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用张量网络方法研究非平衡系统中涨落性质

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Tensor-Network Approaches to the Fluctuation Properties in Nonequilibrium Systems

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内容摘要

在这份研究报告中我们展示张量网络是如何用来在数值上研究非平衡系统中的涨落性质。特别地，我们聚焦于这样的系统，他们的自由度随着系统尺寸呈现指数增长关系，而其中相关量的涨落可以用一些统称为涨落定理的漂亮关系式来量化。张量网络方法被用来计算涨落的特征函数，从这些函数中可以提取出更加细致的信息。

我们首先对于涨落定理给出一个简要的介绍。具体来说，我们在经典统计力学的框架中给出 Jarzynski 恒等式的推导，也基于马尔可夫随机动力学给出 Gallavotti-Cohen 涨落定理的推导。这两个关系式代表了非平衡物理在过去三十年的主要成就。

然后，我们介绍一种张量网络方法，可以用来计算初始处于热平衡态的量子格点系统的功分布。在这个方法中，动力学演化用 Time Evolving Block Decimation (TEBD) 方法模拟，初始的热平衡态可以通过直接 TEBD 方法制备，也可以通过 Minimally Entangled Typical Thermal States (METTS) 方法制备，后者产生一系列典型的态来代表吉布斯正则系综。作为一个示例，我们将此方法应用于处于横场和纵场中的伊辛链。在给定驱动下，可以计算出功分布的矩生成函数，从中验证了量子 Jarzynski 恒等式和一个包含任意可观察量泛函的广义的量子功关系式。

最后，我们将张量网络应用于对非平衡扩散系统中的随机粒子输运做计数统计。这个系统由一个一维的输运通道构成，两端分别接触粒子库。两种张量网络方法被用来实现这样一个应用，它们分别是 Density Matrix Renormalization Group (DMRG, 密度矩阵重整化群) 和 TEBD。输运流的累计量生成函数被数值计算出来，并且和它们的解析解进行对比。我们发现了两者完美吻合，这充分说明了这些方法的有效性。此外，关于输运流的涨落定理也通过验证是成立的。

关键词：非平衡物理，涨落定理，功分布，计数统计，张量网络方法

Abstract

In this report we exhibit how tensor networks can be used to numerically investigate the fluctuation properties in nonequilibrium systems. In particular, we focus on the systems whose degrees of freedom grow exponentially with the system size, and in which the fluctuations of relevant quantities are quantified by some remarkable relations, collectively known as fluctuation theorem. Tensor-network approaches are applied to calculate the characteristic functions of fluctuations that more detailed information can be extracted from.

We start by giving a brief introduction to the fluctuation theorem. Specifically, we present the derivations of the Jarzynski equality in the framework of classical statistical mechanics, and of the Gallavotti-Cohen fluctuation theorem for the Markovian stochastic dynamics. These two relations represent the major advance in nonequilibrium physics in the last three decades.

Then, we introduce a tensor-network approach to calculate the statistics of work done on 1D quantum lattice systems initially prepared in thermal equilibrium states. In this approach, the dynamics is simulated with Time Evolving Block Decimation (TEBD), and the initial thermal equilibrium state is prepared either directly with TEBD or with Minimally Entangled Typical Thermal States (METTS), which generates a set of typical states representing the Gibbs canonical ensemble. As an illustrative example, we apply this approach to the Ising chain in mixed transverse and longitudinal fields. Under a prescribed protocol, the moment generating function for work distribution can be calculated, from which the quantum Jarzynski equality and the generalized quantum work relation involving a functional of an arbitrary observable are tested.

Finally, we apply tensor networks to counting statistics for the stochastic particle transport in an out-of-equilibrium diffusive system. This system is composed of a one-dimensional channel in contact with two particle reservoirs at the ends. Two tensor-network algorithms, namely, Density Matrix Renormalization Group (DMRG) and TEBD, are respectively implemented. The cumulant generating function for the current is numerically calculated and then compared with its analytical solution. Excellent agreement is found, manifesting the validity of these approaches in such an application. Moreover, the fluctuation theorem for the current is shown to hold.

Keywords: Nonequilibrium Physics, Fluctuation Theorem, Work Statistics, Counting Statistics, Tensor-Network Approaches

Contents

Chapter 1

Introduction

The last three decades have witnessed great advance in the field of nonequilibrium statistical physics. In particular, the establishment of various relations, nowadays collectively called fluctuation theorem, have revolutionized our understanding about the dichotomy between microscopic reversibility and macroscopic irreversibility. It is now clear that the microscopic reversibility underpins these relations, whereas the macroscopic irreversibility is interpreted as an emerging property from the statistical level of description. One of these relation is the Jarzynski equality which attracts considerable interests. It is a parameter-free, model-independent relation, and allows to express the free energy difference between two equilibrium states by a nonlinear average over the required work to drive the system in a nonequilibrium process from one state to another. The other notable relation is called Gallavotti-Cohen fluctuation theorem. It is a strikingly simple and general relation which quantifies the large-deviation property of the fluctuating currents flowing across systems maintained in nonequilibrium steady state, and has already been proved in many systems. From this relation, the fluctuation-dissipation theorem, Onsager reciprocal relations and their generalizations can be easily derived.

