

A STUDY ON THE MODELLING OF ACTIVE HEAT BATHS WITH APPLICATIONS TO ACTIVE BROWNIAN HEAT ENGINES

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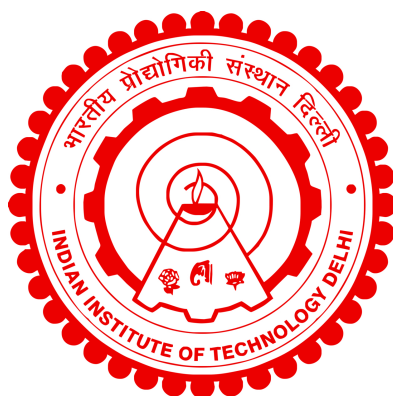
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*The thesis is dedicated to my elder brother late Shyamlal
Majumder and my loving family*

Certificate

This is to certify that the thesis entitled “**A study on the modelling of active heat baths with applications to Active Brownian heat engines**”, submitted by **Rita Majumdar**, **Entry No. 2018PHZ8338**, to the Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy in Physics**, is a record of the original, bonafide research work carried out by her under my supervision and guidance. The thesis has reached the standards fulfilling the requirements of the regulations related to the award of the degree.

The results contained in this thesis have not been submitted in part or in full to any other University or Institute for the award of any degree or diploma to the best of my knowledge.



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Abstract

The central focus of this thesis is understanding small fluctuating active systems, particularly through a thermodynamic perspective. Our approach includes a dual strategy: first, we explore the theoretical and numerical approaches to studying the dynamics of stochastic systems, exploring both Gaussian and non-Gaussian noises. Secondly, we explore the realm of stochastic heat engines to investigate various thermodynamic properties and explore the factors contributing to the enhancement of their performance.

First, we examine the dynamics of a confined overdamped Brownian particle immersed in a thermal bath and subjected to a non-equilibrium bath containing a dilute solution of active particles. Due to confinement, the Brownian particle encounters a harmonic potential. Additionally, it undergoes Poisson shot-noise impulses with a defined amplitude distribution resulting from collisions with active particles within the bath. We derive the stationary solution for the displacement distribution by analyzing the Fokker-Planck equation. We also calculate the moments, including mean, variance, skewness, and kurtosis. Additionally, we calculate an effective temperature using the fluctuation-dissipation theorem and demonstrate the validity of the equipartition theorem for all zero-mean kick distributions, even those resulting in non-Gaussian stationary statistics. In the scenario of Gaussian-distributed active kicks, we observe a transition from Gaussian to non-Gaussian and again re-entry to the Gaussian stationary states with a heavy-tailed leptokurtic distribution across various parameters, consistent with recent experimental findings. Further, we analyze the system's irreversibility by calculating the time asymmetry of cross-correlation functions. In our investigation, we conducted a comprehensive study of the system to lay the groundwork for building a heat engine in the future. We aim to identify the regions where non-Gaussian behavior can be attained and subsequently analyze its impact on engine performance.

Later, we perform an extensive analysis of passive as well as active micro-heat engines with different single-particle stochastic models. Using stochastic thermodynamics, we calculate thermodynamic work, heat, entropy production, and efficiency of passive and active Brownian heat engines through analytical calculation and simulation

techniques and compare both results. We discuss a group of protocols for which exact non-quasistatic calculations can be done, entirely in the passive engine case and partially in the active engines. Then, we summarize our results for a particular protocol. We study the position distributions of the Brownian particle in both passive and active engines. We compare their characteristics in terms of the parameter that measures the competition between the active persistence in the particle position and the harmonic confinement. Our goal is to uncover the correlation between non-Gaussian attributes and efficiency through the computation of excess kurtosis. Our findings indicate that the efficiency of thermal machines can be enhanced or reduced based on the activity within the model, and determining the exact cause solely from the excess kurtosis is not straightforward.

Therefore, we further investigate the model of an active heat engine involving Brownian particles in an active bath, resulting in active Poissonian noise. The positional distribution displays a non-Gaussian leptokurtic fat-tailed shape, and we assess its non-Gaussianity through the calculation of excess kurtosis. Our objective is to directly measure a parameter that correlates with the non-Gaussian behavior of the system, establishing a direct link with the excess kurtosis. For this model, we study two different protocols. We calculate exact analytical expressions for work, heat, and efficiency, which further helps to understand many physical insights about the system. Our research reveals that while there is a general trend of increasing efficiency with increasing excess kurtosis initially, but no particular correlation can be established between these two quantities. This indicates that other factors influenced by activity, besides non-Gaussianity and excess kurtosis, contribute to the observed enhanced efficiency.

