Fractional entropy decay and the third law of thermodynamics

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We report in this paper a theoretical study on the quantum thermodynamic properties of a fractional damping system. Through the analysis, few nontrivial characteristics are revealed, which include (1) a fractional power-law decay entropy function, which provides an evidence for the validity of the third law of thermodynamics in the quantum dissipative region and (2) the varying of the entropy from a nonlinear divergent function to a semilinear decay function with a fractional exponent as the temperature approaches absolute zero.

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I. INTRODUCTION

In theoretical physics, it is of great importance to establish a new theory or discover a fundamental law by exploring new evidence. In the past few years, with the rapid development of research areas such as anomalous diffusion [1–3], quantum thermodynamics [4], and small systems [5], a number of basic problems in statistical physics have been reconsidered. For example, research on small systems has found that the second law of thermodynamics may be violated if the system is driven to a state which is far from equilibrium [6]. However, the validity of the third law is ensured in quantum dissipative environments due to system-reservoir coupling [4,7–9]. These findings have led to a new upsurge of research challenging the foundations of conventional statistical physics.

Recently, enormous progress has been made in the study of fractional Brownian motion (fBm) and related problems [10–12]. Some unusual results have been reported such as ergodic and weak ergodicity-breaking properties in certain kinds of classical fBm processes [13,14]. However, few efforts have been made on fBm in the quantum regime, or even for the systems with some quantum fractional characteristics. Despite the mathematical difficulties due to fractional calculus, more achievements are expected in this challenging field.

Therefore in this paper we report one of our recent studies on the quantum fractional damping (FD) systems. Thermodynamical properties of the system are concerned gradually in the framework of standard fBm. The paper is organized as follows: in Sec. II, we give a clear definition of the so-called fractional damping system from a short review of fBm theory. In Sec. III, the free energy and entropy functions are computed analytically through the convenient methods raised in previous studies. Finally in Sec. IV, we make a short summary of our results and the prospects for further discussions of this subject.

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II. FRACTIONAL BROWNIAN MOTION AND FRACTIONAL DAMPING

In recent years, fractional Brownian motion has attracted considerable attention, since it offers an alternative model of random processes displaying the "Joseph effect" (long-range correlations) [15]. Similar to the standard Brownian motion induced by white noises, fBm is generally believed to originate from the fractional Gaussian noise (fGn) [10,16],

$$\xi(t) = \frac{dx(t)}{dt}, \tag{1}$$

which is zero mean with autocorrelation $\langle\xi(t_1)\xi(t_2)\rangle = 2D_H H(2H-1)|t_1-t_2|^{2H-2}$, where H is the Hurst exponent ranging from 0 to 1. Here $H = 1/2$ corresponds to the standard Brownian motion, $H < 1/2$ and $H > 1/2$ denote the sub- or superdiffusive cases, respectively, and $D_H = [\Gamma(1-2H)\cos(H\pi)]/(2H\pi)$ is the diffusion coefficient identified by the Gamma function $\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}\,dt$.

In general, fBm is regarded as the universal scaling limit of the Langevin dynamics whose microscopic-level correlations transcend to the macroscopic level, but its microscopic-level fluctuations do not. Mathematically, fBm can be described by a generalized Langevin equation containing fractional calculus. The trajectory sample of fBm is a self-affine stationary Gaussian process and is characterized by a standard normal probability distribution in the Boltzmann form:

$$P(x,t) = \frac{1}{\sqrt{2\pi D_H t^{2H}}}\exp\left[-\frac{(x-x_0)^2}{4D_H t^{2H}}\right]. \tag{2}$$

Given the initial conditions such as position x_0, any details about fBm can be revealed by numerically simulating its trajectories.

