Typical pure states and rare events for quantum many-body systems

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I. INTRODUCTION

Recently, considerable attentions have been paid to the fluctuation of the entropy production for mesoscopic transports. In particular, the tails of the probability distribution represent rare but important phenomena for the stochastic thermodynamics. Experimentally, however, it is difficult to sample sufficient number of rare events. The rare events have been explored for a dragged Brownian particle in water, RNA stretching, the electron transport thorough quantum dots, to name only a few. This issue suggests an unsolved problem: How should we sample the rare events? Several numerical methods were developed for the efficient sampling.

In this presentation, we discuss on an alternative way to calculate the probability distribution on the basis of a single sample for quantum many-body systems. Our results treat whole the range of the probability distributions equally well. With the use of the single sample, we can accurately reproduce the full statistics of the ensemble, which is an assembly of many pure states. Hence, the difficulty of sampling the rare events is partially solved.

II. TYPICAL PURE NONEQUILIBRIUM STATES AND PROBABILITY DISTRIBUTION

We use the intrinsic thermal nature of a typical pure state $|\phi\rangle$ on the energy shell $\mathcal{H}_E$. Let us randomly sample a pure state $|\phi\rangle$ from $\mathcal{H}_E$ according to the Haar measure. Then, for an arbitrary observable $\hat{A}$, the expectation value $\langle\phi|\hat{A}|\phi\rangle$ well agrees with the microcanonical average $\langle\hat{A}\rangle_{mc}$ with a probability almost unity[1,2]. For large system size, the equivalence of ensembles claims that the canonical and microcanonical averages for the total system are quantitatively similar. And, we simply denote the microcanonical average as $\langle\hat{A}\rangle_{eq}$.

It is a challenging problem to explore the nonequilibrium processes on the basis of the pure state. We extend the availability of the thermal nature of typical states to the nonequilibrium processes which start from an equilibrium state[3]. We can also construct a class of typical pure nonequilibrium stationary states based on the scattering approach[4], and calculate the stationary current.

The important point is that $\hat{A}$ can be arbitrary higher order polynomials of local operators. For example, $\hat{A}$ can be the exponential of a local operator. One might think that we can distinguish the pure and microcanonical states from the expectation values of higher correlations. However, this is not the case. Hence, we can calculate the characteristic function of, for example, the entropy production $\langle U(t)^\dagger e^{i\xi\beta\hat{H}(t)}U(t)e^{-i\xi\beta\hat{H}(0)}\rangle_{eq}$ on the basis of the pure state $|\phi\rangle$. Here, $\hat{H}(t)$ is the Hamiltonian at time t, and $U(t)$ is the unitary evolution operator. By the Fourier transformation, we can calculate the probability distribution $P(\beta W = a)$ only from a fixed pure state $|\phi\rangle^3$. The deviation roughly satisfies

$$P_{eq}(\beta W = a) = P_\phi(\beta W = a)(1 + \mathcal{O}(\frac{1}{\sqrt{d}})), \qquad (1)$$

where $P_{eq}(\cdot)$ and $P_\phi(\cdot)$ are the probability distributions calculated by the initial microcanonical ensemble and the pure state $|\phi\rangle$. Here, $d = \dim\mathcal{H}_E$ is the dimension of the initial energy shell at an energy scale E. Since d exponentially grows with the system size N, the error is negligible also for relatively small systems. The error estimation (1) is considered as model-independent, and determined only by the absolute value of the probability and the dimension.

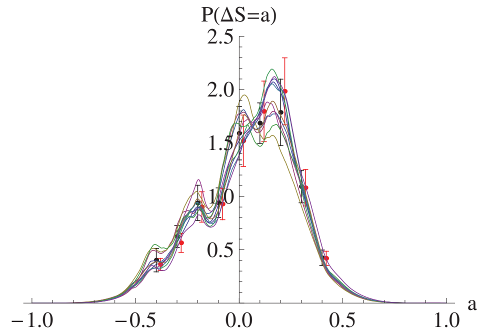

FIG. 1. The probability distribution $P_{eq}(\Delta S = a)$ for the microcanonical ensemble and $P_\phi(\Delta S = a)$ for pure states. The error bars show $P_{eq}(\Delta S = a)/\sqrt{d}$ (red) and fluctuation of 10 randomly sampled pure states (black).

In Fig. 1, we numerically calculate the probability distribution of the entropy production for $N = 10$ sites quantum spin chain which is externally perturbed by a time dependent magnetic field. Here, we ignore the boson or fermion statistics, however, the same argument essentially holds for these cases by constraining both the total energy and the number of particles. This issue is important to explore the energy and particle currents for quantum junctions in nonequilibrium steady states[4]. The Hamiltonian is

$$\hat{H}(t) = -J\sum_{j=1}^{N-1}\sigma_j^z\sigma_{j+1}^z + \sum_{j=1}^{N}\sigma_x + h(t)\sum_{j=1}^{N_s}\sigma_j^z + \gamma\sum_{j=1}^{N}\sigma_j^z. \qquad (2)$$

Here, we use the ferromagnetic exchange energy $J = 1$, and the z component of the magnetic field is $\gamma = 0.5$.

The time-dependent magnetic field $h(t) = \sin 2\pi\omega t$ is acting on the subsystem $0 \leq j \leq N_s$ with $N_s = 2$ and $\omega = 0.4$. The parameter γ controls the integrability. We randomly sample 10 pure states from an energy shell $\mathcal{H}_E$, and calculate the probability distributions. The error bars show the theoretically predicted deviation from the microcanonical case, and the numerical fluctuation. The deviation is in agreement with the theoretical estimation.

The distribution function $P(\beta W = a)$ contains a continuous parameter a, and the error estimation above holds for most of a as verified in Fig. 1. In particular, we can accurately reproduce the tails or large deviations.

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[1] A. Sugita, Nonlinear Phenom. Complex Syst. **10** 192 (2007); cond-mat/0602625 [cond-mat.stat-mech] (2006)
[2] P. Reimann, Phys. Rev. Lett. **99** 160404 (2007)
[3] T. Monnai, and A. Sugita, J. Phys. Soc. Jpn. **83** 094001 (2014)
[4] T. Monnai, and K. Yuasa, Europhysics Letters, **107** 40006