論文の内容の要旨

論文題目

Geometric Approach to Nonequilibrium Statistical Mechanics

(非平衡統計力学への幾何学的アプローチ)

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A geometric perspective often provides us with a deep and intuitive understanding of physics, such as Riemannian geometry in general relativeity, differential geometry with affine connections in gauge theory, and topology in condensed matter physics. It is also useful in the study of statistical mechanics. For example, the thermodynamic length is known to be a natural distance between thermal equilibrium states, quantifying an energetic cost to transform one equilibrium state to another. The metric induced by the thermodynamic length is the classical Fisher metric, which plays an important role in information geometry.

Information geometry concerns a differential-geometric structure of statistical manifolds, whose element represents a probability distributions. Originally, information geometry was considered in the theory of statistical inference. The classical Fisher information, which gives the upper bound on the precision of estimation through the Cramér-Rao inequality, is identified as a natural metric on statistical manifolds. The classical Fisher information is also characterized as the unique monotone metric, which means that it monotonically decreases under information processing. Since a probability distribution on a phase space can be interpreted as a (mixed) state in physics, we can say that for physicists, information geometry treats an informationally natural geometric structure on the space of physical states.

If we consider quantum theory, probability distributions are replaced by density operators. Then, the noncommutativity of operators allows much more abundant structures than the classical information geometry. The quantum Fisher information is again characterized as the monotone metric on the space of density operators, but there are infinitely many types of the quantum Fisher information. In fact, there is a one-to-one correspondence between the quantum Fisher information and an operator monotone function. The physical meaning of the quantum Fisher information has not fully clarified yet. Furthermore, even how to measure it has been elusive.

Another situation where geometry has a close relation to statistical mechanics is thermodynamic control, in which the system is controlled through time-dependent external control parameters. One of the difficulties in analyzing nonequilibrium processes in thermodynamic control is that observable quantities at some time depend not only on the value of the control parameters at that time but also on the entire history of the control. However, when the control is sufficiently slow, the average work performed on the system during the control can be approximated by the squared length of the contour on the space of control parameters, which are measured with the thermodynamic metric. This approximate expression for work opens a way to analyze nonequilibrium processes from a geometrical perspective. There are two problems concerning the evaluation of work in terms of the thermodynamic metric. First, the condition on which this approximate expression is valid is not clear. We need to construct a systematic expansion of the work to clarify the condition. Second, it can evaluate only the average work and cannot evaluate the fluctuations.

In this thesis, we study nonequilibrium statistical mechanics from a geometric perspective. In particular, we (i) examine the relation between quantum information geometry and linear response theory, and (ii) analyze nonequilibrium processes in thermodynamic control and derive a geometric expression for work.

The first original study in this thesis is to understand quantum information geometry based on linear response theory. More concretely, we demonstrate that the quantum Fisher information can be determined by measuring the linear response functions. The central idea is as follows. The quantum Fisher information is quantitatively related to the fluctuations or correlations through the quantum Cramér-Rao inequality. When the system is in thermal equilibrium, such correlations are also quantitatively related to linear response functions to external perturbations. Therefore, we can determine the quantum Fisher information through linear response functions based on these two relations.

For that purpose, we first generalize the fluctuation-dissipation theorem, and establish the quantitative relation between linear response functions and the generalized covariance. Based on the generalized fluctuation-dissipation theorem, we can determine the generalized covariance by measuring linear response functions such as the dynamical susceptibilities and the complex admittances for all frequencies. Since the generalized covariance contains the same amount of information on the quantum state as the quantum Fisher information, we can also experimentally determine the quantum Fisher information in the same way. We demonstrate that our result is applicable to an experimental determination of the skew information, and a validation of skew information-based uncertainty relations.

There are two advantages in our methods to determine the quantum Fisher information. First, once we measure the linear response functions, we can determine any type of the quantum Fisher information. Second, our method does not need quantum state tomography, and therefore can avoid an exponentially large number of measurements even for large systems.

The second original study is on the analysis of work in thermodynamic control. We extend the thermodynamic metric-based expression of work into two directions. One is to obtain a systematic expansion of work from a phenomenological argument, and the other is to obtain a work distribution for overdamped Langevin systems.

First, we derive a systematic expansion of the work assuming the perturbation series expansion and the Taylor expansion of the control parameter. Then we show that the obtained expansion is actually in terms of a small parameter ϵ that characterizes how slowly we control the system, and the leading-order contribution is given by the thermodynamic metric expression. We also discuss the physical picture of the next leading-order contributions to the thermodynamic metric contribution. They can be detected by comparing the excess work in a forward control and a backward control, and are predicted to scale as $1/T^2$ as a function of the total control time T. Since the expansion is derived without assuming the microscopic dynamics, it is valid as long as the perturbation series expansion is valid.

Then, we examine the work distribution in overdamped Langevin systems. We derive the time evolution equation for the moment generating function of the work, and solve it from the lower-order contributions in ϵ. The $O(\epsilon)$ contribution to the generating function reproduces two known facts: the work distribution is Gaussian, and the average work is given by the thermodynamic metric. When we take up to $O(\epsilon^2)$ contributions into account, the work distribution exhibits nonzero skewness, which means that the fluctuation-dissipation relation is violated with scaling $1/T^2$. Furthermore, from the analytic calculation with numerical supports, we conjecture that the n-th cumulant of the work scales as $1/T^{n-1}$ for $n \geq 1$.