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Աշոտ Մաթևոսյան Արթուրի

Ակտիվ ներբջջային պրոցեսների վիճակագրական մեխանիկան

Ա.04.02 - «Տեսական Ֆիզիկա» մասնագիտությամբ ֆիզիկամաթեմատիկական գիտությունների թեկնածուի գիտական աստիճանի հայցման ատենախոսության

ՍԵՂՄԱԳԻՐ

ԵՐԵՎԱՆ - 2024

A. I. ALIKHANYAN NATIONAL SCIENCE LABORATORY
(YEREVAN PHYSICS INSTITUTE)

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Statistical Mechanics of Active Intracellular Processes

SYNOPSIS

of Dissertaion in 01.04.02-“Theoretical Physics” presented for the degree of candidate in physical and mathematical sciences

YEREVAN – 2024

Ատենախոսության թեման հաստատվել է Ա. Ի. Ալիխանյանի անվան ազգային գիտական լաբորատորիայի (ԵրՖԻ) գիտական խորհրդում:

Գիտական ղեկավար՝
Ֆիզ. մաթ. գիտ. թեկնածու Ալլահվերդյան Արմեն Էդուարդի (ԱԱԳԼ)

Պաշտոնական ընդդիմախոսներ՝
Ֆիզ. մաթ. գիտ. դոկտոր Սահակյան Դավիթ Բագրատի (ԱԱԳԼ)
Ֆիզ. մաթ. գիտ. թեկնածու Մկրտչյան Վանիկ Երվանդի (ԱԱԳԼ)

Առաջատար կազմակերպություն՝
Ֆիզիկայի Կիրառական Պրոբլեմների Ինստիտուտ, Երևան, ՀՀ

Ատենախոսության պաշտպանությունը կայանալու է 2024 թ. սեպտեմբերի 10-ին՝ ժամը 14:00-ին, ԱԱԳԼ-ում գործող ԲԿԳԿ-ի 024 «Ֆիզիկայի» մասնագիտական խորհրդում (Երևան, 0036, Ալիխանյան եղբայրների փ. 2):

Ատենախոսությանը կարելի է ծանոթանալ ԱԱԳԼ-ի գրադարանում:
Սեղմագիրն առաքված է 2024 թ. օգոստոսի 10-ին:

Մասնագիտական խորհրդի գիտական քարտուղար՝
Ֆիզ. մաթ. գիտ. դոկտոր Հրաչյա Մարուքյան

The subject of the dissertation is approved by the scientific council of A. I. Alikhanyan National Science Laboratory (YerPhI).

Scientific supervisor:
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Official opponents:
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Leading organization:
Institute of Applied Problems of Physics, Yerevan, Armenia

The defense will take place on the 10th of September 2024 at 14:00 during the “Physics” professional council’s session of HESC 024 acting within AANL (2 Alikhanyan brothers str., 0036, Yerevan).

The dissertation is available at the AANL library.
The synopsis is sent out on the 10th of August 2024.

Scientific secretary of the special counsel:
Doctor of phys-math. sciences Hrachya Marukyan

GENERAL DESCRIPTION OF THE WORK

Thermodynamics, an empirical science developed in the 19th century by Carnot, Clausius, and Kelvin, describes energy and matter transformations in quasi-equilibrium macroscopic systems, introducing key concepts such as entropy and irreversibility [1–3]. Thermodynamic systems consist of microscopic components governed by quantum or classical dynamics, necessitating the foundations of phenomenological thermodynamics to be based on statistical mechanics. This field bridges macro and micro descriptions and addresses non-equilibrium phenomena in physics [4–8].

The Gibbs distribution is central to equilibrium statistical mechanics, linking the probability of system states in phase space to its Hamiltonian, with thermodynamic quantities derived as averages over this distribution.

This thesis explores the influence of external static magnetic fields, which do not affect classical systems in thermodynamic equilibrium. The magnetic field's inherent connection to rotations is evident in classical electrodynamics, where it acts as a pseudo-vector similar to angular momentum [9]. Thus, the second aim of this thesis is to identify open problems in the statistical mechanics of rotating systems and investigate non-equilibrium relaxation of angular momentum.

In equilibrium classical statistical mechanics, static magnetic fields have no effects as they do not perform work or appear in the system's energy expression, resulting in an equilibrium distribution independent of magnetic fields [10]. This insight, known as the Bohr-van Leeuwen theorem, underscores the necessity of quantum mechanics to explain magnetism [2, 11, 12]. However, magnetic field effects can be considered within classical mechanics by relaxing the assumption of equilibrium [13, 14].

Non-equilibrium systems are widespread, evident in living organisms, fluid flows, and chemical reactions, among other phenomena [15–17]. Although equilibrium states are rare in nature, quasi-equilibrium concepts such as Langevin and Fokker-Planck equations are useful for studying non-equilibrium systems [4, 6]. These equations uphold fluctuation and fluctuation-dissipation theorems (FDT), linking equilibrium and non-equilibrium thermodynamics [18]. The FDT connects equilibrium fluctuations with the system's response to small external perturbations, exemplified by the Einstein relation for the diffusion coefficient [18].

Statistical mechanics problems often consider a large system divided into a smaller subsystem of interest (the "system") and a larger quasi-equilibrium subsystem (the "thermostat" or "bath") [2]. The system interacts with the thermostat, exchanging energy, particles, linear momentum, and angular momentum. Non-equilibrium can arise either from the system's perturbation and relaxation or from the thermostat's non-equilibrium state, leading to non-equilibrium steady states (NESS) [4, 18]. NESS generalizes equilibrium states, lacking time-reversal symmetry and supporting persistent currents.

In recent years, studying the processes within living cells has garnered significant attention due to its fundamental importance in understanding biological functions and behaviors [19] . The main motivation of our work is to understand the function of ATPase, a group of enzymes responsible for generating ATP molecules, the energy currency of the cell Even the tiniest change in the function of ATPase can significantly impact the growth and function of the entire organism. Rotation plays a pivotal role in the function of ATPase [20–22] : the flow of protons drives the rotation of the central stalk, which subsequently induces conformational changes in the catalytic part, thereby facilitating ATP synthesis (Figure 1). However, in such a microscopic system, rotation does not occur in a purely mechanical sense but rather should be understood through the principles of statistical mechanics [23].

We develop advanced tools and extend the principles of non-equilibrium statistical mechanics to study rotating systems out of equilibrium [13, 14, 23]. Our research not only enhances the under-

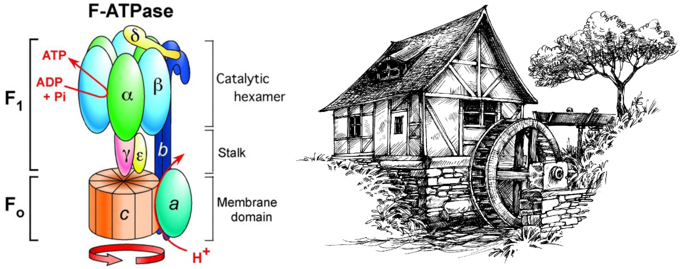

Figure 1: (left) Schematic models of the F-ATPase. The membrane extrinsic (F_1) sector, catalytic hexamers ($\alpha_3\beta_3$), stalk, and membrane domain (F_0) are shown. Red arrows represent the direction of the chemical reaction, subunit rotation (C, γ, ϵ), and proton transport in physiological conditions. **(right)** The rotation of ATPase is analogous to that of a watermill. For ATPase, rotation is driven by the flow of protons along the electrostatic potential gradient across a membrane, whereas a watermill rotates due to water flowing along a gravitational potential gradient. Unlike the macroscopic watermill, ATPase operates on a microscopic scale, and its rotational dynamics are best understood within the framework of statistical mechanics. This molecular turbine effectively converts the energy from the proton gradient into the chemical energy of ATP, mirroring how a watermill transforms the energy of falling water into mechanical work.

standing of biological systems but also has potential applications in other fields beyond biology (plasma physics, astrophysics, turbulence and classical mechanics).

This thesis explores three physical systems connected to a non-equilibrium thermostat [13, 14, 23], emphasizing rotational motion and angular momentum. Magnetic fields can impact non-equilibrium systems, creating rotating NESS for charged particles and inducing NESS in thermostats based on their non-equilibrium traits [13, 14]. Furthermore, non-equilibrium states with kinetic origins unveil unique stochastic dynamics of angular momentum [23].