सारांश

इस थीसिस का मुख्य उद्देश्य कम उच्चावचों वाली सक्रिय प्रणालियों को समझना है, विशेष रूप से उष्मागतिकी परिप्रेक्ष्य के माध्यम से। यह अध्ययन दो भिन्न दृष्टिकोण से किया गया है। सर्वप्रथम, हम स्टोकेस्टिक प्रणालियों की गतिशीलता का अध्ययन करने के लिए सैद्धांतिक और संख्यात्मक मानकों का पता लगाते हैं, जिसके अंतर्गत गॉसियन और गैर-गॉसियन दोनों का अध्ययन प्रस्तुत किया गया है। तत्पश्चात, हम विभिन्न थर्मोडायनामिक गुणों की जांच करने और उनके प्रदर्शन को बढ़ाने में योगदान देने वाले कारकों का पता लगाने के लिए स्टोकेस्टिक हीट इंजन के कार्य सीमाओं का अध्ययन करते हैं।

अध्ययन के प्रथम भाग में हम ऊष्मा स्रोत में डूबे हुए एक सीमित सक्रिय ब्राउनियन कण की गतिशीलता की जांच करते हैं, जबकि ब्राउनियन कण सक्रिय कणों के निम्न सांद्रता वाले असाम्य स्रोत के अधीन होते हैं। पाश की उपस्थिति में, ब्राउनियन कण एक हार्मोनिक बल के अंतर्गत गति करता पाया जाता है। इसके अतिरिक्त, यह स्रोत के सक्रिय कणों के साथ टकराव के परिणामस्वरूप परिभाषित आयाम वितरण के साथ पॉइसन लघु-प्रायिक आवेगों से भी गुजरता है। हम फोकर-प्लैंक समीकरण का विश्लेषण करके विस्थापन वितरण के लिए साम्य हल प्राप्त करते हैं। हम माध्य, विचरण, तिरछापन और कर्टोसिस सहित अन्य गुणों की भी गणना करते हैं। इसके अतिरिक्त, हम उतार-चढ़ाव-अपव्यय प्रमेय का उपयोग करके एक प्रभावी तापमान की गणना करते हैं और सभी शून्य-माध्य किक वितरणों के लिए समविभाजन प्रमेय की वैधता प्रदर्शित करते हैं, यहां तक कि गैर-गॉसियन स्थिर आंकड़ों के परिणामस्वरूप भी। गॉसियन-वितरित सक्रिय किक के परिदृश्य में, हम गॉसियन से गैर-गॉसियन में संक्रमण देखते हैं और हाल के प्रायोगिक निष्कर्षों के अनुरूप, विभिन्न मापदंडों में भारी टेल वाले लेप्टोकर्टिक वितरण के साथ गॉसियन के अध्ययन में पुनः प्रवेश करते हैं। इसके अतिरिक्त, हम क्रॉस-सहसंबंध कार्यों की समय विषमता की गणना करके सिस्टम की अपरिवर्तनीयता का विश्लेषण करते हैं। अपनी जांच में, हमने भविष्य में ताप इंजन के निर्माण के लिए आधार तैयार करने के लिए प्रणाली का व्यापक अध्ययन किया। हमारा लक्ष्य उन क्षेत्रों की पहचान करना है जहां गैर-गॉसियन व्यवहार प्राप्त किया जा सकता है और बाद में इंजन प्रदर्शन पर इसके प्रभाव का विश्लेषण किया जा सकता है।

