTPQ) state, which is an analytically-tractable example of thermal pure states in general systems. In particular, the formula for the 2REE is greatly simplified under reasonable assumptions based on thermodynamic behaviors of the system. The whole curve of the 2REE $S_2(\ell)$, including the deviation from a linear volume law scaling $S_2 \propto \ell$, is determined by only two parameters. We illustrated a practical advantage of the formula by numerically computing the 2REE of the cTPQ states and fitting it by the formula. The formula extracts the density of the 2REE more accurately than other naive ways based on the linear volume law. Furthermore, we discuss the universality of the formula by referring the “scrambling”, or dephasing of the coefficients, of wave functions of general pure states. We conjecture that our formula of the 2REE will apply to “scrambled” pure states which include thermal pure states.

In Chapter 3, we study the 2REE of stationary pure states after quantum quench by numerical exact diagonalization. Such stationary states are considered to be an example of thermal pure states when the thermalization takes place. Numerical results are perfectly consistent with the conjecture proposed in Chapter 2. When the stationary pure states are scrambled due to the time-evolution after quantum quench, the 2REE of those states is well fitted by our formula. In addition, we show that fitting of the experimental data of the 2REE in ultracold atoms (A. M. Kaufman *et al.*, Science **353**, 794 (2016)) by our formula works quite well, which supports the usefulness of our formula in experiments on the EEs.

In Chapter 4, as another example of thermal pure states, energy eigenstates in general integrable/non-integrable systems are investigated. We again employ numerical exact diagonalization and calculate the 2REE of energy eigenstates in one-dimensional spin chains. Our results suggest that the 2REE of non-integrable models obeys the formula derived in Chapter 2 while that of integrable models does not. Although a recent study by Lu and Grover (T.-C. Lu and T. Grover, arXiv:1709.08784 (2017)) derived a different functional form of the volume law for energy eigenstates of non-integrable models as ours, we claim that our formula is still meaningful in extracting information of the system in the thermodynamic limit from finite size systems and telling non-integrable models from integrable models.

In Chapter 5, we summarize our results in this thesis and present possible future directions of the study.

The result in this thesis will contribute to link quantum mechanics with thermodynamics, whose connection is a long-standing problem since the early days of the discovery of quantum mechanics. Our results can also be seen as an extension of the previous studies of pure state thermodynamics to one of the most important non-local quantities in quantum many-body systems, i.e., the REE. In addition, our formula gives an accurate prediction of the density of the 2REE in the thermodynamics limit from a result in finite size systems, so it is surely of use in numerical/experimental studies on the entanglement entropy in the future.