We investigate the effects of weak magnetic fields on living organisms, addressing the credibility and reproducibility of experimental reports [24–27]. The physical mechanisms underlying these effects in molecular biology remain unclear [28–30]. We propose a mechanism for the influence of weak magnetic fields on the stochastic motion of ions, crucial in biological processes [9, 31], showing that ions acquire non-zero average angular momentum when equilibrium is disrupted by active processes.

Further, we revisit the Bohr-van Leeuwen theorem by examining a classical charged Brownian particle interacting with an equilibrium thermal bath. Although the particle does not "feel" the magnetic field per the theorem, its interaction with the bath induces non-equilibrium states in the bath. Using the Caldeira-Leggett model, we show that a magnetic field induces long-term changes in the bath, leading to average angular momentum in uncharged bath oscillators [8, 11, 32–34].

Our final investigation examines the persistence of rotation in systems where the confining potential is not perfectly symmetrical, leading to the decay of angular momentum. We extend the question of integrals of motion under weak perturbations [35, 36], deriving a coarse-grained stochastic differential equation describing the decay of angular momentum. Our results align with numerical simulations, enhancing the understanding of integrals of motion in weakly perturbed systems.

Relevance of the research topic

The research topic presented in the thesis, focusing on the non-equilibrium statistical mechanics of rotating systems, is of significant relevance for several reasons:

- **Biological Implications of Magnetic Fields.** The study of weak magnetic fields' effects on biological systems is crucial for understanding magnetobiology and its implications for cellular processes and medical applications [13, 24].
- **Advancement in Non-Equilibrium Physics.** This research contributes significantly to non-equilibrium physics by exploring systems far from equilibrium and elucidating the role of fluctuation-dissipation theorems, bridging the gap between macroscopic and microscopic descriptions [4, 14, 18].
- **Conservation Laws.** Understanding the behavior of conserved quantities, such as angular momentum, in systems with weakly violated symmetries is vital for refining our understanding of symmetry and conservation laws in physical systems [13, 14, 35, 36].
- **Practical Applications.** The practical applications of this research range from biomedical diagnostics and therapeutics to nanoscale device design, industrial process optimization, and advancements in aerospace engineering and robotics [13, 14, 16].
- **Future Research Directions.** Future research directions include determining the adiabatic invariant in rotating systems, refining the Caldeira-Leggett model to incorporate the Generalized Gibbs distribution, and exploring fluctuation-dissipation relations in active matter systems, offering new theoretical insights and practical advancements in various scientific and engineering disciplines.

In summary, this research addresses fundamental questions in statistical mechanics and thermodynamics, offering new insights into non-equilibrium phenomena and the effects of magnetic fields. The implications span from biological systems to advanced technologies, making this an essential area of study for both theoretical and applied physics.

The aims of the thesis

- **Equilibrium vs. Non-Equilibrium:** This thesis explores the complex dynamics of non-equilibrium systems influenced by external perturbations, bridging the gap between equilibrium and non-equilibrium statistical mechanics using tools like the Langevin and Fokker-Planck equations [4, 6].
- **Magnetic Field Effects and Magnetobiology:** Investigating the influence of weak magnetic fields on non-equilibrium biological systems, this research proposes a mechanism where ions accumulate angular momentum, potentially altering protein functions and explaining observed magnetic field effects in biology [13, 24].
- **Angular Momentum and Conservation Laws:** Focusing on the dissipation of angular momentum in nearly symmetric systems, this thesis derives a stochastic differential equation for its behavior, extending the Caldeira-Leggett model to provide a microscopic foundation for macroscopic observations in rotating systems [22, 23].

Scientific novelty.

The scientific novelty of this thesis lies in its significant contributions to the field of non-equilibrium statistical mechanics, particularly in the context of magnetobiology and rotating systems. Here are the key points of novelty:

- **Explaining the effects of weak magnetic fields on biological systems:** This research proposes a new mechanism for weak magnetic fields influencing ion motion in biological systems, potentially altering protein function. This mechanism addresses the gap in understanding magnetobiological effects, often overshadowed by thermal fluctuations, thereby advancing the field of magnetobiology [13, 27].

- **Long-term impact of magnetic fields on thermostats:** By extending the Caldeira-Leggett model to include the effects of an external magnetic field, this study demonstrates that magnetic fields induce a non-equilibrium steady state in the bath oscillators, challenging the traditional view that magnetic fields have no effect on equilibrium states [14, 32–34].
- **Stochastic dynamics of angular momentum in weakly rotationally symmetric systems:** Introducing a novel stochastic differential equation to describe the decay of angular momentum in systems with weakly violated rotational symmetries, this research provides new insights into the persistence and dissipation of angular momentum, validated through numerical simulations [23, 35, 36].

Overall, these findings push the boundaries of our understanding in non-equilibrium statistical mechanics, with implications across diverse fields from biophysics to materials science.

Practical and theoretical significance.

The research presented in this thesis holds significant theoretical and practical importance. Theoretically, it advances our understanding of non-equilibrium statistical mechanics, especially in the context of rotational systems and the effects of magnetic fields. By challenging the constraints of the Bohr-van Leeuwen theorem, the work opens new avenues for exploring how classical systems can exhibit magnetism when driven out of equilibrium [13, 14, 23]. Practically, the findings have profound implications for fields such as magnetobiology, where the observed non-equilibrium rotation of ions under weak magnetic fields offers a plausible mechanism for altering protein functions, potentially explaining many experimentally observed yet poorly understood phenomena in living organisms [24, 27]. Additionally, the insights gained into the behavior of thermostats and the conservation of angular momentum in nearly symmetric systems could influence the design and analysis of molecular machines and other technologies reliant on rotational dynamics [22]. Thus, this research not only bridges fundamental gaps in our understanding of thermodynamics and statistical mechanics but also provides a basis for future technological innovations.

Approbation of the work.

The results of the thesis were reported at the conferences ”4-th MATINYAN Seminar” (Yerevan, 2022), ”5-th MATINYAN Seminar” (Yerevan, 2023) and have been discussed at the seminars of the Alikhanian National Science Laboratory.

Publications.

Three papers are published on the topic of the thesis [13, 14, 23].

Structure of the thesis.

The thesis consists of an introduction, three additional Chapters, a conclusion and a list of references. It contains 130 pages, including 16 figures.

CONTENT OF THE THESIS

Introduction

We reviewed the scientific literature related to the topic of the thesis. We established a high-level overview of the research and provided the general aims of the study. Moreover, scientific significance, novelty and practical value are also established. Short overview is provided for widely used topics in the thesis, such as Langevin and Fokker-Planck equations, Bohr-van Leeuwen theorem and Caldeira-Leggett model. The thesis is organized into chapters and they can be read independently.

Chapter 1

§1.1: Introduction

The introduction discusses the controversial effects of weak, static magnetic fields on biological systems, often supported by irreproducible experiments [25–27]. Significant effects of weak diamagnetism in biological systems occur only at high magnetic fields ($\sim 20\,\mathrm{T}$). Though theories suggest weak fields could influence ion motion [9], the minimal theoretical impact is due to the large disparity between friction-induced relaxation time (less than 10^{-9} s) and the magnetic timescale (greater than 10^{-3} s) [28, 30]. This study proposes mechanisms for weak magnetic fields to influence ion motion by including cellular white noise, sustaining cyclotron motion, and affecting cation-driven protein processes [37], bypassing the Bohr-van Leeuwen theorem. It also explores stochastic trajectories and autocorrelation functions, examining overdamped and underdamped regimes with the thermal bath's memory effects.

§1.2: The Model

This section examines the Langevin equation for ions in external potentials generated by membranes or proteins, disregarding electrostatic interactions between ions to focus on thermal bath interactions and external forces [9]. The Langevin equation, normalized by mass m, incorporates terms for friction with memory, potential gradient forces, Lorentz force from an external magnetic field $\boldsymbol{B}$, an equilibrium thermal noise $\boldsymbol{\eta}(t)$, and a non-equilibrium noise $\boldsymbol{\xi}(t)$ from fluctuating potentials [6, 38, 39]:

$$\dot{\boldsymbol{v}}(t) = -\gamma \int_{t_0}^{t} \mathrm{d}t' \kappa \mathrm{e}^{-\kappa|t-t'|} \boldsymbol{v}(t') - \nabla_{\boldsymbol{r}} V(\boldsymbol{r}) + \frac{Q}{m} \boldsymbol{v} \times \boldsymbol{B} + \frac{1}{m} \boldsymbol{\eta}(t) + \frac{1}{m} \boldsymbol{\xi}(t) , \tag{1}$$

The Gaussian noises $\boldsymbol{\eta}(t)$ and $\boldsymbol{\xi}(t)$ have defined properties, with $\boldsymbol{\eta}(t)$ adhering to the fluctuation-dissipation relation (FDR): it has autocorrelation $\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij} q\,(\theta/2) \exp(-\kappa\,|t-t'|)$ with intensity $q = 2m\gamma k_B T$, ensuring noise correlation and friction memory share the same exponential decay [38, 39].

