Noncanonical statistics of a finite quantum system with non-negligible system-bath coupling

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The canonical statistics describes the statistical properties of an open system by assuming its coupling with the heat bath is infinitesimal in comparison with the total energy in thermodynamic limit. In this paper, we generally derive a noncanonical density matrix for the open system with a finite coupling to the heat bath, which deforms the energy shell to effectively modify the conventional canonical way. The obtained noncanonical distribution reflects the back action of system on the bath and thus depicts the statistical correlations between two subsystems by the mutual information as a result of energy conservation.

I. INTRODUCTION

Statistical mechanics describes the average properties of a system without referring to all its microscopic states. In most situations, the validity of the canonical statistical description is guaranteed in the thermodynamic limit, which requires that, while the degrees of freedom of the heat bath is infinite, the system-bath coupling approaches infinitesimal. However, if the system only interacts with a small heat bath with finite degrees of freedom, the system-bath interaction cannot be ignored compared with the energy of the heat bath. The properties of such a finite system have recently attracted a lot of attention with regard to both experiments [1,2] and theories [3–11].

Initiated from the pioneering work of Gibbs, the canonical statistics until now has been built on a rigorous foundation. For instance, if a pure state of the universe is assumed, then the canonical form of the system reduced density matrix is guaranteed by Levy's lemma [12–15]. Nevertheless, the conventional canonical statistics still cannot describe well the thermodynamic behavior of the finite system when the sufficiently large system-bath interaction is taken into consideration. The statistics of an open system with considerable system-bath coupling has been studied by harmonic oscillator [4,16] and spin [17] systems. In this paper, we generally consider an effective system-bath coupling by assuming the bath possesses a much more dense spectrum than that of the system, and then the system-bath interaction energy can be treated as the deformation of the energy shell for the total system. Therefore, the canonical density matrix of the system is modified to be a noncanonical one. This modified distribution obviously implies that corrections are necessary for the finite-system thermodynamic quantities in canonical statistics, such as average internal energy and its fluctuation.

The rest of the paper is organized as follows. In Sec. II we derive an effective Hamiltonian of the total system by perturbation theory; via this Hamiltonian the noncanonical statistical distribution without referring to any specific model

is presented. To further illustrate the novel thermodynamic properties of the finite system by noncanonical statistics, a model of coupled harmonic oscillators is introduced in Sec. III, and the statistical quantities such as internal energy, fluctuation, and the mutual information between two subsystems are calculated. We conclude in Sec. IV.

II. FINITE SYSTEM-BATH COUPLING

We generally consider a composite coupled system, which can be divided into a system S with Hamiltonian H_S and a heat bath B with Hamiltonian H_B. The coupling between the system and the bath can be generally described by H_I. Then we have the total Hamiltonian $H = H_S + H_B + H_I$. The system and the bath have the following spectrum decompositions:

$$H_S = \sum_n E_n |n\rangle\langle n|, \tag{1}$$

$$H_B = \sum_{j=1}^{N} \sum_{k_j} \epsilon_{k_j} |k_j\rangle\langle k_j| \otimes \prod_{i \neq j}^{N} I_i. \tag{2}$$

Here $|n\rangle$ is the eigenstate of the system with the corresponding eigenenergy E_n. The heat bath is composed of N noninteracting particles, the eigenstate of the jth particle is $|k_j\rangle$ with the corresponding eigenenergy ϵ_{k_j}, and I_i is the identity operator of the Hilbert space of the ith particle. In the following, we will use the notation $|\vec{k}\rangle = \prod_{j=1}^{N} |k_j\rangle$, $\vec{k} = (k_1, k_2, \ldots, k_N)$, to present the eigenstate of H_B and denote $\epsilon(\vec{k}) = \sum_{j=1}^{N} \epsilon_{k_j}$ as its eigenenergy. Usually, the energy spectrum of the system is much sparser than the heat bath, i.e.,

$$\min |E_n - E_m| \gg \max |\epsilon(\vec{k}) - \epsilon(\vec{l})|, \tag{3}$$

which holds for the neighboring energy levels n and m ($\vec{k}$ and $\vec{l}$) of the system (bath) (see Fig. 1).