1.1 Motivation

1.2 Outline

The purpose of the present report is to show how tensor-network approaches can be used to numerically calculate the statistics of relevant quantities in nonequilibrium systems. In fact, this nowadays constitutes one of very active subfields of statistical physics. This report is organized as follows.

Chapter 2

Fluctuation Theorem

Fluctuation theorem is one of the greatest triumphs in the search for general statements regarding the dynamics of systems far from equilibrium. It represents a collection of relations in similar structure, concerning the comparison between the probabilities of forward and time-reversed trajectories. These relations are as a consequence of microreversibility, a fundamental symmetry of Nature. They can be considered as a generalization of the second law of thermodynamics. Close to equilibrium, the fluctuation theorem reduces to the fluctuation-dissipation relations such as the Green-Kubo relation for the transport coefficient. Moreover, they also implies the Onsager reciprocal relations as well as the generalized nonlinear ones up to arbitrary order. In this chapter, we give a very detailed analytical derivation of two most well-known relations, the Jarzynski equality and the Gallavotti-Cohen fluctuation theorem.

2.1 Jarzynski Equality

In 1997, Jarzynski proved a remarkable relation,

$$\left\langle \mathrm{e}^{-\beta W} \right\rangle = \mathrm{e}^{-\beta \Delta F}, \tag{2.1}$$

where W is the work done on a system that is initially in thermal equilibrium and driven out of equilibrium by an external force evolving under a protocol which is parameterized by λ from the value A to B. $\Delta F = F_B - F_A$ denotes the free energy difference between the final equilibrium ensemble and the initial equilibrium ensemble, and $\langle \cdot \rangle$ stands for the average over the repetition of driving [1–5]. This relation was later called Jarzynski equality, allowing to express the free energy difference between two equilibrium states by a nonlinear average over the required work to drive the system in a nonequilibrium process from one state to the other. From the Jarzynski equality, the Clausius inequality can be immediately obtained as a corollary, $\langle W \rangle \geq \Delta F$, thus in accord with the second law of thermodynamics.

We now derive the Jarzynski equality in the framework of classical statistical physics. Let's consider a system described by the Hamiltonian $H(x;\lambda)$, where $x \equiv (\mathbf{q}, \mathbf{p})$ denotes the microstate and λ represents the external control parameter. When this system is equilibrated with a thermal environment, its microstate can be viewed as a random variable sampled from the Boltzmann-Gibbs distribution

$$\mathcal{P}_\lambda^{\mathrm{eq}}(x) = \frac{1}{Z_\lambda} \mathrm{e}^{-\beta H(x;\lambda)}. \tag{2.2}$$

The partition function and free energy are given by the familiar expressions:

$$Z_\lambda = \int \mathrm{d}x \, \mathrm{e}^{-\beta H}, \qquad F_\lambda = -\beta^{-1} \ln Z_\lambda. \tag{2.3}$$

Under a driven protocol $\lambda_t, 0 \leq \lambda \leq \tau$, after being prepared in equilibrium, the system evolves in time as λ is switched from $\lambda_0 = A$ to $\lambda_\tau = B$. Because the system is thermally isolated in this process, the work done on the system is simply the net change in its internal energy

$$W(x_0) = H(x_\tau(x_0); B) - H(x_0; A). \tag{2.4}$$

Here, $x_\tau(x_0)$ denotes the final coordinate in phase space, conditioned that the trajectory launched from the initial coordinate x_0. The left-hand side of Eq. (2.1) is then an average of $\exp[-\beta W(x_0)]$ over the initial conditions sampled from the equilibrium distribution (2.2) at $\lambda = A$:

$$\begin{aligned} \langle \mathrm{e}^{-\beta W} \rangle &= \int \mathrm{d}x_0 \mathcal{P}_A^{\mathrm{eq}}(x_0)\, \mathrm{e}^{-\beta W(x_0)} \\ &= \frac{1}{Z_A} \int \mathrm{d}x_0\, \mathrm{e}^{-\beta H(x_\tau(x_0); B)} \\ &= \frac{1}{Z_A} \int \mathrm{d}x_\tau \left| \frac{\partial x_\tau}{\partial x_0} \right|^{-1} \mathrm{e}^{-\beta H(x_\tau; B)}, \end{aligned} \tag{2.5}$$

where we have changed the variables of integration from x_0 to $x_\tau(x_0)$. Such a change of variable is permitted since there is a one-to-one correspondence between final and initial coordinates under Hamiltonian evolution. The additional factor in the last line is the Jacobian associated with the change of variables. Since the volume of phase space is conversed by the Liouville theorem [6], this factor is exactly unity. Hence

$$\langle \mathrm{e}^{-\beta W} \rangle = \frac{1}{Z_A} \int \mathrm{d}x_\tau \mathrm{e}^{-\beta H(x_\tau; B)} = \frac{Z_B}{Z_A} = \mathrm{e}^{-\beta \Delta F}. \tag{2.6}$$

Q.E.D.