Estimates of model parameters are given, which help to elucidate the physical behavior of the ions in these conditions.

§1.3: Diamagnetism in Harmonic Potential

This section discusses the transition from the Langevin equation (1) to the Fokker-Planck (FP) equation to determine the stationary regime for a particle, where the probability density of ion motion becomes time-independent [6, 39]. In the context of a confining harmonic potential, this stationary state is achieved swiftly, within approximately 10^{-9} seconds. For a magnetic field along the z-axis ($\boldsymbol{B} = \hat{\boldsymbol{e}}_z b$), we get the key result

$$\langle L \rangle = -b \frac{q_{\mathrm{w}}}{\gamma m^2 \kappa^2} , \tag{2}$$

(a)
(b)
(c)
(d)

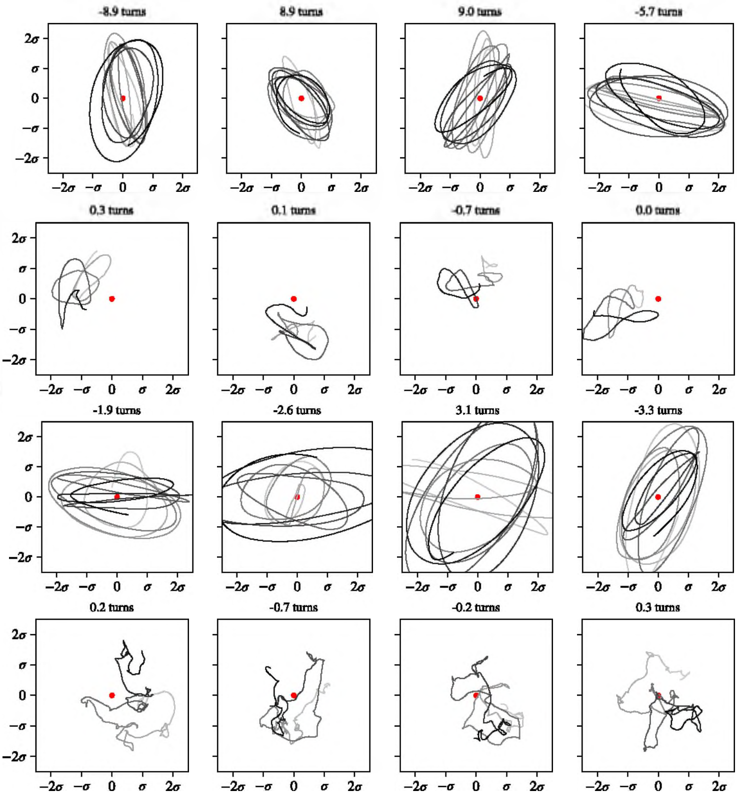

Figure 2: Random trajectories in the (x, y) plane. The darker (brighter) points refer to recent (earlier) times, total trajectory time is τ, $\sigma \equiv \sqrt{\langle x^2 \rangle} = \sqrt{\langle y^2 \rangle}$. **(a)** underdamped due to memory: $b = 1, \gamma = 100, \kappa = 10, \omega_0 = 90, \tau = 30$, **(b)** moderately damped: $b = 1, \gamma = 100, \kappa = 10, \omega_0 = 10, \tau = 30$, **(c)** underdamped due to strong potential confinement: $b = 1, \gamma = 100, \kappa = 1000, \omega_0 = 1000, \tau = 3$, and **(d)** overdamped: $b = 1, \gamma = 100, \kappa = 1000, \omega_0 = 20, \tau = 30$.

together with expressions form $\langle v_x^2 + v_y^2 \rangle$ and $\langle x^2 + y^2 \rangle$. These results indicate a diamagnetic response, where $\langle L \rangle / B < 0$. The magnetic moment is given by $\mathcal{M}_c = -\frac{q_w}{q} \frac{k_B T Q^2 B}{m^2 \kappa^2}$. Comparison with quantum diamagnetic and paramagnetic moments indicates that while $\mathcal{M}_c$ is smaller than the electronic diamagnetic moment of water, it may exceed the spin paramagnetic moment at the same temperature [12].

§1.4: Autocorrelation, Characteristic Times, and Numerical Results

In this section, the stochastic motion of an ion in a harmonic potential with a magnetic field is studied using the complex coordinate $\zeta = x + \mathrm{i}y$, where rotations in the xy plane are described by the phase of ζ. The autocorrelation function $\langle \zeta(t_1) \zeta^*(t_2) \rangle$ is derived, showing that the ion's motion can be distinguished between underdamped (rotational) and overdamped regimes based on the roots of the characteristic equation.

Numerical solutions using the Euler-Maruyama method [39] are presented, showing the influence of parameters such as κ, γ, and ω_0 on the ion's trajectory. Various regimes are visualized: underdamped due to memory (Figure 2 (a)), moderately damped (Figure 2 (b)), underdamped due to strong potential confinement (Figure 2 (c)), and overdamped (Figure 2 (d)). The spread of the angle variable (turns) $\int_0^t \Omega(s)\, ds$ is used to visualize these different behaviors across figures.

§1.5: Summary

In this section, the chapter is summarized. Future research directions include the study of stochastic cyclotron motion fluctuations, the metastability of nonequilibrium states, resonance phenomena under time-dependent fields, electrostatic interactions between ions, and potential applications to active matter and ion channels, especially in the context of COVID-19 related research [9, 28, 29].

Chapter 2

§2.1: Introduction

The introduction introduces the concept and sets the stage for a detailed exploration of how a static magnetic field can influence the random motion of particles in a fluid, a phenomenon that is central to understanding various biological and physical processes.

According to Bohr-van Leeuwen (BvL) theorem, charged classical particles do not experience magnetic fields in equilibrium, implying that equilibrium magnetic influences should be explained by quantum mechanics [2, 10, 40]. This theorem precludes equilibrium classical magnetism, which has potential applications in fields such as plasma physics and biophysics, where magnetic fields influence systems like fusion research, charged colloidal liquids, and biological processes involving metal ions (Na^+, K^+, Ca^{2+}) crucial for molecular biology [9, 25, 27, 28, 31]. Biophysical responses to static magnetic fields might be looked for in the quantum domain, however, it is not likely that all biophysical influences of magnetic fields can be accounted for by quantum models [28]. Classical effects of a static magnetic field on the Brownian motion of a charged particle, described by the Langevin equation, are investigated using the Caldeira-Leggett model [8, 11, 32–34]. The study reveals that the magnetic field induces long-term changes in the bath state, such as a sizable average angular momentum in bath oscillators, distinct from linear momentum and energy behaviors [8,41]. This analysis extends to understanding the behavior of angular momentum, linear momentum, and energy at the system-bath interface, emphasizing that while the bath can store angular momentum long-term, linear momentum is eventually dissipated from its observables.

§2.2: The Model

This section presents the Caldeira-Leggett model, which we use to describing the motion of ions in external potentials within a biological context [8, 11, 32–34]. We consider a classical particle with position vector $\boldsymbol{R}$, unit charge, and unit mass interacting with a magnetic field $\boldsymbol{B}$. Subject to a rotation-symmetric harmonic potential, the particle's Lagrangian is

$$\mathcal{L}_S = \frac{1}{2}\dot{\boldsymbol{R}}^2 - \frac{1}{2}\omega_0^2 \boldsymbol{R}^2 + \boldsymbol{A}(\boldsymbol{R})\dot{\boldsymbol{R}}\,, \tag{3}$$

where vector potential $\boldsymbol{A}(\boldsymbol{R})$ generates a static, homogeneous magnetic field $\boldsymbol{B} = \operatorname{curl}\boldsymbol{A}$. The particle couples to a bath of N harmonic oscillators with coordinates $\boldsymbol{r}_k$, masses m_k, frequencies ω_k. The potential energy of the particle-bath interaction is assumed to be bilinear with coupling constants c_k. Thus, the bath+interaction Lagrangian reads

$$\mathcal{L}_B = \sum_{k=1}^{N} \left[\frac{m_k}{2}\dot{\boldsymbol{r}}_k^2 - \frac{m_k\omega_k^2}{2}\left(\boldsymbol{r}_k - \frac{c_k \boldsymbol{R}}{m_k\omega_k^2}\right)^2 \right], \tag{4}$$

And the full Lagrangian is $\mathcal{L} = \mathcal{L}_S + \mathcal{L}_B$. Due to rotational symmetry around the axis of uniform $\boldsymbol{B}$, there is a modified angular momentum conservation.

