Entropy and Its Quantum Thermodynamical Implication for Anomalous Spectral Systems

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Abstract

The state function entropy and its quantum thermodynamical implication for two typical dissipative systems with anomalous spectral densities are studied by investigating on their low-temperature quantum behavior. In all cases it is found that the entropy decays quickly and vanishes as the temperature approaches zero. This reveals a good conformity with the third law of thermodynamics and provides another evidence for the validity of fundamental thermodynamical laws in the quantum dissipative region.

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I. INTRODUCTION

The widespread interest on dissipative environments in recent years has highlighted the critical role that it plays in the study of mesoscopic systems [1], statistical mechanics [2, 3], quantum computation and fundamental quantum physics [4, 5]. In particular, the quantum thermodynamic properties of such stochastic coupling open systems has long been a hot spot of chemistry and physics [6, 7]. Whereas many new facets of old results have emerged bringing out lots of subtle issues. It is important to be cautious to question the validity of fundamental laws especially the three laws of thermodynamics.

Of all the fundamental laws in thermodynamics, the third law which is contributed by W. H. Nernst in the critical analysis of various chemical and electrochemical reactions bears prominent consequences for quantum mechanics and low-temperature physics studies [8–10]. It confirmed the fact that the absolute zero temperature is unattainable because of the immediate coincidence between the isotherm and the isentrope (adiabat) [10]. Therefore the Carnot engine can never reach 100% efficiency for any finite temperature.

Great progress in thermodynamics attributed to this law has been witnessed in curing the known deviations by quantum statistical mechanics and interactions among particles according to common wisdom, although some unfulfillment may still exist. Intriguingly it has been found that finite dissipation helps to ensure the third law rather than deviate it [11, 12]. Further investigations sequentially illuminated the predominance of anomalous couplings in assuring the third law [13]. However, the mechanism of how quantum dissipation influences the low-temperature thermodynamic properties of the system is still an important subject needs to be clarified. Meanwhile, the recent widespread interest in the low-temperature behavior of small systems has provided a new point of viewing the pivotal role that dissipative environment plays in a virginal physical field of study, namely, quantum thermodynamics, for which the validity of the third law is an unavoidable subject to be elucidated.

Basing on these considerations, in this paper we devote our mind to the state function entropy of two typical quantum dissipative systems with anomalous spectral density, dedicating to elucidate its properties of evolving with temperature and quantum thermodynamical implication. In Sec. III, the remarkable integral method which is to be used in getting the free energy and entropy is briefly retrospected. Sec. III gives the explicit expression of entropy for two typical anomalous spectral systems. Sec. IV serves as a summary of our
II. INTEGRAL METHOD

In an earlier paper by G.W. Ford, et al. [14] a remarkable integral method was presented which provided us a convenient shortcut to calculate the free energy and entropy of a complex dissipative system [15–18]. The primary procedure is to begin with writing the free energy of the quantum oscillator as

\[ F(T) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \text{Im} \left\{ \frac{d\log \alpha(\omega + i0^+)}{d\omega} \right\}, \]

where \( f(\omega, T) \) is the free energy of a single oscillator of frequency \( \omega \), given by \( f(\omega, T) = k_B T \log[1 - \exp(-\hbar \omega/k_B T)] \) with the zero-point contribution \( \hbar \omega/2 \) being omitted. While \( \alpha(\omega) \) denotes the generalized susceptibility which can be got from the corresponding equation of motion of the system. After accomplishing this integration, the entropy of the quantum oscillator can then easily be got from a single derivation as

\[ S(T) = -\frac{\partial F(T)}{\partial T}. \]

Since the function \( f(\omega, T) \) in Eq. (1) vanishes exponentially for \( \omega \gg k_B T/\hbar \), the total integrand is then confined only to low frequencies as \( T \to 0 \) and the free energy together with the entropy then can be calculated by expanding the factor multiplying \( f(\omega, T) \) in the powers of \( \omega \). So what is essentially left to be determined in the following is the generalized susceptibility \( \alpha(\omega) \) which can be resulted from analytically solving the quantum Langevin equation (QLE)

\[ M\dddot{x} + M \int_0^t dt' \gamma(t-t')\dot{x}(t') + \partial_x U(x) = \xi(t), \]

where \( \gamma(t) \) is the memory friction function and \( \dot{\xi}(t) \) is the random force operator with zero mean, its correlation obeys the quantum fluctuation-dissipation theorem [6, 19]

\[ \langle \xi(t)\xi(t') \rangle_s = \frac{\beta \hbar}{\pi} \int_0^\infty d\omega J(\omega) \coth(\frac{\beta \hbar \omega}{2}) \cos(t - t'), \]

where \( \langle \cdots \rangle_s \) denotes the quantum symmetric average operation and \( \beta = 1/k_B T \) is the inverse temperature.
In the case of harmonic potential \( U(x) = \frac{1}{2}M\omega_0^2 x^2 \), the QLE is linear and its solution can be obtained by Fourier transformation as

\[
\tilde{x}(\omega) = \alpha(\omega)\tilde{\xi}(\omega),
\]

