論 文 の 内 容 の 要 旨

論文題目　Thermodynamic relations on irreversibility in nonequilibrium systems
（非平衡系の不可逆性に関する熱力学的関係）

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Physical systems in the real world are basically operated and maintained in nonequilibrium states. To carry out a particular function, the system unavoidably consumes energy from some resources or exchanges energy with its surroundings somehow. It is well known that thermodynamic systems undergoing irreversible processes are always accompanied by thermodynamic costs, which place fundamental limits on systems' operational performance. For example, molecular motors convert the chemical energy stored in ATP into a directed movement; thus, the more energy is dissipated, the farther the motor can travel. Moreover, one might intuitively expect a trade-off relation between the dissipation cost and the fluctuation of the displacement. Unveiling such latent relations distinguishes the possible from the impossible and deepens our understanding of the underlying mechanisms of physical systems, thus providing insights into the design principles of optimal artificial machines.

Over the past few decades, there has been a flurry of research to understand the thermodynamics of small systems, resulting in two comprehensive frameworks: stochastic thermodynamics and quantum thermodynamics. Stochastic thermodynamics mainly focuses on the thermodynamic aspects of classical systems far from equilibrium, whereas quantum thermodynamics deals with quantum systems in which quantum effects emerge. These theoretical frameworks allow us to investigate the physical properties of microscopic systems that are subject to significant fluctuations. One of the central quantities in thermodynamics is entropy production, which characterizes the irreversibility of thermodynamic processes. In nonequilibrium steady-state systems, entropy production quantifies the amount of heat dissipated into the environment. In the context of biological processes, entropy production reflects the free energy lost in the spontaneous relaxation to perform a specific function. Furthermore, entropy production sets universal limits to the efficiency of thermal machines, such as heat engines and refrigerators. Therefore, revealing new relations on irreversibility and estimating the degree of irreversibility have become important research topics.

In recent years, a powerful inequality known as thermodynamic uncertainty relation (TUR) has been discovered for nonequilibrium systems described by Markov jump processes and overdamped Langevin equations. The TUR asserts a trade-off between the uncertainty of time-integrated currents (a statistical measure) and entropy production (a thermodynamic measure), i.e., high precision of currents is unattainable without increasing the associated entropy production. Remarkably, the TUR not only quantifies our intuition --- higher accuracy requires more cost --- for the first time but also imposes a lower bound on entropy production in terms of moments of currents. Nevertheless, questions remain about how entropy production constrains the current fluctuation in other stochastic dynamics and whether a tighter lower bound on entropy production can be derived given additional information.

Such research questions are addressed in two separate parts of this thesis. In the first part of this thesis, we focus on investigating the TUR in various dynamics from both theoretical and practical perspectives. Motivated by the numerical fact that the TUR is no longer valid in some stochastic dynamics, we derive novel TURs for a wide range of observables, which are not limited to time-integrated currents. Employing an information-theoretic approach, we obtain TURs for steady-state underdamped Langevin dynamics and for Langevin systems driven by an external time-dependent control protocol. Our derived bounds indicate that the entropy production cannot solely constrain the fluctuation of observables in the finite times, and other complementary contributions such as the dynamical activity are required. Going beyond the Markovian systems and adopting another approach based on the fluctuation theorem, we derive TURs for non-Markovian systems, including time delay, measurement and feedback control, and semi-Markov processes. The obtained TURs imply that in addition to the entropy production, non-Markovian contributions such as the information flow and memory effects play an important role in suppressing observable fluctuations. Along with theoretical results, we also propose a TUR-based method, which exactly estimates entropy production for overdamped Langevin dynamics and returns a tightest lower bound of entropy production for Markov jump processes. The proposed method provides an effective and efficient tool to infer dissipation in biological and physical systems from experimental data.

In the second part of the thesis, we aim to tighten the lower bound of the total entropy production, thus sharpening the second law of thermodynamics. Specifically, we derive geometrical bounds on the irreversibility in both quantum and classical Markovian open

systems that satisfy the detailed balance condition. Using information geometry, we prove that irreversible entropy production is bounded from below by a modified Wasserstein distance between the initial and final states, thus strengthening the Clausius inequality in the reversible-Markov case. The modified metric can be regarded as a discrete-state generalization of the Wasserstein metric, which has been used to bound dissipation in continuous-state Langevin systems. Notably, the derived bounds can be interpreted as the quantum and classical speed limits, implying that the associated entropy production constrains the minimum time of transforming a system state.

The thesis presents various thermodynamic relations on the irreversibility of thermodynamic processes, which connect physical quantities such as dissipation, thermodynamic length, observable fluctuations, dynamical activity, and evolution speed in both classical and quantum open systems.