The system-bath interaction H_I is weak compared to H_0, which reads

$$H_I = \sum_{j=1}^{N} \sum_{n,n',k_j,k'_j} g_{nk_j,n'k'_j} |n,k_j\rangle\langle n',k'_j| \otimes \prod_{i \neq j}^{N} I_i \tag{4}$$
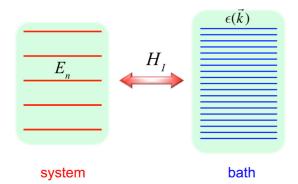
FIG. 1. (Color online) The energy spectra of the system and the heat bath. The spectral density of the heat bath should be much larger than the system.

with $|n,k_j\rangle \equiv |n\rangle \otimes |k_j\rangle$. To obtain the canonical density matrix ρ_S of the system, we usually start with a microcanonical density matrix of the system and its heat bath,

$$\rho_{\mathrm{mic}} = \frac{P_{V(E,\delta)}}{\dim V(E,\delta)}, \qquad (5)$$

without considering H_I, and then trace over the heat bath, i.e., $\rho_S = \mathrm{Tr}_B \rho_{\mathrm{mic}}$. The density of matrix ρ_{mic} describes a microcanonical ensemble which is assumed in an energy shell $[E, E + \delta]$ with δ a small energy scale, $\delta \ll E$, and

$$V(E,\delta) = \mathrm{Span}\{|n,\vec{k}\rangle : E \leqslant E_n + \epsilon(\vec{k}) \leqslant E + \delta\} \qquad (6)$$

is the subspace of $H_S + H_B$ associated with this energy shell, and $P_{V(E,\delta)}$ is the projection operator to $V(E,\delta)$. Then the probability of finding the state $|n\rangle$ in this canonical ensemble is

$$P_n(E) = \langle n|\rho_S|n\rangle = \frac{\Omega(E - E_n, \delta)}{\dim V(E,\delta)}, \qquad (7)$$

where $\Omega(E - E_n, \delta) = \dim V_n(E - E_n, \delta)$ and

$$V_n(E - E_n, \delta) = \mathrm{Span}\{|n,\vec{k}\rangle : E - E_n \leqslant \epsilon(\vec{k})$$
$$\leqslant E - E_n + \delta\} \qquad (8)$$

represents the subspace of $H_S + H_B$ associated with the subenergy shell $[E - E_n, E - E_n + \delta]$ when the system state is fixed at $|n\rangle$, obviously, $V(E,\delta) = \sum_n \bigoplus V_n(E - E_n, \delta)$.

In certain cases that the heat bath is no longer infinitely large, and the system-bath interaction energy is small but should not be complete neglected, the reduced density matrix of the system can be obtained by perturbatively considering H_I. The first-order perturbation effect of these off-diagonal terms with $n \neq n'$ can be ignored under the condition

$$\left| \frac{g_{nk_j, n'k_j'}}{E_{n'} - E_n + \epsilon_{k_j'} - \epsilon_{k_j}} \right| \ll 1. \qquad (9)$$

However, for the terms with $n = n'$, the above condition $|g_{nk_j, nk_j'}(\epsilon_{k_j'} - \epsilon_{k_j})^{-1}| \ll 1$ will be violated due to the properties of the energy spectra given in Eq. (3). Thus the diagonal terms can contribute to the system behaviors and should be kept in the interaction Hamiltonian [16], which yields

$$H_I \approx \sum_{j=1}^{N} \sum_{n,k_j,k_j'} g_{nk_j,nk_j'} |nk_j\rangle\langle nk_j'| \otimes \prod_{i \neq j}^{N} I_i. \qquad (10)$$
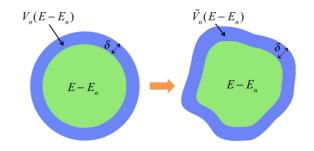

FIG. 2. (Color online) The subenergy shell without and with the consideration of the system-bath coupling are schematically shown in a manner analogous to classical phase space.

Then the total effective Hamiltonian has the diagonal form with respect to the eigenstates of the system, i.e.,

$$H_{\mathrm{eff}} = \sum_n [E_n + h(n)]|n\rangle\langle n| \qquad (11)$$

with

$$h(n) = \sum_{j=1}^{N} \sum_{k_j,k_j'} (\epsilon_{k_j} \delta_{k_j,k_j'} + g_{nk_j,nk_j'})|k_j\rangle\langle k_j'| \otimes \prod_{i \neq j}^{N} I_i. \qquad (12)$$