(5)

where \( \tilde{x}(\omega) = \int_{-\infty}^{\infty} dt x(t) \exp(i\omega t) \) and similarly noting is true for \( \tilde{\xi}(\omega) \). This results in the generalized susceptibility

\[
\alpha(\omega) = \left[-M\omega^2 - iM\omega\gamma(\omega) + M\omega_0^2\right]^{-1}.
\]

(6)

### III. ENTROPY AND ITS QUANTUM THERMODYNAMICAL IMPLICATION

Essentially, for arbitrary systems the expression of the generalized susceptibility \( \alpha(\omega) \) can be easily obtained given the Fourier transform of the memory friction function is known. For example, supposing \( \tilde{\gamma}(\omega) \) can be written in the following form of complex

\[
\tilde{\gamma}(\omega) = \text{Re}[\tilde{\gamma}(\omega)] + i\text{Im}[\tilde{\gamma}(\omega)],
\]

(7)

then after some algebra, we will obtain in the low-frequency limit

\[
\text{Im} \left\{ \frac{d \log \alpha(\omega)}{d\omega} \right\} = \frac{\omega_0^2 (1 + \omega \frac{d}{d\omega}) + \omega^2 (1 + \text{Im}[\tilde{\gamma}(\omega)] - \omega \frac{d}{d\omega})}{(\omega_0^2 - \omega^2)^2 + \omega^2 \tilde{\gamma}(\omega)^2} \text{Re}[\tilde{\gamma}(\omega)] \approx \frac{(1 + \omega \frac{d}{d\omega})\text{Re}[\tilde{\gamma}(\omega)]}{\omega_0^2}. \]

(8)

Since it has been confirmed in previous studies for the quantum dissipative systems \([6, 16, 20]\)

\[
\text{Re}[\tilde{\gamma}(\omega)] = \frac{1}{M} \frac{J(\omega)}{\omega},
\]

(9)

this provides a fundamentally convenient way to investigate the thermodynamical properties of the system via the spectral density \( J(\omega) \) in case of not knowing the explicit form of \( \tilde{\gamma}(\omega) \). Here in the following, the state function entropy of two typical quantum dissipative systems with anomalous spectral is studied using above-mentioned relations.
FIG. 1: The spectral density of the Drude and non-Ohmic (e.g. $\delta = 0.8$ and $\delta = 1.2$) system as functions of the frequency compared with the Ohmic case ($\delta = 1.0$), where dimensionless parameters such as $M = 1.0$ and $\omega_r = \gamma_d = \gamma = 1.0$ are used while $\omega_d = 5.0$.

A. Drude system

Firstly, let us consider the particular case of the system with a frequency-dependent Drude type of spectral density \[ J(\omega) = M\gamma\omega \frac{1}{1 + \omega^2/\omega_d^2}, \] (10)
where $\gamma$ is the friction constant and $\omega_d$ a Drude cut-off frequency. Seen in Fig.1 when the relevant frequencies of the system are much lower than $\omega_d$, the reservoir described by Eq.(10) behaves like an Ohmic bath with constant effective damping strength $\gamma$. The Drude model is therefore always be treated as a type of generalized Ohmic spectral.

After some algebra we obtain in the low-frequency limit

$$\text{Im}\left\{\frac{d\log \alpha(\omega)}{d\omega}\right\} = \frac{\gamma}{\omega_0^2} \frac{1 - \omega^2/\omega_d^2}{(1 + \omega^2/\omega_d^2)^2} \approx \frac{\gamma}{\omega_0^2}. \tag{11}$$

Hence, we get the expression of the free energy of quantum oscillator at low temperature,

$$F(T) = \frac{\gamma k_B T}{\pi \omega_0^2} \int_0^{\infty} d\omega \log[1 - \exp(-\hbar \omega/k_B T)]$$

$$= -\frac{\pi}{6} \hbar \gamma \left(\frac{k_B T}{\hbar \omega_0}\right)^2. \tag{12}$$
The entropy thus reads

\[ S(T) = -\frac{\partial F(T)}{\partial T} = \frac{\pi}{3} \gamma \left( k_B T \frac{k_B T}{\hbar \omega_0^2} \right). \tag{13} \]

Seen from it, the large-frequency cut-off of the Drude spectral is revealed to have no influence on the low-temperature properties of the quantum dissipative system. A kind of linear decaying entropy identical to the case of typical Ohmic friction is obtained. As \( T \to 0 \), \( S(T) \) vanishes principle to \( T \), in perfect conformity with the third law of thermodynamics.

**B. non-Ohmic system**

In order to have more intensive understanding on the system’s low-temperature quantum properties, we turn in the following to the non-Ohmic damping system which is another type of dissipative systems with anomalous spectral.