Solving the Euler-Lagrange equations, we derive a Langevin equation for the particle, incorporating a friction kernel $\zeta(t)$ and noise $\boldsymbol{\xi}(t)$ due to the bath's random initial state. Given the initial Gibbsian density of the bath and the arbitrary initial density of the particle, a fluctuation-dissipation relation $\langle \xi_\alpha(t)\xi_\beta(t')\rangle = T\delta_{\alpha\beta}\zeta(t-t')$ holds.

In the thermodynamic limit with $N \to \infty$, and under a dense frequency limit $\delta\omega \to 0$ and weak coupling $c_n \to 0$, an Ohmic friction and white noise are reproduced in the Langevin equation by the specific choice $\omega_n = \delta\omega\, n$ and $c_n = \sqrt{2\gamma\omega_n^2 m_n \delta\omega/\pi}$.

§2.3: The Bohr-van Leeuwen theorem

This section discusses the Bohr-van Leeuwen theorem, which states that in classical mechanics, static magnetic fields have no effect on the net magnetization of electrons in thermal equilibrium [2, 10, 40]. The theorem highlights the necessity of quantum mechanics to explain magnetic phenomena, as classical physics cannot account for magnetism. It also mentions that the theorem does not apply to non-equilibrium steady states, allowing for magnetization in classical mechanics under certain conditions [13].

The fluctuation-dissipation relation ensures that the particle's state, governed by the Langevin equation, relaxes to a Gibbsian density [8, 11, 32–34]. This steady-state density is proportional to $\exp\left(-\frac{1}{2}(\boldsymbol{V}^2 + \omega_0^2\boldsymbol{R}^2)/T\right)$ and notably does not include the magnetic field $\boldsymbol{B}$. Consequently, the average angular momentum calculated with respect to steady-state distribution is zero, illustrating the Bohr-van Leeuwen theorem for Brownian motion. This exclusion of the magnetic field $\boldsymbol{B}$ from the equilibrium density applies to any confining potential [10, 40].

§2.4: Angular momentum of bath modes

This section discusses the angular momentum of bath modes, which are the collective motions of particles in a fluid that act as a thermal bath. Writing position $\boldsymbol{R} = (X, Y, Z)$, se start from a initial distribution with the following moments:

$$\left\langle X^2\right\rangle = \left\langle Y^2\right\rangle = \sigma_X\, T/\omega_0^2, \quad \left\langle V_x^2\right\rangle = \left\langle V_y^2\right\rangle = \sigma_V\, T, \tag{5}$$

where $\sigma_X = \sigma_V = 1$ refers to the equilibrium second moments of the initial state.

The long-time average angular momentum $L(\omega)$ (the component along the magnetic field $\boldsymbol{B}$) of a bath oscillator with frequency $\omega = \omega_k$ evaluates to

$$L(\omega) = \delta\omega\, \frac{4\gamma|\boldsymbol{B}|T}{\pi} \times \frac{(\omega^2-\omega_0^2)\left((1-\sigma_V)\omega^2 + (1-\sigma_X)\omega_0^2\right)}{\left((\omega^2-\omega_0^2-b\omega)^2+\gamma^2\omega^2\right)\left((\omega^2-\omega_0^2+b\omega)^2+\gamma^2\omega^2\right)}. \tag{6}$$

This shows that even though bath oscillators are not charged, they acquire a non-zero angular momentum. This means that the long-time state of the bath feels the magnetic field $\boldsymbol{B}$. The dependence of the angular momentum on the oscillator frequency is plotted in Figure 3.

We emphasize that $L(\omega) \neq 0$ due to initially non-equilibrium state of the particle, since $L(\omega) = 0$ whenever $\sigma_X = \sigma_V = 1$; cf. (6). Next, we confirm that (6) is consistent with the average angular momentum conservation (2.4) between $t = 0$ and $t = \infty$:

$$\int_0^\infty \mathrm{d}\omega\, L(\omega) = -\frac{Tb(1-\sigma_X)}{\omega_0^2} = |\boldsymbol{B}|\, [\langle X^2\rangle_0 - \langle X^2\rangle_\infty], \tag{7}$$

where $\langle X^2\rangle_0$ and $\langle X^2\rangle_\infty$ are the initial and final values; cf. (5). Even for $\sigma_X = 1$ we can have $L(\omega) \neq 0$ due to $\sigma_V \neq 1$ in (6). Hence, $L(\omega) \neq 0$ need not be driven by the conservation law; see Fig. 3. Now $L(\omega)$ changes its sign at $\omega = \omega_0$ and goes to zero as $\sim \omega^{-4}$ for $\omega \gg \max[\omega_0, \gamma, b]$; i.e. two sets of oscillators rotate in different directions, as Fig. 3 shows.

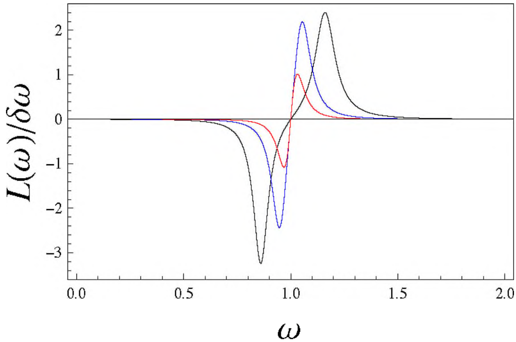

Figure 3: $L(\omega)/\delta\omega$ versus ω for $T = 1$, $\omega_0 = 1$, $\gamma = 0.1$, $\sigma_X = 1$, $\sigma_V = 0.1$; cf. (6, 5). Curves refer to different magnetic fields (2.2) (from bottom to top): $\boldsymbol{B} = 0.3$ (black), $\boldsymbol{B} = 0.1$ (blue), $\boldsymbol{B} = 0.03$ (red).

§2.5: Energy of bath modes

This section delves into the magnetic field's influence on interaction-induced corrections to the energy of a bath mode. The average energy $E(\omega_k)$ of the bath mode with frequency $\omega = \omega_k$ is defined as

$$E(\omega_k) = \frac{m_k}{2}\left\langle \dot{\boldsymbol{r}}_k^2 \right\rangle + \frac{m_k\omega_k^2}{2}\left\langle \boldsymbol{r}_k^2 \right\rangle + \left\langle \boldsymbol{R}^2 \right\rangle \frac{c_k^2}{2m_k\omega_k^2} - c_k \left\langle \boldsymbol{R}\cdot\boldsymbol{r}_k \right\rangle, \tag{8}$$

where the averages are taken over the initial distribution. The full conserved energy of the particle plus the bath is the sum of $E(\omega_k)$ over all modes, plus the mean energy $\langle \frac{1}{2}\dot{\boldsymbol{R}}^2 + \frac{\omega_0^2}{2}\boldsymbol{R}^2\rangle$ of the particle. In the limit $t \to \infty$, $E(\omega)$ is derived as

$$E(\omega) \;=\; 3T - \delta\omega\left(2\varepsilon(\omega) + \varepsilon(\omega)|_{B=0}\right), \qquad \text{where} \tag{9}$$

$$\varepsilon(\omega) \;=\; \frac{T\gamma}{2\pi} \times \frac{\omega^2(b^2+\gamma^2) + \left(\omega^2-\omega_0^2\right)^2}{(\omega^2-\omega_0^2-b\omega)^2+\gamma^2\omega^2}\,\frac{(1-\sigma_V)\omega^2+(1-\sigma_X)\omega_0^2}{(\omega^2-\omega_0^2+b\omega)^2+\gamma^2\omega^2}. \tag{10}$$

The thermal energy $3T$ is consistent with the equipartition theorem. The interaction-induced factor proportional to $\delta\omega$ comprises $2\varepsilon(\omega)$ from the (x, y)-components influenced by the magnetic field $\boldsymbol{B}$, and $\varepsilon(\omega)|_{B=0}$ from the z-component. This factor vanishes for $\sigma_X = \sigma_V = 1$. Thus, the long-term mean energy of the mode, in contrast to the particle's mean energy, exhibits a magnetic field dependence, albeit weaker than the dependence observed in (6), where the magnetic field effect predominates due to the zero angular momentum without interaction. The interaction-driven term in $E(\omega)$ represents a small correction to the leading term $2T$.

