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Statistical Mechanics for Athermal Fluctuation



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Kiyoshi Kanazawa

Statistical Mechanics for Athermal Fluctuation

Non-Gaussian Noise in Physics

Doctoral Thesis accepted by Kyoto University, Kyoto, Japan



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Supervisor's Foreword

When random variables are added, their sum tends to obey the Gaussian distribution regarding their large number limit. This fact is the result of the central limit theorem in probability theory. Thus, fluctuation around the average value is always characterized by the Gaussian distribution, which forms the basis of equilibrium statistical mechanics. Even in nonequilibrium situations, the fluctuation theorem, which is the result of the Gaussian fluctuations, plays an important role. Therefore, properties associated with the Gaussian fluctuations, which are important in many cases, are well understood. Nevertheless, non-Gaussian fluctuations are ubiquitous in nature. This is counter-intuitive because we may consider that non-Gaussian fluctuations should be irrelevant because of the central limit theorem. To understand such situations. In this book, Kiyoshi Kanazawa answers these questions through analysis of the physics of non-Gaussian noise.

To survive non-Gaussian noise, a system must be free from the central limit theorem. To understand this we need to recall the fundamental theorem of mathematics known as the Lévy–Ito decomposition in which any Lévy process can be decomposed into a Wiener process and compound Poisson processes. This mathematical theorem suggests that both thermal Gaussian fluctuations and athermal non-Gaussian fluctuations, or jump processes, should coexist if the non-Gaussian noise is still relevant in the thermodynamic limit. The detailed mechanism of the appearance of non-Gaussian noise is clearly explained in this book.

However, the mathematical description of non-Gaussian fluctuations has not yet been well developed, even though the description of the Gaussian fluctuation is well established. I believe that this book provides the first systematic mathematical description of non-Gaussian noises in terms of the detailed description of the stochastic calculus of random variables. This book also discusses anomalous transport between athermal environments and energy-pumping through athermal systems.

One characteristic worthy of mention is the self-contained description for Gaussian fluctuations. Indeed, Part I which represents almost half of this book is devoted to a review of the stochastic theory of thermally fluctuating systems including Markovian stochastic calculus, the kinetic theory of dilute gases, the Langevin equation and its microscopic derivation, the stochastic calculus for a single trajectory, and stochastic energetics. This means that this book can be used as a concise textbook for modern nonequilibrium statistical mechanics. Thus, I recommend this book to graduate students who are interested in nonequilibrium statistical mechanics as a modern and self-contained textbook for stochastic analysis of systems agitated by Gaussian noise or non-Gaussian noise.

Kyoto, Japan March 2017 Prof. Hisao Hayakawa

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K. Kanazawa, T. Sagawa, and H. Hayakawa, "Stochastic Energetics for Non-Gaussian Processes" Physical Review Letters **108**, 210601–210605 (2012).

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Chapter 1 Introduction to Physics of Fluctuation

1.1 Background: Physics of Thermal Fluctuation

Recent experimental development has enabled us to investigate fluctuating small systems in detail (e.g., biological [1–4], colloidal [5–7], and electrical systems [8–10]). For example, trajectories of microscopic quantities can be experimentally observed in addition to the ensemble averages of macroscopic quantities as illustrated in Fig. 1.1a. The techniques of single molecule manipulation furthermore have enabled us to control small systems (see Fig. 1.1b for a schematic of the optical trap [12]). Correspondingly, theoretical frameworks for small fluctuating systems are topics of wide interest from the viewpoint of statistical mechanics and thermodynamics to answer several natural and important questions: *How do we make stochastic models of fluctuations? What is the thermodynamic quantities for small systems, such as work and heat? What is the theoretical bound for the energy efficiency of small heat engines?* These questions are important even in understanding practical issues, such as efficiencies of molecular motors in biology [13].

One of theoretical approaches to these questions is applications of stochastic processes. From the viewpoint of statistical mechanics, modeling fluctuations from microscopic dynamics has been an interesting issue [14–18]. For example, the Langevin equation is derived for thermal fluctuating systems and is analyzed in the formulation of stochastic processes. This methodology is useful even for modeling nonequilibrium fluctuations [19–23]. From the viewpoint of thermodynamics, stochastic energetics (or stochastic thermodynamics) [24–29] has recently attracted wide interest among researchers of statistical physics. Stochastic energetics is a thermodynamic formulation based on the Gaussian stochastic processes, whereby thermodynamic quantities, such as work and heat, are introduced on the level of a single trajectory. Indeed, the recent studies on the nonequilibrium equalities [8–10, 29–41], such as the fluctuation theorem and the Jarzynski equality, are often investigated using stochastic energetics, and this formulation is intensively generalized toward information processing [42–49] and steady state thermodynamics [28, 37, 50].

