

論文の内容の要旨

Dynamics and Thermodynamics of Coupled Quantum Oscillators (結合量子振動子系の動力学と熱力学)

氏名 青木 隆明

In general, it is difficult to isolate a quantum system; the system always interacts with its environment, which causes decoherence and dissipation of the system. Such a system is called an open quantum system. The total system, which consists of the system of interest and the environment, may be isolated and its dynamics can be unitary. As the degrees of freedom of the environment is huge, however, pursuing the total dynamics is generally beyond our computational ability. Besides, the dynamics of the environment itself is typically of little interest. Thus, we usually focus on the dynamics of the open system by taking the partial trace over the degrees of freedom of the environment.

In the theory of open quantum systems, it is often assumed that the environment is in a thermal equilibrium (Gibbs) state at the initial time. We call such an environment a bath. Because of the interaction with the bath, the dynamics of the system is not unitary; it is not described by the Schrödinger equation nor by the von Neumann equation. We do not have a simple form of the time-evolution equation for the system for a general coupling. Nonetheless, when the coupling is weak enough for the time scale of the bath to be much shorter than that of the system, the dynamics of the system is called Markovian; under several approximations its dynamics can be described by a simple form of the time-evolution equation called the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL)-type Markovian master equation. This equation comprises two parts; one is related to the dynamics induced by the Hamiltonian of the system and the other is related to the decoherence which comes from the interaction with the bath.

There is a procedure to derive the GKSL equation from the microscopic Hamiltonian of the system, the bath, and their interaction. In the derivation, we need the complete set of the eigenstates of the Hamiltonian of the system. When the system is simple like a two-level system and a harmonic oscillator, we know the eigenstates and can derive the explicit form of the GKSL equation. On the other hand, when the system is complicated like a Kerr-nonlinear parametric oscillator (KPO), which we study in this thesis, only several eigenstates of the Hamiltonian are known, and

hence it is difficult to derive its GKSL equation. Instead in the literature, as a decoherence part of the GKSL equation for a KPO, the decoherence part of the GKSL equation for a harmonic oscillator is often used. As this decoherence part is not derived from the microscopic Hamiltonian of the total system which consists of a KPO and its environment, it is doubtful whether this decoherence part accurately describes the decoherence of the KPO. Indeed, we derive the GKSL equation for a KPO starting from the microscopic Hamiltonian of the total system comprised of the KPO and a bath of harmonic oscillators, finding a different form of the decoherence term.

We compare the dynamics of a KPO under our GKSL equation and that under the GKSL equation in the literature. As a result, we find that the excitation error of a KPO under our GKSL equation is smaller than that under the GKSL equation in the literature. In particular, in the low-temperature limit of the bath, we find that the state of a KPO under our GKSL equation is mostly confined to the cat subspace, which is spanned by KPO's two degenerate ground states. This is desirable when we use a KPO as a qubit for a quantum computer, whose mission is to reduce as many errors as possible. We claim that it is essential to employ our more accurate GKSL equation to reproduce this desirable result.

On the other hand, we also study in this thesis a total system made up of coupled harmonic oscillators in a star configuration, in which the central harmonic oscillator (system of interest) is coupled to a finite number of surrounding harmonic oscillators (bath). When the initial state of the total system is a Gaussian state, not only the dynamics of the system of interest but also the dynamics of the total system including the bath can be pursued. Even when the size of the bath is finite, we can set the parameters so that the finite-time dynamics of the system of interest may be well approximated by the GKSL equation.

An open quantum system and a bath is one of the typical setups in the research field of quantum thermodynamics, which explains microscopic thermodynamic changes of microscopic quantum systems coupled to macroscopic ones. One of the most fundamental problems in quantum thermodynamics is how to define thermodynamic quantities such as the thermodynamic entropy, the temperature, heat, and work. Of particular importance is the thermodynamic entropy because it characterizes the irreversibility of thermodynamics. This is why researchers have suggested several definitions of thermodynamic entropy and various ones of entropy production and of its rate. Nevertheless, there is no consensus for now.

There is active research into the relation between non-Markovianity of the dynamics of an open quantum system and a negative entropy production rate of the total system. However, there is no agreement about this relation mainly because there is no unified definition of the entropy production rate or of non-Markovianity. On the other hand, when an open quantum system is under the GKSL-type Markovian dynamics, it is widely believed that the entropy production rate of the total system is non-negative, and researchers often use the von Neumann entropy production rate, which is the negated time-derivative of the von Neumann relative entropy between the reduced state of the system and the reference stationary state of the GKSL equation. There is an implicit assumption in the form of the von Neumann entropy production rate that the size of a bath is so macroscopically large that its temperature does not change during the dynamics. Although the temperature of the whole bath does not change macroscopically, the temperature of a part of the bath can change microscopically. The von Neumann entropy production rate cannot take this microscopic temperature change into account.

In order to take this microscopic temperature change into account, we consider the quantum model of coupled harmonic oscillators in a star configuration. As the initial state of the total system, we prepare the tensor product of the Gibbs states of the system and the bath. As a result, we find that every harmonic oscillator is always in a Gibbs state with a time-dependent temperature. This allows us to define the thermodynamic entropy for each harmonic oscillator in a similar way to the definition in equilibrium thermodynamics and statistical mechanics. We can

treat every harmonic oscillator on an equal footing thanks to the initial state that we adopted. We define the nonequilibrium thermodynamic entropy of the total system as the summation of the thermodynamic entropy of each harmonic oscillator. We analytically confirm that our total thermodynamic entropy satisfies the third law of thermodynamics. We find numerically that our total thermodynamic entropy production rate can be negative though the finite-time dynamics of the central harmonic oscillator (the system of interest) is well approximated by the GKSL-type Markovian master equation, while our total thermodynamic entropy satisfies the second law of thermodynamics. This contrasts with the von Neumann entropy production rate, which is always positive. This difference originates in our microscopically treating the harmonic oscillators in the bath. We can pursue the time evolution of the temperature of each harmonic oscillator in our formulation. We hence find that the temperatures of the harmonic oscillators in the bath which have almost the same frequency as the system change due to the interaction. Our thermodynamic entropy production rate takes this into account, while the von Neumann entropy production rate does not. Therefore, when the size of the bath is finite, our thermodynamic entropy production rate is preferable.