However, instead of focusing on the microscopic characteristics of the pure fBm dynamics, we present here a statistical exploration of the quantum thermodynamic properties of a particular type of dissipative systems which exhibit fBm, namely, the fractional damping (FD) system. Mathematically it can be expressed as a generalized system-plus-reservoir Hamiltonian model of quantum oscillators [17–19]. The

Heisenberg equations of motion for this system lead to the following Langevin equation written in good quantum numbers [20–23]:

$$m\ddot{x} + \int_0^t \eta(t-t')\dot{x}(t')\,dt' + \partial_x U(x) = \xi(t), \tag{3}$$

where x is the coordinate operator of the system oscillator commuting with its momentum p by $[x,p] = i\hbar$, $\eta(t) = \eta_\alpha t^{-\alpha}/\Gamma(1-\alpha)$ is the frictional kernel with fractional exponent $0 < \alpha < 1$, $\Gamma(s)$ is the gamma function, η_α is the strength constant, $U(x)$ is the potential energy of the external force, $\xi(t)$ is a stationary fractional Gaussian noise whose correlation obeys the quantum fluctuation-dissipation theorem [24,25]

$$\langle \xi(t)\xi(t')\rangle_s = \frac{\beta\hbar}{\pi}\int_0^\infty d\omega J(\omega)\coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(t-t'), \tag{4}$$

where $J(\omega) \propto \eta_\alpha\omega^\alpha$ is the spectral density of the sub-Ohmic bath, $\beta = 1/k_BT$ is the inverse temperature, and $\langle\cdots\rangle_s$ denotes the quantum symmetric average operation.

III. ENTROPY AND THE THIRD LAW

In the study of quantum thermodynamics, it is a matter of prime importance to obtain the entropy function. But before this, the free energy of the system must first be calculated. According to the remarkable formula [26–29]

$$F(T) = \frac{1}{\pi}\int_0^\infty d\omega f(\omega,T)\,\mathrm{Im}\left\{\frac{d\log\Psi(\omega+i0^+)}{d\omega}\right\}, \tag{5}$$

this can easily be achieved. Here $f(\omega,T) = k_BT\log[1-\exp(-\hbar\omega/k_BT)]$ is the free energy of a single oscillator with the zero-point contribution $\hbar\omega/2$ neglected, and $\Psi(\omega)$ is the generalized susceptibility which can be derived from Eq. (3) through a series of Fourier transformations.

Since $f(\omega,T)$ in Eq. (5) vanishes exponentially for $\omega \gg k_BT/\hbar$, the whole integrand is actually confined to low frequencies as $T \to 0$. The free energy of the system can then be calculated by expanding $\Psi(\omega)$ in the powers of frequency ω. In the particular case of a harmonic potential $U(x) = \frac{1}{2}m\omega_0^2x^2$, we have from Eq. (3)

$$\Psi(\omega) = \tilde{x}(\omega)/\tilde{\xi}(\omega) = \left[-m\omega^2 - m\eta_\alpha(i\omega)^\alpha + m\omega_0^2\right]^{-1}. \tag{6}$$

Note that a special factor $(i\omega)^\alpha$ is met in the calculation of $\Psi(\omega)$ which should be addressed carefully, but we remember in mathematics that $(i)^\alpha = \cos(\alpha\pi/2) + i\sin(\alpha\pi/2)$. Then after some algebra, we obtain in the low-frequency limit

$$\begin{aligned}\mathrm{Im}&\left\{\frac{d\log\Psi(\omega)}{d\omega}\right\}\\ &= \frac{\eta_\alpha\omega^{\alpha-1}\left[\alpha\left(\omega_0^2-\omega^2\right)+2\omega^2\right]\sin\frac{\alpha\pi}{2}}{\eta_\alpha^2\omega^{2\alpha} - \eta_\alpha\omega^\alpha\left(\omega^2-\omega_0^2\right)\cos\frac{\alpha\pi}{2} + \left(\omega^2-\omega_0^2\right)^2}\\ &\cong \frac{\alpha\eta_\alpha\omega^{\alpha-1}}{\omega_0^2}\sin\left(\frac{\alpha\pi}{2}\right).\end{aligned} \tag{7}$$

