Formalisms of Quantum Fluctuation Theorem

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非平衡系の正負エントロピー生成の生起確率の比が物質定数を含まない形でバランスすることが古典系で広く成立することが知られており、FluctuationTheorem (FT) と呼ばれている。以前、量子系への拡張を仕事演算子を定義して行いプランク定数の2乗に比例する補正があることを特定のモデルで示した。一方、Kurchan によってこれと古典極限では一致する等価でない定式化がなされていたが両者の関係ははっきりしていなかった。今回は両者の関係を明確にする。これによって量子補正の起源が理解される。

1 Quantum Fluctuation Theorem

Since the discovery by Evans, Cohen and Morriss[1], many types of fluctuation theorem(FT) has been presented both for deterministic, and stochastic systems. Though the systems and the definition of entropy production differ, FT has a universal form.

$$\log \frac{P(\Sigma_t = A)}{P(\Sigma_t = -A} = A \tag{1}$$

Here, $P(\Sigma_t = A)$ is the probability that the entropy production during time 0 to t is some value A. Contrary to FT for classical systems, FT for quantum systems has not been well understood. In order to generalize FT to quantum systems(QFT), it is necessary to identify entropy production or work done externally. And two procedures are available:

(a)Measure flows of energy, particle numbers etc. and evaluate the entropy production or work done as accumulated value of the flows.

(b)Measure energy, particle numbers etc.twice and evaluate the entropy production or work done as the difference of the two observed values.

These two procedures are not equivalent in quantum systems. In this letter, we clarify the relationship between procedure (a) and (b).

1.1 Work Operator Formalism

We show an example of procedure (a). Consider a particle trapped by a harmonic potential which moves one-dimensionally through ideal Bose gas.

$$H(t) = \frac{p^2}{2m} + \frac{k}{2}(q - f(t))^2 + \frac{1}{2} : \int d\lambda((p_\lambda - \kappa_\lambda q)^2 + \omega_\lambda^2 q_\lambda^2) : \tag{2}$$

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) The system is in equilibrium with inverse temperature β

) At time $t=0$, the harmonic potential starts to move, where its center follows the trajectory $x=f(t)$.(f(0)=0 is assumed.)

We define the work operator $\Sigma_t \equiv \beta(U^\dagger H(0)U - H(0))$ and concern its spectrum distribution $P(\Sigma_t = A) \equiv \mathrm{Tr}(\frac{1}{Z}e^{-\beta \mathrm{H}(0)}\delta(\Sigma_t - \mathrm{A}))$. By straightforward calculation, one finds $\log\frac{P(\Sigma_t=A)}{P(\Sigma_t=-A)} = (1+\hbar^2\epsilon_2 + O(\hbar^4))A$. Where ϵ_2 does not depend on system parameters (at least for $f(t)$ proportional to t).

1.2 2times observation formalism

Here, we summarize the result obtained by Kurchan[3]. Assume that the time evolution unitary operator during time 0 to t U satisfies $U^\dagger = U^*$. This is achieved for the system perturbed periodically in time. And the whole system is initially obeys canonical ensemble with inverse temperature β. Then perform the observation of energy H at 0 and t. The energy change is $\Sigma_t = \beta(E_n - E_m)$. Then the probability that Σ_t is A, $P(\Sigma_t = A) = \Sigma_{m,n}\frac{1}{Z}e^{-\beta E_m}|\langle n|U|m\rangle|^2\delta(A-\beta(E_n - E_m))$ satisfies FT relation with no quantum deviation. The essence of the derivation is the symmetry of characteristic function $\phi_2(\xi) \equiv \int dAP(\Sigma_t = A)e^{-i\xi A} = \phi_2(-i+\xi)^*$.

2 Work Operator Formalism and 2times Observation Formalism

The difference between procedure (a) and (b) becomes very clear by considering the characteristic functions of $P(\Sigma_t = A)$ for both approaches, $\phi_1(\xi)$and $\phi_2(\xi)$. One has the following expressions:

$$\begin{aligned}\phi_1(\xi) &= \int dAP(\Sigma_t = A)e^{-i\xi A} = \langle e^{-i\xi\beta(U^\dagger H(0)U - H(0))}\rangle \\ \phi_2(\xi) &= \langle e^{-i\xi\beta U^\dagger H(0)U}e^{i\xi\beta H(0)}\rangle\end{aligned} \tag{3}$$

So far, the quantum deviation of FT seen in work operator approach is considered as the result of the uncommutativity of $U^\dagger H(0)U$ and $H(0)$.

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