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Fig. 1.1 a Schematic of the singular trajectory of fluctuating systems associated with thermal baths. The bead moves randomly because of the thermal fluctuation. Trajectories are experimentally observed, for example, using the total internal microscopy [11]. **b** Schematic of the optical tweezers, which are applicable to manipulate the bead arbitrarily. The bead is trapped by the laser potential and is moving around the focus point of the laser

1.2 Toward Physics of Athermal Fluctuation

While thermal fluctuations has been intensively studied in statistical mechanics and thermodynamics, athermal fluctuations have not been systematically investigated yet because they are essentially in nonequilibrium steady states. Athermal fluctuations are experimentally interesting topics in biological [51, 52], electrical [53–56], and granular [57–61] systems, which are preserved in nonequilibrium steady states by external energy injection. They are experimentally reported to be characterized by their non-Gaussianity [51–61], and are theoretically studied on the basis of non-Gaussian models [62–70]. We then naturally encounter the following questions:

- (Q1) **Statistical mechanics for athermal fluctuation**: *What is the minimal model of athermal stochastic systems? How do we systematically derive such a model from microscopic dynamics?*
- (Q2) **Thermodynamics for athermal fluctuation**: *How do we formulate a thermodynamic framework for athermal stochastic systems? What are the unique characters of athermal fluctuation different from the conventional thermodynamic phenomena?*

In this thesis, the answers to these questions are presented in both approaches of statistical mechanics and thermodynamics. To answer the question Q1, a statistical mechanical approach is developed by introducing a minimal stochastic model for athermal fluctuation [69, 70]: A Langevin-like equation with non-Gaussian noise is derived from microscopic dynamics for a wide class of athermal systems. We focused on the system size expansion, which was a microscopic foundation of the conventional Langevin equation, and have generalized its formulation toward the athermal stochastic systems. We have finally clarified the mechanism behind the emergence of the non-Gaussianity in athermal fluctuations. As an analytically solvable model, a granular rotor under viscous friction is investigated to numerically examine the validity of our formulation.

Analytical properties of general non-Gaussian Langevin equations are also studied systematically in this thesis even in the presence of with nonlinear friction terms [70]. By considering an asymptotic expansion for a large frictional coefficient, a full-order asymptotic formula is presented for the steady distribution function. The first-order

truncation of our formula leads to the independent-kick model, which was phenomenologically introduced in Ref. [58]. We further show that the high-order correction terms directly correspond to multiple-kicks during relaxation by introducing a diagrammatic representation. As a demonstration of our formulation, a granular rotor under the Coulomb friction is addressed theoretically and numerically.

To answer the question Q2, we next study a thermodynamic formulation for athermal stochastic systems. We first present a generalization of stochastic energetics for general non-Gaussian processes [65]. Stochastic energetics has been formulated as a mathematical theory of stochastic processes, where technical problems exist in terms of the stochastic product (stochastic integral) for definition of thermodynamic quantities. To introduce thermodynamic quantities, the Stratonovich product is known to be appropriate for Gaussian stochastic processes by applying the ordinary stochastic chain rule. We then discuss what kind of product is appropriate for definition of thermodynamic quantities for general non-Gaussian stochastic processes. Concretely, three kinds of products are defined for smoothed stochastic processes (the Itô, Stratonovich, and * products), and the ordinary stochastic chain rule is derived for an arbitrary stochastic process by using a mixed product, where multiple products coexist. This stochastic chain rule is applied to the reformulation of stochastic energetics for general non-Gaussian stochastic dynamics.

On the basis of the above thermodynamics formulation, distinctive phenomena in athermal systems are studied [66, 67] from the viewpoint of energetics. We first study energy transport between two athermal baths, and derive fundamental laws on the statistics of heat current: the generalized Fourier law and the generalized fluctuation relation. Remarkably, the direction of heat current depends on the properties of the heat conducting wire, showing the explicit absence of the zeroth law for athermal systems. We further show that the zeroth law recovers if we fix the kind of the conducting device by introducing an indicator to characterize the direction of heat current. As a demonstration, we study energy transport between two granular motors.

Finally, the energy pumping is studied from athermal fluctuations [67]. We focus on an electrical circuit with avalanche diodes as an experimentally realizable example, and theoretically study extracted work from athermal fluctuation. A positive amount of work is shown extractable from the athermal fluctuation in cyclic manipulations, even for finite-speed protocols.