§2.6: Linear momentum

The conservation of linear momentum in a Brownian particle system is explored by analyzing how the linear momentum is transferred from the particle to the bath. The study reveals that for a free Brownian particle ($\omega_0 = \mathbf{B} = 0$), the linear momentum conservation is expressed as $\frac{\mathrm{d}}{\mathrm{d}t}\left[\sum_{k=1}^{N} \frac{c_k}{\omega_k^2} \dot{\boldsymbol{r}}_k(t) + \boldsymbol{V}(t)\right] = 0.$, where $\boldsymbol{V}(t)$ is the momentum of the Brownian particle and $\frac{c_k}{\omega_k^2}\dot{\boldsymbol{r}}_k(t)$ is part of the mode's momentum $m_k\dot{\boldsymbol{r}}_k$. For long times, the particle's velocity thermalizes, but its position does not. The average linear momentum of a bath mode, $\frac{c_k}{\omega_k^2}\langle\dot{\boldsymbol{r}}_k\rangle$, oscillates over time. When considering the collective momentum in the thermodynamic limit, the integral $\sum_{\omega_1}^{\omega_2} \frac{c_k}{\omega_k^2}\langle\dot{\boldsymbol{r}}_k\rangle$ shows that the collective momentum for non-zero frequencies decays as $O(t^{-1})$ for large times. However, the total bath momentum remains non-zero and equals the initial particle momentum $\langle\boldsymbol{V}(0)\rangle$, as derived from $\sum_{k=1}^{N} \frac{c_k}{\omega_k^2}\dot{\boldsymbol{r}}_k(t) = \langle\boldsymbol{V}(0)\rangle$. This suggests that the momentum is transferred to the zero-frequency mode, resulting in no observable motion for long times.

Comparison with angular momentum reveals key differences: single mode angular momentum converges to a time-independent value, while linear momentum oscillates and dissipates in the long-time limit.

§2.7: Brownian charge in viscous fluid

This section investigates the behavior of a spherical Brownian charge (radius a) in an incompressible viscous fluid. We write the Navier-Stokes equation [42], where the center of mass $\boldsymbol{R}$ of the particle follows the Langevin equation. The fluid's velocity field $\boldsymbol{u}(\boldsymbol{r},t)$ satisfies

$$\partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\nabla\hat{p} + \nu\nabla^2\boldsymbol{u} \quad \text{with} \quad \nabla\cdot\boldsymbol{u} = 0 \tag{11}$$

and the boundary condition $\boldsymbol{u}(\boldsymbol{r},t) = \dot{\boldsymbol{R}}(t) \equiv \boldsymbol{V}(t)$ on the surface of the sphere ($|\boldsymbol{r}-\boldsymbol{R}(t)| = a$) [42]. Assume the Reynolds number $\mathrm{Re} = |\boldsymbol{V}|a/\nu \ll 1$ and the product $\mathrm{St}\cdot\mathrm{Re} \ll 1$, with Strouhal number $\mathrm{St} = a/(\tau|\boldsymbol{V}|)$, where τ is a characteristic time of the Brownian motion. Then the Stokes flow approximation yields $\boldsymbol{u}(\boldsymbol{r},t) = \hat{\boldsymbol{u}}(\boldsymbol{r}-\boldsymbol{R}(t),t)$ [42], where

$$\hat{\boldsymbol{u}}(\boldsymbol{r},t) = \frac{3}{4}\frac{a}{r}\left(\left(1+\frac{a^2}{3r^2}\right)\boldsymbol{V}(t) + \left(1-\frac{a^2}{r^2}\right)\frac{(\boldsymbol{V}(t)\cdot\boldsymbol{r})\boldsymbol{r}}{r^2}\right). \tag{12}$$

Integrating the average flow over time results in a non-zero net displacement of the fluid, described by $\int_0^\infty \langle\boldsymbol{u}(\boldsymbol{r},t)\rangle \mathrm{d}t = -\frac{3a}{4r^3}\frac{T(1-\sigma_x)}{\omega_0^2}\frac{1}{\gamma}(\boldsymbol{B}\times\boldsymbol{r})$, despite the equilibrium state yielding $\langle\boldsymbol{u}(\boldsymbol{r},t)\rangle = 0$.

§2.8: Summary

This section provides a concise summary of the findings of Chapter 2. The main unresolved question is whether these findings are specific to the Caldeira-Leggett model, which is pertinent for liquid descriptions [8], or if they extend to more realistic bath models. Preliminary hypotheses suggest that the non-spontaneous nature of bath angular momentum might persist in more general models due to the conservation law, whereas the spontaneous aspect could be unique to linear models.

Chapter 3

§3.1: Introduction

The conservation of angular momentum modifies the equilibrium statistical mechanics, described by a microcanonical density that includes angular momentum conservation and a generalized Gibbs distribution for subsystems [2]. Practical applications include rotary molecular motors, like the ATP synthase enzyme, rotating atomic clusters, and classical Brownian charges under magnetic fields [14, 22]. The study aims to extend insights into turbulence, where large vortices decay into smaller ones due to viscous forces, and relate to the Kolmogorov-Arnold-Moser theorem on integrable systems [17,35,36].

This section introduces the idea of canonical and microcanonical distributions, as well as establishing their equivalence for non-rotating thermodynamics systems.

§3.2: Mesoscopic description of the system

This section delves into the intermediate scale between microscopic and macroscopic levels, where the behavior of systems is described in terms of collective variables. This mesoscopic approach is crucial for understanding the weak non-conservation of angular momentum in the context of statistical mechanics, particularly when the systems is not in equilibrium.

The ergodic microcanonical ensemble $\delta(E - H(\zeta))$ with ζ the phase-space coordinates, where only the total energy is conserved, corresponds to the Gibbs canonical distribution $\exp(-\beta H_{\text{sub}}(\zeta_{\text{sub}}))$ for subsystem phase-space coordinates ζ_{sub}, with $\beta = T^{-1}$ inverse temperature. A single particle in a closed system is described by the Langevin equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r} = \boldsymbol{v}\,, \quad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{v} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}) - \gamma \boldsymbol{v} + \sqrt{2\gamma T}\,\boldsymbol{\xi}(t)\,, \quad \langle \boldsymbol{\xi}_i(t)\boldsymbol{\xi}_j(t')\rangle = \delta_{ij}\,\delta(t-t')\,, \tag{13}$$

combining deterministic friction $-\gamma\boldsymbol{v}$ and stochastic white noise $\sqrt{2\gamma T}\,\boldsymbol{\xi}(t)$, where γ and noise amplitude satisfy the Fluctuation-Dissipation relation [6]. The subsystem Hamiltonian $H_{\text{sub}}(\zeta_{\text{sub}}) = \frac{\boldsymbol{v}^2}{2} + V(\boldsymbol{r})$ leads to the canonical distribution as the stationary solution [6]. Extending this to a particle in a rotating environment with angular velocity $\boldsymbol{\Omega} = \hat{\boldsymbol{e}}_z\Omega$ and temperature T, the Langevin equation (13) is modified to

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r} = \boldsymbol{v}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{v} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}) - \gamma\,(\boldsymbol{v} - \boldsymbol{\Omega}\times\boldsymbol{r}) + \sqrt{2\gamma T}\,\boldsymbol{\xi}(t)\,, \tag{14}$$

accounting for local equilibrium and isotropic thermal noise by adjusting the friction term to $\gamma(\boldsymbol{v} - \boldsymbol{\Omega}\times\boldsymbol{r})$. Through the corresponding Fokker-Planck equation, we confirm that the modified canonical distribution $\rho_{\text{c}}(\zeta_{\text{sub}}) \propto \exp\left(-\beta\, H_{\text{sub}}(\zeta_{\text{sub}}) - \alpha\, L_{z,\text{sub}}(\zeta_{\text{sub}})\right)$ is a stationary solution if potential $V(\boldsymbol{r})$ is rotation symmetric, indicating consistency with the rotational framework.