अध्ययन के शेष भाग में, हम विभिन्न एकल-कण स्टोकेस्टिक मॉडल के साथ निष्क्रिय और साथ ही सक्रिय माइक्रो-हीट इंजन का व्यापक विश्लेषण करते हैं। स्टोकेस्टिक थर्मोडायनामिक्स का उपयोग करते हुए, हम विश्लेषणात्मक गणना और सिमुलेशन तकनीकों के माध्यम से निष्क्रिय और सक्रिय ब्राउनियन ताप इंजनों के उष्मागतिकीय कार्य, ऊष्मा, एन्ट्रॉपी उत्पादन और दक्षता की गणना करते हैं और दोनों परिणामों की तुलना करते हैं। हम प्रोटोकॉल के एक समूह पर चर्चा करते हैं जिसके लिए सटीक गैर-क्वासिस्टैटिक की गणना की जा सकती है, पूर्णतया निष्क्रिय इंजन मामले में और आंशिक रूप से सक्रिय इंजन में। तत्पश्चात, हम एक विशेष प्रोटोकॉल के लिए अपने परिणामों को संक्षेप में प्रस्तुत करते हैं। हम निष्क्रिय और सक्रिय दोनों इंजनों में ब्राउनियन कण के स्थिति वितरण का अध्ययन करते हैं। हम उनकी विशेषताओं की तुलना उन मानकों के संदर्भ में करते हैं जो कण स्थिति में सक्रिय दृढ़ता और दोलन पाश के बीच प्रतिस्पर्धा को मापता है। हमारा लक्ष्य अतिरिक्त कर्टोसिस की गणना के माध्यम से गैर-गॉसियन विशेषताओं और दक्षता के बीच संबंध को उजागर करना है। हमारे निष्कर्षों से संकेत मिलता है कि मॉडल के भीतर गतिविधि के आधार पर थर्मल मशीनों की दक्षता को बढ़ाया या घटाया जा सकता है। केवल अतिरिक्त कर्टोसिस से सटीक मानक निर्धारित करना एक कठिन

विधि है। इसलिए, हम एक सक्रिय ऊष्मा इंजन के मॉडल की आगे जांच करते हैं, जिसमें सक्रिय बाथ में ब्राउनीयन कण शामिल होते हैं, जिससे सक्रिय पॉइसोनियन शोर उत्पन्न होता है। स्थितिजन्य वितरण एक गैर-गौसियन लेण्टोकर्टिक फैट-टेल्ड आकार प्रदर्शित करता है, और हम इसकी गैर-गौसियनता का मूल्यांकन अतिरिक्त कुटोसिस की गणना के माध्यम से करते हैं। हमारा उद्देश्य एक ऐसे पैरामीटर को सीधे मापना है जो प्रणाली के गैर-गौसियन व्यवहार के साथ सहसंबद्ध हो, अतिरिक्त कुटोसिस के साथ सीधे संबंध स्थापित करते हुए। इस मॉडल के लिए, हम दो अलग-अलग प्रोटोकॉल का अध्ययन करते हैं। हम कार्य, ऊष्मा, और दक्षता के लिए सटीक विश्लेषणात्मक अभिव्यक्तियाँ गणना करते हैं, जो प्रणाली के बारे में कई भौतिक अंतर्दृष्टि समझने में और मदद करती हैं। हमारा शोध यह प्रकट करता है कि जबकि प्रारंभ में अतिरिक्त कुटोसिस बढ़ने के साथ दक्षता बढ़ने की एक सामान्य प्रवृत्ति होती है, लेकिन इन दो मात्राओं के बीच कोई विशेष सहसंबंध स्थापित नहीं किया जा सकता है। यह संकेत करता है कि गतिविधि से प्रभावित अन्य कारक, गैर-गौसियनता और अतिरिक्त कुटोसिस के अलावा, देखी गई बढ़ी हुई दक्षता में योगदान करते हैं।

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Abbreviations

Th	Thermal system
RT	Run and Tumble
CN	Colored Noise
AOUP	Active Ornstein Uhlenbec Process
PSN	Poisson Shot Noise
UCNA	Unified Colored Noise Approximation
PDF	Probability Distribution Function
FPE	Fokker Planck Equation
FDR	Fluctuation Dissipation Relation

Symbols

T_h (T_1)	Temperature of the hot reservoir
T_c (T_2)	Temperature of the cold reservoir
Q_h (Q_1)	The amount of heat absorbed from the hot reservoir
Q_c (Q_2)	The amount of heat rejected to the cold reservoir
W and P	Total extracted work and Power output
η_C and η_{CA}	Carnot efficiency and Curzon and Ahlborn efficiency
η and η_C^{eff}	efficiency and effective Carnot efficiency
S and $\dot{S}$	entropy and entropy production rate
k_B	Boltzmann Constant
U	Internal energy
κ	Stiffness of harmonic oscillator
$\xi(t)$	Gaussian white noise
$\eta(t)$	Active noise
ω	Average no of kick per unit time
γ	Friction coefficient