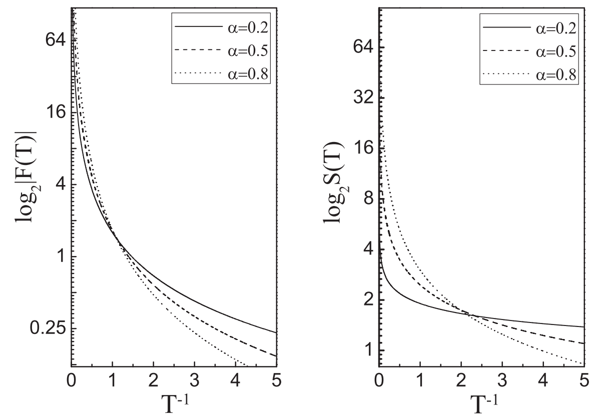

FIG. 1. Free energy and entropy of the FD system as a function of the inverse temperature. Dimensionless parameters in use are $\eta_\alpha = \hbar\omega_0 = k_B = 1.0$.

This leads to an analytical expression of the free energy

$$\begin{aligned}F(T) &\cong \frac{\alpha\eta_\alpha k_BT}{\pi\omega_0^2}\sin\left(\frac{\alpha\pi}{2}\right)\int_0^\infty d\omega\omega^{\alpha-1}\log[1-e^{-\hbar\omega/k_BT}]\\ &= -\frac{\alpha\eta_\alpha\hbar}{\omega_0^{1-\alpha}}\sin\left(\frac{\alpha\pi}{2}\right)\Gamma(\alpha)\zeta(\alpha+1)\left(\frac{k_BT}{\hbar\omega_0}\right)^{\alpha+1},\end{aligned} \tag{8}$$

where a special integral $\int_0^\infty dyy^\nu\log(1-e^{-y}) = -\Gamma(\nu+1)\zeta(\nu+2)$ is relevant with $\Gamma(s)$, the gamma function, and $\zeta(z) = \Sigma_{n=1}^\infty\frac{1}{n^z}$, Riemann's ζ function.

With this knowledge, the entropy function of the frictional damping system can then be evaluated as

$$\begin{aligned}S(T) &= -\frac{\partial F(T)}{\partial T}\\ &= \frac{\alpha(\alpha+1)\eta_\alpha}{\omega_0^2(\hbar/k_B)^{\alpha+1}}\sin\left(\frac{\alpha\pi}{2}\right)\Gamma(\alpha)\zeta(\alpha+1)T^\alpha.\end{aligned} \tag{9}$$

Here we emphasize that as $T \to 0$, $S(T)$ decays rapidly, providing more evidence for the validity of the third law of thermodynamics in the quantum region.

In order to further reveal the quantum thermodynamic properties of the FD system, we plot in Fig. 1 the free energy and

TABLE I. Comparison of the thermodynamic properties of various conventional quantum dissipative systems with different spectra density $J(\omega)$. A replacement $\mathcal{D}(\omega) = d\log\Psi(\omega)/d\omega$ is used for simplicity.

Type of QD systems	$J(\omega)$	$\mathrm{Im}\{\mathcal{D}(\omega)\}$	$F(T)$	$S(T)$
Harmonic[a]	ω	Const.	T^2	T
Ohmic[b]	ω	Const.	T^2	T
Drude[c]	ω	Const.	T^2	T
Harmonic velocity[a]	ω^3	ω	T^3	T^2
Blackbody radiation[b]	ω^3	ω^2	T^4	T^3
Harmonic acceleration[a]	ω^5	ω^3	T^5	T^4
Non-Ohmic[c]	ω^δ	$\omega^{\delta-1}$	$T^{\delta+1}$	T^δ
Fractional damping	ω^α	$\omega^{\alpha-1}$	$T^{\alpha+1}$	T^α
Arbitrary chosen bath[b]	$\omega^{\nu+1}$	ω^ν	$T^{\nu+2}$	$T^{\nu+1}$

[a]Reference [8].
[b]Reference [4], where $\nu \in (-1,1)$.
[c]Reference [9], where $\delta \in (0,2)$.