The model's limitations include the typically constant phenomenological friction coefficient γ, which realistically depends on temperature and density, increasing with temperature due to more frequent particle collisions, as observed in the temperature-dependent viscosity of the Lennard-Jones gas [43]. We also study the case of space-dependent $\gamma(\boldsymbol{r})$.

§3.3: Weak non-conservation of angular momentum

We investigate the dynamics of N interacting particles subjected to an external potential $V(\boldsymbol{r}) = \frac{1}{2}\left(a^2(1+\epsilon)^2\,x^2 + a^2(1-\epsilon)^2\,y^2 + a_z^2\,z^2\right)$, where $\epsilon \neq 0$ breaks the rotational symmetry around the z-axis, leading to a non-conservation of the angular momentum component L_z.

We consider weak pairwise interactions via translationally and rotationally invariant potentials $\sum_{i<j} \mathcal{U}(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$ and this makes the system ergodic so that it will approach equilibrium. Deriving from the Newton equations, the rate of change of L_z is shown to depend on the external potential's torque, yielding $\frac{dL}{dt} = 4a^2\epsilon\sum_{i=1}^{N} x_i y_i$ where $(x_i, y_i, z_i) \equiv \boldsymbol{r}_i$ is the position of i-th particle. Assuming a separation of timescales, we express $\sum_i x_i y_i$ as a sum of its time-average term $\langle xy\rangle$ and a fluctuating term $h(t)$. For large N, the fluctuating term is approximated as Gaussian noise by the Central Limit Theorem. The deterministic part of $\frac{dL}{dt}$ depends on the time-averaged $\langle xy\rangle$, which is calculated to be non-zero due to ϵ. The decay rate of L is derived as $\tau_L \propto \epsilon^{-2}$, assuming ergodicity and a quasi-stationary distribution for the system. Furthermore, fluctuations are characterized by

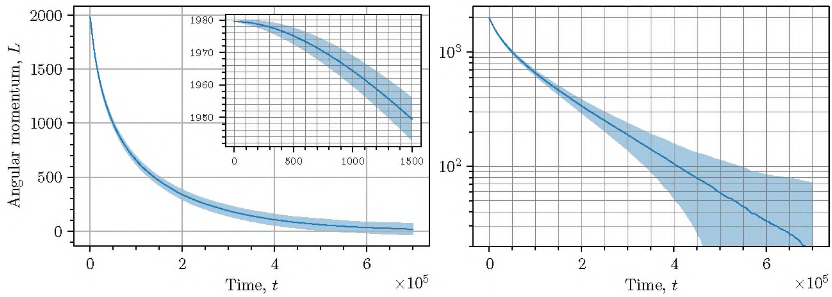

Figure 4: This figure illustrates the relaxation of total angular momentum L. The solid line is the ensemble average over 1200 simulations with the same initial E and L. The shaded region surrounding the line corresponds to one standard deviation of the values within the ensemble. The inset shows the relaxation just after the violation of the rotational symmetry. For a different perspective, the same plot is presented on the right side with a logarithmic scale.

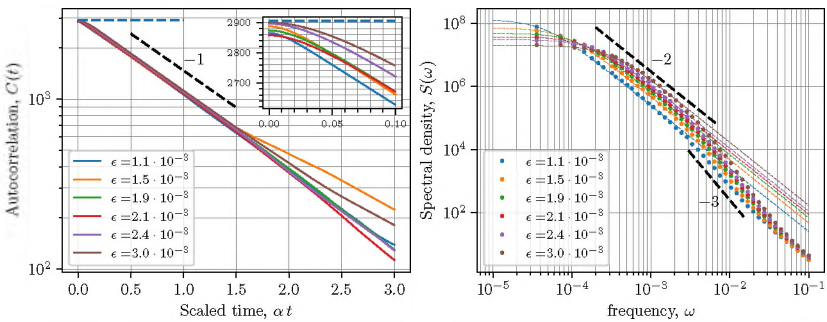

Figure 5: (left) Autocorrelation function of $L(t)$ in the steady state, when L fluctuates around 0. The horizontal axis corresponds to the time, scaled by decay rate α. The horizontal dashed line corresponds to the steady-state fluctuations, while the other dashed line denoted the -1 slope, demonstrating exponential decay of the autocorrelation function. Deviation from the slope is due to statistical noise. Inset provides a magnified view of the same plot at smaller times. **(right)** Calculated spectral density (points) is compared to the analytical Lorentzian spectral density. The discrepancy at high ω is due to short-time correlations of colored noise, which we assumed to be white in (15).

the autocorrelation function of $h(t)$, leading to a Langevin equation for $L = L_z$ that includes a drift term and a diffusion term with Gaussian noise:

$$\frac{\mathrm{d}}{\mathrm{d}t}L = \frac{4a^2\epsilon^2}{\gamma}\frac{2\Omega NT}{a^2-\Omega^2}\frac{a^2(a^2+\gamma^2)}{a^4+\gamma^2\Omega^2} + 4a^2\epsilon\sqrt{\frac{NT^2(a^2+\gamma^2)}{\gamma(a^2-\Omega^2)(a^4+\gamma^2\Omega^2)}}\,\xi_h(t). \tag{15}$$

This is a stochastic differential equation for L, but the right-hand side depends on Ω and T. In the next section, we derive the angular velocity and temperature as a function of the angular momentum: $\Omega(L)$ and $T(L)$, thus (15) will be a closed Langevin equation for L.

§3.4: Canonical and microcanonical distributions

This section explores the relationship between the microcanonical and canonical ensembles, particularly focusing on how the parameters of the microcanonical distribution L and E relate to the canonical parameters T and Ω to form a closed stochastic differential equation for L, c.f. (15). By considering a partitioned N-particle system into a subsystem and a bath, and leveraging the equivalence of ensembles under conditions such as $N \gg 1$, small subsystem energy, and weak subsystem-bath interactions, it is shown that the canonical distribution is a valid approximation of the marginalized microcanonical distribution for the subsystem [1,5]. The Hamiltonian of the system is expressed as $H = H_{\text{sub}} + H_{\text{bath}} + H_{\text{interaction}}$, with $H_{\text{interaction}}$ being negligible among the rest.

Using this framework, the conserved total energy E and angular momentum L are related to subsystem quantities T and Ω:

$$\Omega(L,E) = \frac{E}{L}\left(\sqrt{1+\frac{3a^2L^2}{E^2}}-1\right) \quad \text{and} \quad T(L,E) = \frac{E}{3N}\left(2-\sqrt{1+\frac{3a^2L^2}{E^2}}\right), \tag{16}$$

This illustrates that temperature increases as angular momentum decays when angular momentum decays with conserved energy, indicating a conversion of rotational motion into chaotic motion. Furthermore, during relaxation, the system monotonically contracts in the x-y plane but expands along the z direction.

§3.5: Numerical Simulations

This section presents our results from molecular dynamics simulations validating mesoscopic descriptions (14). We simulate 523 particles in an external quadratic potential with weak Lennard-Jones interactions. The ensemble equivalence at low densities is established, while it breaks down at high densities due to strong interactions and non-Gaussian distributions.

We also examine the relaxation of angular momentum under anisotropic potentials (Figure 4) and find that the friction constant γ evolves, because the temperature of the system increases. We present various methods of estimation of phenomenological γ coefficient from the numerical simulations.

We further investigate angular momentum fluctuations, deriving autocorrelation and spectral density functions, which match analytical predictions, wee Figure 5.

§3.6: Summary

This section provides a concise summary of the findings of Chapter 3 and sets up the future research directions, which include exploring non-uniform friction constants, collisionless relaxation scenarios, and the implications of trivial microcanonical ensembles, while also considering practical applications like work extraction from rotating systems and determining the correct adiabatic invariant for such systems.

CONCLUSIONS

This thesis investigates a range of non-equilibrium phenomena influenced by magnetic fields. Our exploration begins with the contentious topic of weak magnetic fields affecting living organisms. The primary challenge lies in the competition between weak magnetic fields and strong thermal fluctuations within the cellular environment. By closely examining the stochastic movements of ions under weak static magnetic fields, we reveal that ions can accumulate a certain average angular momentum. This rotational motion is proposed as a mechanism for altering protein function, potentially explaining observed phenomena in magnetobiology.