1.3 Organization of This Thesis

This thesis consists of two parts: review on statistical mechanics and thermodynamics for thermal fluctuation (Chaps. 2–6, Part I) and its theoretical extension for athermal fluctuation (Chaps. 7–12, Part II). The contents in each part are described below (see Fig. 1.2 for chapter connection):



Fig. 1.2 Schematic of the chapter connection in this thesis

Part I

Background of the study in this thesis is reviewed from the viewpoint of statistical mechanics and thermodynamics for thermal fluctuation in Part I. From Chap. 2 to Chap. 4, statistical mechanics of thermal fluctuation is formulated on the basis of the stochastic processes and molecular kinetic theory. In Chaps. 5 and 6, stochastic energetics for the Langevin equation is reviewed utilizing the stochastic calculus. The details of each chapter are presented below:

- **Chapter 2**: a brief introduction is provided to the Markovian stochastic processes. In particular, the correspondence between stochastic differential equations (SDEs) and master equations are shown for various examples.
- Chapter 3: molecular kinetic theory is formulated from microscopic dynamics for many-body systems of hard spheres. The pseudo-Liouville equation is derived first and the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy is derived from the pseudo-Liouville equation. The Boltzmann equation is then deduced by assuming molecular chaos from a systematic calculation. Using this method, a stochastic model of one-dimensional Brownian motion (e.g., the Rayleigh particle) is derived from microscopic dynamics.
- **Chapter** 4: the Langevin equation is reviewed in terms of thermodynamics and microscopic derivation. We first review the Langevin equation and its consistence with equilibrium thermodynamics. The Langevin equation is then derived from microscopic dynamics by the system size expansion. As the demonstrations, several problems are solved: the Rayleigh particle, a nonequilibrium Rayleigh particle, and a granular motor. We finally remark unsolved problems in the original system size expansion, which is solved in Chaps. 7 and 8.
- Chapter 5: the mathematical theory of stochastic calculus is reviewed for general Markov processes. Trajectories for Markov processes are generally singular, and selection of multiplication between stochastic variables is an important issue. We review the Itô integral and the Itô-type SDE, and the corresponding differential rules. In the special case of the Gaussian noise, the Itô rule is valid to simplify the differential rule (the Itô formula). Various stochastic integrals are also studied in terms of the ordinary chain rule and the Wong-Zakai theory.
- **Chapter 6**: stochastic energetics is reviewed for the Langevin equation. Realistic setups where the Langevin equation is valid are first explained, and thermodynamic quantities (i.e., work and heat) are introduced on the level of a single trajectory. The nonequilibrium identities and the second law of thermodynamics are finally derived for the Langevin dynamics.

Part II

The main results of this thesis are presented in Part II. In Chaps. 7 and 8, we present a formulation of statistical mechanics for athermal fluctuations. In Chaps. 9 and 11, a thermodynamic formulation for athermal fluctuation is shown by extending stochastic energetics. The details of the chapters are presented below:

- **Chapter** 7: a systematic derivation of a Langevin-like non-Gaussian equation is presented from microscopic dynamics. Mathematical characters of the non-Gaussian Langevin equation are first studied and its asymptotic derivation from master equations is shown by generalizing the system size expansion. Under the condition where the thermal friction is sufficiently large, the non-Gaussian properties are dominant with the central limit theorem violated. As a demonstration, we address a granular motor under viscous friction and derive the non-Gaussian Langevin equation as its reduced stochastic dynamics.
- **Chapter 8**: the formulation in Chap. 7 is generalized for nonlinear systems. We also study the analytical properties of the non-Gaussian Langevin equation. Using a perturbation for large friction, a full-order asymptotic formula is derived for the steady probability distribution function. We show that the first-order approximation of our formula leads to the independent-kick model, and high-order correction terms correspond to multiple-kick during relaxation. A granular motor under Coulombic friction is analyzed as a realistic example.
- **Chapter 9**: stochastic energetics is formulated for general non-Gaussian stochastic dynamics. Markovian stochastic processes are reformulated using the smoothed δ -function, and three types of products are introduced between a stochastic variable and the smoothed δ -function: the Itô, Stratonovich, and * products. By introducing mixed products, where multiple products coexist, the ordinary chain rule is derived for an arbitrary Markovian stochastic dynamics. We finally apply this formulation to stochastic energetics for general non-Gaussian processes.
- Chapter 10: energy transport between athermal reservoirs are studied by applying stochastic energetics for non-Gaussian processes. The statistics of heat current between athermal reservoirs is investigated for a simple stochastic model driven by non-Gaussian fluctuation, and generalizations of the Fourier law and the fluctuation theorem are obtained. We also find a violation of the zeroth law of thermodynamic, whereby the direction of heat current depends on the heat conducting wire. As a demonstration, heat conduction between two granular motors is studied with the aid of the method developed in Chap. 7.
- Chapter 11: energy pumping from athermal fluctuation is studied in the formulation of stochastic energetics. As an experimentally realizable setup, we consider an electrical circuit under avalanche noise, whose dynamics is governed by the non-Gaussian Langevin equation. Extracted work and power from the non-Gaussian athermal noise is studied through a cyclic manipulation, and a positive amount of work is theoretically found to be extracted even for finite-speed protocols regardless of the spatial symmetry of the system.
- Chapter 12: we conclude this thesis with some remarks and future perspectives.

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Part I Review on Stochastic Theory for Fluctuating Thermal Systems