The non-Ohmic type of spectral emerges in various frameworks in physics \[6, 22, 23\]. For example, quantized chaotic systems might exhibit non-Ohmic fluctuations due to semiclassically implied long time power-law correlations \[24–26\]. Other examples may appear in the context of a many-particle system \[27, 28\], where the hierarchy of states and associated couplings, ranging from the single-particle levels to the exponentially dense spectrum of complicated many particle excitations, can lead to a very structural non-Ohmic band profile describing the residual interactions. As is seen in Fig. 1, in any cases the typical spectral is not like “white noise”.

In general, the non-Ohmic spectral density is written in the following form

\[ J(\omega) = M \gamma_\delta \left( \frac{\omega}{\omega_r} \right)^\delta, \tag{14} \]

where \( \delta \) is the power exponent taking values between 0 and 2, \( \gamma_\delta \) is the symmetrical friction constant tensor, and \( \omega_r \) denotes a reference frequency allowing for \( \gamma_\delta \) to have the dimension of a viscosity at any \( \delta \).

In the low-frequency limit we have

\[ \text{Im} \left\{ \frac{d \log \alpha(\omega)}{d\omega} \right\} = \frac{\delta \gamma_\delta \omega^{\delta-1}}{\omega_0^2 \omega_r^\delta}. \tag{15} \]
FIG. 2: The free energy and entropy of the Drude ($\delta = 1.0$) and non-Ohmic (e.g. $\delta = 0.5$ and $\delta = 1.6$) system as functions of the inverse temperature. Where dimensionless parameters such as $\hbar \omega_r = k_B = \gamma_\delta = 1.0$ as well as $\omega_0 = 1.0$ are used.

Hence, we get the expression of the free energy at low temperature

$$F(T) = \frac{\delta \gamma_\delta k_B T}{\pi \omega_0^2 \omega_r^\delta} \int_0^\infty d\omega \omega^{\delta - 1} \log[1 - \exp(-\hbar \omega/k_B T)]$$

$$= -\Gamma(\delta + 1)\zeta(\delta + 1) \frac{\gamma_\delta \hbar \omega_r}{\pi \omega_0^2} \left(\frac{k_B T}{\hbar \omega_r}\right)^{\delta + 1}.$$  (16)

The entropy thus reads

$$S(T) = \Gamma(\delta + 2)\zeta(\delta + 1) \frac{\gamma_\delta k_B T}{\pi \omega_0^2} \left(\frac{k_B T}{\hbar \omega_r}\right)^{\delta},$$  (17)

where the gamma function $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$ and the Riemann’s zeta-function $\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$ is used. With this result we conclude again that $S(T) \to 0$ as $T \to 0$ in agreement with the third law as is shown in Fig. 2. In all cases the entropies are revealed to decay as a $\delta$ order power function of the temperature. This is much different from that of the Drude system as well as the general Ohmic case. Formally it results from the fact that Eq. (15) has a factor $\omega^{\delta - 1}$ whereas the corresponding result of Eq. (11) is independent of the frequency. But actually its essential reason lives in the fact that the coupling strength between the system and the reservoir of these two damping systems is completely different from each other.
FIG. 3: The entropy of the non-Ohmic system as functions of the friction exponent $\delta$ at various $T$. Where dimensionless parameters such as $\hbar \omega = k_B = \gamma = 1.0$ as well as $\omega_0 = 1.0$ are used.

For more detailed information, we plot in Fig.3 the entropy of the non-Ohmic systems as functions of the friction exponent $\delta$ at different $T$. From which we can see that the entropy of the non-Ohmic systems evolves non-monotonically only if the system temperature is very low. This reveals a common influence of the non-Ohmic damping on the quantum thermodynamic properties of the system. Comparing $S(T)$ in the sub-Ohmic ($0 < \delta < 1$) and super-Ohmic ($1 < \delta < 2$) range with that of the Ohmic case ($\delta = 1$) one can found not all the non-Ohmic damping case is beneficial to the quantum dissipative system. Because the low-temperature quantum behavior tends to be annihilated in the limit of sub- or super-Ohmic range of damping. This is a particular conclusion resulted only from the study of non-Ohmic damping systems.

IV. SUMMARY AND DISCUSSION

In summary, we have studied in this paper the low-temperature thermodynamical properties of two typical anomalous quantum dissipative systems by deriving the entropy function from the spectral density. In all cases it is found that the entropy decays quickly and vanishes as the temperature approaches zero in good conformity with the third law of thermodynamics. The results obtained in this study provides another evidence for the validity of fundamental laws in the quantum dissipative region and may turn out to be relevant to experiments in nanoscience where one always tests the quantum thermodynamics of small
systems coupled to a heat bath. Experimentally, this work may also provide useful information for some other studies such as those in connection with the radiation of black-body.

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