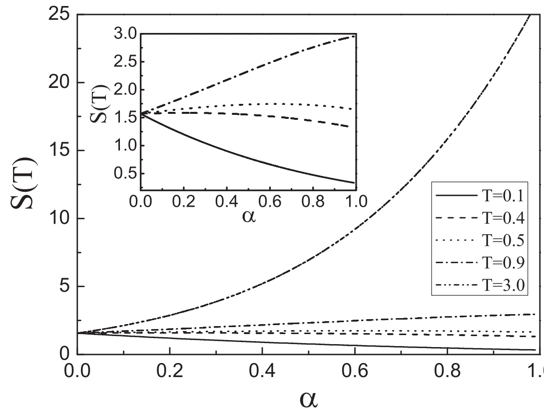

FIG. 2. Entropy of the FD system plotted as a function of the fractional exponent at various system temperatures. Inserts: local amplification of the linear curves. Dimensionless units are used as those of Fig. 1.

entropy as a function of the inverse temperature for different α. From this we can see that in all cases the entropy decays rapidly. and the decay rate increases as the increasing of α. This reminds us of the previous results because the power law decay of $S(T)$ has been witnessed in various quantum dissipative systems such as those listed in Table I. The difference lies mainly in that the power-law decay of the entropy in the FD system is characterized by the fractional exponent α. Then, one may argue, was it a coincidence or an inevitable consequence?

To clarify this question, we give in Table I a comparison of the temperature-dependent decay of the entropy functions for different quantum dissipative systems. The arguments of other quantities including the power spectra density $J(\omega)$ for each system are listed as well. From Table I one may notice that the exponent of $S(T)$ for each case is identical to that of $J(\omega)$ except for the two structured baths (harmonic velocity and harmonic acceleration). Alternatively, given that the spectra densities of the systems were identified by a universal power exponent, the entropy decay of each quantum dissipative system then can be classified with the same trend of the power law, regardless of the exponent α, δ, ν, or others. Therefore in our opinion, the fractional entropy decay of the FD system is an inevitable result under quantum thermodynamics.

To get a deeper understanding into the quantum thermodynamics of the FD system, we present in Fig. 2 a further investigation of the α dependence of $S(T)$ for different system temperatures. From this we can see that $S(T)$ varies from a nonlinear divergent function to a semilinear decay function of α as the temperature decreases. In the low-temperature limit, it decays approximately in a standard linear form. This is a nontrivial phenomenon. Despite that the intrinsic mechanism is not clear in the current calculations, we believe that new physics may exist in the FD systems.

IV. SUMMARY AND DISCUSSION

In conclusion, to date we have had a preliminary understanding of the quantum thermodynamic properties of the FD system. The free energy and entropy functions are calculated analytically, which have fractional power-law decay characteristics as the temperature goes to absolute zero. This represents further evidence for the validity of the third law of thermodynamics, even in the quantum dissipative region. Moreover, our results show some nontrivial phenomena including that $S(T)$ varies from a nonlinear divergent function to a semilinear decay function of α as the temperature reduces gradually. All these findings show that although the FD system is not a real system of fBm, there are many interesting things deserving further investigations.

We note that among all kinds of stochastic processes that produce subdiffusion, fBm may be a model particularly relevant to subcellular transport. For example, the negative and long-range correlation appearing as $H < 1/2$ has been observed in subdiffusing mRNA molecules [30], RNA proteins, and chromosomal loci within *E. coli* cells [31]. In a similar way, fBm can be used to describe unbiased translocations [32,33], the dispersion of apoferritin proteins in crowded dextran solutions [34], and lipid molecules in lipid bilayers [35]. Hence, although several aspects for the understanding of fBm and FD systems remain formidable, we expect that this work could motivate the continuous demystification of this seemingly simple subject.

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