Next, we delve into the interaction of charged particles with a thermal environment. Using the Caldeira-Leggett model to represent the thermal bath of numerous oscillators, we study the minimal influence of a charged particle on the thermostat. In the presence of an external magnetic field, the final equilibrium state of the particle does not sense the magnetic field, consistent with the Bohr-van Leeuwen theorem. However, during relaxation, the charged particle induces a non-equilibrium steady state (NESS) in the thermal bath. Uncharged bath oscillators acquire significant average angular momentum, segregating into two groups with different oscillation directions based on frequency. Thus, while the magnetic field's impact on the Brownian charge is imperceptible in equilibrium, it manifests in the surrounding environment over the long term.

Finally, we address the non-equilibrium statistical mechanics of rotating systems, focusing on the behavior of conserved quantities when symmetries are weakly violated. By investigating the non-conservation of angular momentum in nearly rotationally symmetric systems, we derive a stochastic differential equation for the total angular momentum and validate it through extensive numerical simulations. This work enhances our understanding of how minor imperfections in rotational symmetry affect the conservation and dissipation of angular momentum.

Our research has raised numerous intriguing questions for future investigation. The field of statistical thermodynamics in rotating systems, though well-established, still holds significant unanswered questions that warrant thorough exploration using modern statistical physics tools and methodologies. One key question involves identifying the adiabatic invariant in systems with multiple conserved quantities. In a microcanonical ensemble where only energy is conserved, the phase-space volume serves as the adiabatic invariant, with entropy linked to the logarithm of this volume. This principle extends to quantum systems, where the number of states is proportional to the state space volume. However, identifying the adiabatic invariant in rotating systems, where both energy and total angular momentum are conserved, remains a challenge. Our objective is to determine this invariant form in rotating systems.

Another promising direction is extending the Caldeira-Leggett model to accommodate the Generalized Gibbs distribution. The Caldeira-Leggett model provides a microscopic description of the thermostat, reproducing the Langevin equation. In Chapter 3, we extended the Langevin equation for rotating systems. Our next goal is to derive this Langevin equation from a microscopic model of a rotating bath, such as the Caldeira-Leggett model.

Additionally, I am exploring active matter, particularly the fluctuation-dissipation relations in active systems and their potential generalizations. Starting with a mesoscopic model that explicitly introduces activity, I aim to observe its effects on the macroscopic scale.

PUBLICATIONS IN THE TOPIC OF THESIS

(1) A. Matevosyan and A. E. Allahverdyan, “Nonequilibrium, weak-field-induced cyclotron motion: A mechanism for magnetobiology,” *Physical Review E*, vol. 104, no. 6, 2021.

(2) A. Matevosyan and A. E. Allahverdyan, “Lasting effects of static magnetic field on classical Brownian motion,” *Physical Review E*, vol. 107, no. 1, 2023

(3) A. Matevosyan, “Weak (non) conservation and stochastic dynamics of angular momentum,” *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2024, no. 5, 2024

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Մաթևոսյան Աշոտ Արթուրի

Ակտիվ ներբջջային պրոցեսների վիճակագրական մեխանիկան

Ամփոփագիր

Թերմոդինամիկան էմպիրիկ գիտություն է, որը մշակվել է Կարնոյի, Կլաուզիուսի և Քելվինի կողմից 19-րդ դարում: Այն նկարագրում է էներգիայի և նյութի փոխակերպումները քվազի-հավասարակշռված մակրոսկոպիկ համակարգերում՝ սահմանելով այնպիսի հիմնական հասկացություններ, ինչպիսիք են էնտրոպիան և անդարձելիությունը: Թերմոդինամիկական համակարգերը բաղկացած են միկրոսկոպիկ բաղադրիչներից, որոնք ունեն քվանտային կամ դասական դինամիկա, ինչը պահանջում է, որ ֆենոմենոլոգիական թերմոդինամիկայի հիմքերը հիմնված լինեն վիճակագրական մեխանիկայի վրա: Վերջինս կապում է մակրո և միկրո նկարագրությունները, ինչպես նաև նկարագրում է ֆիզիկայի ոչ հավասարակշիռ երևույթները:

Գիբսի բաշխումը առանցքային դեր ունի հավասարակշիռ վիճակագրական մեխանիկայում. այն կապ է հաստատում ֆազային տարածության մեջ բաշխման ֆունկցիայի և Համիլտոնյանի միջև:

Այս թեզը ուսումնասիրում է արտաքին հաստատուն մագնիսական դաշտերի ազդեցությունը, որոնք չեն ազդում դասական հավասարակշիռ համակարգերի վրա: Այսպիսով, այս թեզի երկրորդ նպատակն է բացահայտել բաց խնդիրները պտտվող համակարգերի վիճակագրական մեխանիկայում և ուսումնասիրել իմպուլսի մոմենտի ոչ հավասարակշռված մարումը:

Հավասարակշիռ դասական վիճակագրական մեխանիկայում հաստատուն մագնիսական դաշտերը ազդեցություն չունեն, քանի որ լորենցի ուժը աշխատանք չի կատարում: Հետևաբար, հավասարակշիռ բաշխումը անկախ է մագնիսական դաշտից: Այս պատկերացումը, որը հայտնի է որպես Բոր-վան Լյուվենի թեորեմ, ընդգծում է քվանտային մեխանիկայի անհրաժեշտությունը մագնիսականությունը բացատրելու համար: Այնուամենայնիվ, մագնիսական դաշտի ազդեցությունները կարելի է դիտարկել դասական մեխանիկայի շրջանակներում՝ խախտելով հավասարակշռության պայմանը:

Ոչ հավասարակշռության համակարգերը բազմազան են, օրինակ կենդանի օրգանիզմները, հոսող հեղուկները և քիմիական ռեակցիաները, ի թիվս այլ երևույթների: Գոյություն ունեն գործիքներ ոչ հավասարակշիռ համակարգերի ուսումնասիրության համար, ինչպիսիք են Լանժևինի և Ֆոկեր-Պլանկի հավասարումները: Այս հավասարումները բավարարում են ֆլուկտուացիոն-դիսիպացիոն թեորեմը (ՖԴԹ), որոնք սերտորեն կապում է հավասարակշիռ և ոչ հավասարակշիռ թերմոդինամիկան: ՖԴԹ-ը կապ է հաստատում հավասարակշիռ ֆլուկտուացիաների և փոքր արտաքին խոտորումների նկատմամբ համակարգի արձագանքի միջև: Նման օրինակ է Էյնշտեյնի առնչությունը դիֆուզիոն գործակցի համար:

Վերջին տարիներին կենդանի բջիջներում տեղի ունեցող գործընթացների ուսումնասիրությունը զգալի ուշադրություն է գրավել կենսաբանական գործառույթների և վարքագծի ըմբռնման համար դրա հիմնարար կարևորության պատճառով: Մեր աշխատանքի հիմնական մոտիվացիան ATPase-ի ֆունկցիան հասկանալն է՝ սպիտակուցային համակարգ, որը սինթեզում է էներգակիր ATP մոլեկուլները՝ բջջի էներգիայի միավորը: Նույնիսկ ATPase-ի ֆունկցիայի ամենափոքր

փոփոխությունը կարող է զգալիորեն ազդել ամբողջ օրգանիզմի աճի և ֆունկցիայի վրա: Պտույտը առանցքային դեր է խաղում ATPase-ի գործառույթում. պրոտոնների հոսքը խթանում է կենտրոնական ռոտորի պտույտը, որը հետագայում առաջացնում է կոնֆորմացիոն փոփոխություններ կատալիտիկ մասում՝ դրանով իսկ խթանում ATP-ի սինթեզը: Այնուամենայնիվ, նման միկրոսկոպիկ համակարգում պտույտը տեղի է ունենում ոչ թե զուտ մեխանիկական իմաստով, այլ ավելի շուտ պետք է հասկանալ և նկարագրել վիճակագրական մեխանիկայի սկզբունքների միջոցով:

Վիճակագրական մեխանիկայի խնդիրները հաճախ դիտարկում են մեծ համակարգ, որը բաժանված է ավելի փոքր ենթահամակարգի (այսուհետ «համակարգ») և ավելի մեծ քվազի-հավասարակշիռ ենթահամակարգի (այսուհետ «թերմոստատ»): Համակարգը փոխազդում է թերմոստատի հետ՝ փոխանակելով էներգիա, մասնիկներ, իմպուլս և իմպուլսի մոմենտ:

Այս թեզը ուսումնասիրում է երեք ֆիզիկական համակարգեր՝ փոխազդող ոչ հավասարակշիռ թերմոստատի հետ՝ կենտրոնանալով պտտվող շարժման և անկյունային իմպուլսի վրա: Մագնիսական դաշտերը կարող են ազդել ոչ հավասարակշիռ համակարգերի վրա այս կամ այն ձևերով: Բացի այդ, ոչ հավասարակշիռ վիճակները, որոնք ունեն կինետիկ ծագում, բացահայտում են անկյունային իմպուլսի յուրահատուկ ստոխաստիկ դինամիկա:

Մենք ուսումնասիրում ենք թույլ մագնիսական դաշտերի ազդեցությունը կենդանի օրգանիզմների վրա՝ անդրադառնալով փորձարարական հաշվետվությունների արժանահավատությանը և վերարտադրելիությանը: Մոլեկուլային կենսաբանության մեջ այս ազդեցությունների հիմքում ընկած ֆիզիկական մեխանիզմները մնում են անհասկանալի: Մենք առաջարկում ենք թույլ մագնիսական դաշտերի՝ իոնների ստոխաստիկ շարժման վրա ազդեցության մեխանիզմ: Այս իոնները կարևոր նշանակություն ունեն կենսաբանական գործընթացներում: Մենք ցույց ենք տալիս, որ իոնները ձեռք են բերում ոչ զրոյական միջին իմպուլսի մոմենտ, երբ հավասարակշռությունը խախտվում է ակտիվ գործընթացներով:

Այնուհետև, մենք վերանայում ենք Բոր-վան Լյուվենի թեորեմը՝ ուսումնասիրելով դասական լիցքավորված բրոունյան մասնիկը, որը փոխազդում է հավասարակշիռ թերմոստատի հետ: Թեև մասնիկը չի «զգում» մագնիսական դաշտը՝ ըստ թեորեմի, նրա փոխազդեցությունը թերմոստատի հետ առաջացնում է ոչ հավասարակշռված վիճակներ թերմոստատի համար: Օգտագործելով Կալդեիրա-Լեգետի մոդելը, մենք ցույց ենք տալիս, որ մագնիսական դաշտը առաջացնում է թերմոստատի երկարկյաց փոփոխություններ, որի հետևանքով թերմոստատի չլիցքավորված տատանակները ձեռք են բերում պտույտ:

Մեր վերջին հետազոտությունը ուսումնասիրում է պտտական համակարգերի կայունությունը, որտեղ արտաքին պոտենցիալը կատարյալ սիմետրիկ չէ, ինչը հանգեցնում է իմպուլսի մոմենտի մարմանը: Մենք ընդլայնում ենք շարժման ինտեգրալների հարցը թույլ խոտորումների դեպքում՝ ստանալով մակրոսկոպիկ ստոխաստիկ դիֆերենցիալ հավասարում, որը նկարագրում է իմպուլսի մոմենտի մարումը: Մեր արդյունքները համընկնում են թվային սիմուլյացիաների հետ՝ ընդլայնելով մեր պատկերացումները շարժման ինտեգրալների վերաբերյալ թույլ խոտորված համակարգերում:

Ашот Матевосян Артурович

Статистическая механика активных внутриклеточных процессов

Резюме

Термодинамика - эмпирическая наука, разработанная в 19 веке Карно, Клаузиусом и Кельвином, описывает превращения энергии и вещества в квазиравновесных макроскопических системах, вводя такие ключевые понятия, как энтропия и необратимость. Термодинамические системы состоят из микроскопических компонентов, управляемых квантовой или классической динамикой, что требует, чтобы основы феноменологической термодинамики основывались на статистической механике. Эта область объединяет макро- и микроописания и рассматривает неравновесные явления в физике.

Распределение Гиббса занимает центральное место в равновесной статистической механике, связывая вероятность состояний системы в фазовом пространстве с ее гамильтонианом, а термодинамические величины выводятся как средние значения по этому распределению.

В этой работе исследуется влияние внешних статических магнитных полей, которые не влияют на классические системы, находящиеся в термодинамическом равновесии. Неотъемлемая связь магнитного поля с вращением очевидна в классической электродинамике, где оно действует как псевдовектор, аналогичный моменту импульса. Таким образом, вторая цель данной работы - выявить открытые проблемы в статистической механике вращающихся систем и исследовать неравновесную релаксацию углового момента.

В равновесной классической статистической механике статические магнитные поля не оказывают никакого влияния, поскольку они не выполняют работу и не проявляются в выражении энергии системы, что приводит к равновесному распределению, независимому от магнитных полей. Это открытие, известное как теорема Бора-ван Левена, подчеркивает необходимость квантовой механики для объяснения магнетизма. Однако эффекты магнитного поля можно рассматривать в рамках классической механики, ослабив предположение о равновесии.

Неравновесные системы широко распространены, проявляясь, среди прочего, в живых системах, потоках жидкостей и химических реакциях. Хотя равновесные состояния редки в природе, квазиравновесные концепции, такие как уравнения Ланжевена и Фоккера-Планка, полезны для изучения неравновесных систем. Эти уравнения поддерживают теоремы флуктуации и флуктуационно-диссипативной теории (FDT), связывающие равновесную и неравновесную термодинамику. FDT связывает колебания равновесия с реакцией системы на небольшие внешние возмущения, примером чего может служить соотношение Эйнштейна для коэффициента диффузии.

В последние годы изучению процессов, происходящих в живых клетках, уделяется значительное внимание в связи с его фундаментальной важностью для понимания биологических функций и поведения. Основная цель нашей работы - понять функцию ATPase, группы ферментов, ответственных за выработку молекул АТФ, энергетической валюты клетки. Даже малейшее изменение в функции ATPase может существенно повлиять на рост и функционирование всего организма. Вращение играет ключевую роль в функционировании ATPase: поток протонов вращает центральный стержень,

который впоследствии вызывает конформационные изменения в каталитической части, тем самым способствуя синтезу ATP. Однако в такой микроскопической системе вращение происходит не в чисто механическом смысле, а скорее должно быть понято с помощью принципов статистической механики.

В задачах статистической механики часто рассматривается большая система, разделенная на меньшую подсистему, представляющую интерес ("система"), и более крупную квазиравновесную подсистему ("термостат" или "ванна"). Система взаимодействует с термостатом, обмениваясь энергией, частицами, линейным импульсом и угловым моментом. Неравновесие может возникать либо из-за возмущения системы, либо из-за неравновесного состояния термостата, что приводит к неравновесным устойчивым состояниям (NESS). NESS обобщает равновесные состояния, в которых отсутствует симметрия обращения времени и поддерживаются постоянные токи.

В данной работе рассматриваются три физические системы, подключенные к неравновесному термостату, с акцентом на вращательное движение и момент импульса. Магнитные поля могут влиять на неравновесные системы, придавая вращательное движение заряженным частицам и вызывая вращение термостатов в зависимости от их неравновесных характеристик. Кроме того, неравновесные состояния с кинетическим происхождением обнаруживают особую стохастическую динамику углового момента.

Мы исследуем воздействие слабых магнитных полей на живые организмы, проверяя достоверность и воспроизводимость результатов экспериментов. Физические механизмы, лежащие в основе этих эффектов в молекулярной биологии, остаются неясными. Мы предлагаем механизм влияния слабых магнитных полей на стохастическое движение ионов, имеющее решающее значение в биологических процессах, показывая, что ионы приобретают ненулевой средний угловой момент, когда равновесие нарушается активными процессами.

Далее мы пересматриваем теорему Бора-ван Левена, исследуя классическую заряженную броуновскую частицу, взаимодействующую с равновесной термальной ванной. Хотя частица, согласно теореме, не "чувствует" магнитное поле, ее взаимодействие с ванночкой вызывает в ванночке неравновесные состояния. Используя модель Калдейры-Леггетта, мы показываем, что магнитное поле вызывает долговременные изменения в ванне, приводящие к среднему угловому моменту в незаряженных генераторах bath.

В нашем заключительном исследовании рассматривается устойчивость вращения в системах, где ограничивающий потенциал не является идеально симметричным, что приводит к уменьшению углового момента. Мы расширили вопрос об интегралах движения при слабых возмущениях, выведя крупнозернистое стохастическое дифференциальное уравнение, описывающее уменьшение углового момента. Наши результаты согласуются с результатами численного моделирования, что улучшает понимание интегралов движения в слабовозмущенных системах.