2.2 Gallavotti-Cohen Fluctuation Theorem

Chapter 3

Conclusion and Perspectives

The present report has been devoted to study of the nonequilibrium systems with tensor-network approaches, with the focus on the fluctuation properties of relevant quantities. The characteristic functions quantifying the fluctuations are numerically calculated.

Appendix A

Numerical Details and Code Implementations

> *Computer programming is an art, because it applies accumulated knowledge to the world, because it requires skill and ingenuity, and especially because it produces objects of beauty. A programmer who subconsciously views himself as an artist will enjoy what he does and will do it better.*
>
> — Donald E. Knuth

Computer programming plays an increasing important role in scientific research. It has de-facto become a pillar in scientific research, to be complementary with theory and experiment. A scientist might first build a model to describe a physical system according to the underlying physical laws, then use a computer to calculate the results and visualize them. This is now a widely adopted paradigm in scientific community. This appendix is devoted to the numerical details and code implementations about the DMRG approach to counting statistics. The required software and code written in C++ are presented in detail. Some explanatory remarks are also given.

Required Software

The following listed software are those minimal requirements for the code presented in next section to be compiled and executed correctly.

- Ubuntu 22.04 – one of the most popular distribution of Linux operating system. Other version might also be OK, but it is highly recommended to use the most recent one.
- g++ – an open-source C++ compiler included in GCC (GNU Compiler Collection). It can be installed on Ubuntu with the command `sudo apt install g++`.
- GNU Make – a utility that facilitates compiling a program from source code. It reads from a file named `Makefile` which includes a set of instructions to be executed. It can be installed on Ubuntu with the command `sudo apt install make`. Readers are referred to Ref. [7] for detailed account.
- GSL (GNU Scientific Library) – an open-source library for C/C++ programmers. It is licensed under the GNU General Public License (GPL). It can be installed on Ubuntu with the command `sudo apt install gsl-bin libgsl27 libgsl-dbg libgsl-dev`. The reference manual for this library is Ref. [8].
- ITensor (Intelligent Tensor) – an open-source library for performing tensor computation. It provides both C++ and Julia version, whereas the former is used here. The installation instructions comes with the downloaded source code from here. Readers are referred to Ref. [9] for more details.

C++ Code for DMRG Approach to Counting Statistics

In the following, we show the code, which are written in separate text files:

- `Class_model.h`.

Listing A.1: `Class_model.h`.

```
#include <iostream>
#include <fstream>
#include <iomanip>
#include <cmath>
#include <vector>
#include <itensor/all.h>

class Cmodel
{
	public:
		static itensor::Real m_D;
		static itensor::Real m_Delta_x;
		static int m_L;
		static int m_N_L;
		static int m_N_R;
		static int m_Dim;
		static itensor::IndexSet m_phys_indices;
		static itensor::IndexSet m_mpo_bond_indices;
		static std::vector<itensor::ITensor> m_mpo;

		static void initialization(int, int, int, int);
		static void parameterization(itensor::Real);
		static itensor::Real A();


		std::vector<itensor::ITensor> m_mps;
		int m_center;

		Cmodel(void);
		Cmodel(const Cmodel &);
		void print(std::string, int);
		void canonication(int, int, itensor::Real);
		itensor::Real Q(void);
		itensor::Real P(int, int);
		Cmodel &operator=(const Cmodel &);
		std::vector<itensor::ITensor> prime(void);

	private:
		static itensor::Real factorial(int);
		static std::vector<itensor::ITensor> idmps(void);
};
```

Appendix B

关于此模板

PKUreport 是一个针对北京大学博士后研究工作报告的 LaTeX，其制作符合北京大学博士后出站报告提交说明。

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使用

- 使用 TeX Live 套装，该套装适用 Unix-like/Microsoft Windows/macOS 操作系统。
- 使用 xelatex 编译方式。
- 使用 biber 作为参考文献宏包 biblatex 的后台处理程序。

编译步骤

- `xelatex Report.tex`
- `biber Report`
- `xelatex Report.tex`
- `xelatex Report.tex`

一些具体说明

- 模板的主文件是 Report.tex，在其中可以添加章。每一章的所有相关文件放入一个子文件夹中。每一个子文件夹的路径通过 \path 定义。
- 摘要、致谢、文章发表分别写在相应的 tex 文件中。
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许可证

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Publications

This report is based on the first two of the following journal articles:

- **Jiayin Gu**, Fan Zhang, and H. T. Quan, *Tensor-Network Approach to Work Statistics for 1D Quantum Lattice Systems*, Phys. Rev. Res., 4, 033139 (2022).
- **Jiayin Gu** and Fan Zhang, *Tensor-Network Approaches to Counting Statistics for the Current in a Boundary-Driven Diffusive System*, New J. Phys., 24, 113022 (2022).
- Yu-Xin Wu, **Jiayin Gu** and H. T. Quan, *Full Counting Statistics and Fluctuation Theorem for the Currents in the Discrete Model of Feynman's Ratchet*, Phys. Rev. E, 106, 014154 (2022). (co-corresponding author)