Here $h(n)$ describes the heat-bath Hamiltonian corresponding to the system state $|n\rangle$. It can be further diagonalized as $h(n) = \sum_{j=1}^{N} \sum_{\alpha_j} \varepsilon_{\alpha_j}(n)|\alpha_j\rangle\langle\alpha_j| \otimes \prod_{i \neq j}^{N} I_i$, with the eigenstate $|\vec{\alpha}\rangle = \prod_{j=1}^{N} |\alpha_j\rangle$ and the corresponding eigenenergy $\varepsilon(\vec{\alpha},n) = \sum_{j=1}^{N} \varepsilon_{\alpha_j}(n)$. The new energy spectrum of the heat bath $\varepsilon(\vec{\alpha},n)$ is changed compared with the original energy spectrum $\epsilon(\vec{k})$ due to the system-bath coupling.

This system-bath coupling is usually negligible when we study the thermalized state of the system in a large heat bath. However, in the situation of finite system statistics, it is crucial to consider the system-bath interaction energy for the relatively small heat bath. The effective Hamiltonian Eq. (11) is already diagonalized with diagonal elements $E(n,\vec{\alpha}) = E_n + \varepsilon(\vec{\alpha},n)$. Then it is straightforward to define the new subspace

$$\tilde{V}(E,\delta) = \mathrm{Span}\{|n,\vec{\alpha}(n)\rangle : E \leqslant E_n + \varepsilon(\vec{\alpha},n) \leqslant E + \delta\}, \qquad (13)$$

corresponding to $V(E,\delta)$, by substituting $|n,\vec{k}\rangle$ with $|n,\vec{\alpha}(n)\rangle$ and $\epsilon(\vec{k})$ with $\varepsilon(\vec{\alpha},n)$. In the same way, we define

$$\tilde{V}_n(E - E_n, \delta) = \mathrm{Span}\{|n,\vec{\alpha}(n)\rangle : E - E_n \leqslant \varepsilon(\vec{\alpha},n)$$
$$\leqslant E - E_n + \delta\} \qquad (14)$$

and $\tilde{\Omega}(E - E_n, \delta) = \dim \tilde{V}_n(E - E_n, \delta)$. We schematically illustrated the deformation of the subenergy shell in Fig. 2. The diagonal term of the system reduced density matrix $\tilde{\rho}_S$ is

$$\tilde{P}_n(E) = \frac{\tilde{\Omega}(E - E_n, \delta)}{\dim \tilde{V}(E,\delta)}, \qquad (15)$$

which considers the correction of the canonical density matrix ρ_S due to the system-bath interaction; thus we name $\tilde{\rho}_S$ the noncanonical density matrix of the system and $\tilde{P}_n(E)$ the noncanonical distribution.

To further obtain an explicit expression of $\tilde{P}_n(E)$, we introduce the entropy defined by $S(E) = k_B \ln \Omega(E,\delta)$, where k_B is the Boltzmann constant. We note that, the function form

of $\Omega(E,\delta)$ is dependent on the Hamiltonian H; thus with or without the considering of H_I, the deformation of energy shell yields $\Omega(E,\delta)$ and $\tilde{\Omega}(E,\delta)$ have different expressions. Therefore, we should keep in mind that $S(E)$ is actually a functional of $V(E,\delta)$, i.e., $S(E) \equiv S[V(E,\delta)]$. When the system is in the state $|n\rangle$, the entropy can be expanded as [18]

$$\tilde{S}(E - E_n) = S(E - E_n) + \delta_n S(E - E_n)$$
$$\approx S(E) - \frac{\partial S(E)}{\partial E}E_n + \phi_n, \qquad (16)$$

where

$$\phi_n = \delta_n S(E) - \frac{\partial[\delta_n S(E)]}{\partial E}E_n. \qquad (17)$$

The term $\delta_n S(E - E_n)$ is the functional variation of $S(E - E_n)$, where the subscript n means that the functional variation also depends on the state of system. In the above derivation, we actually assume a small deformation of the energy shell, i.e., when N is large, there is a small difference between $\Omega(E - E_n,\delta)$ and $\tilde{\Omega}(E - E_n,\delta)$. This difference vanishes in the thermodynamic limit as shown in Ref. [4] for a concrete example. As E_n is still small compared with E, then we can expand $S(E - E_n)$ to the first order, and ϕ_n represents the first-order approximation of $\delta_n S(E - E_n)$. The derivative terms of $S(E)$ can be evaluated by the idea from classical phase space: Since $\Omega(E)$ is the dimension of the subspace $V(E,\delta)$, it is proportional to the volume of the energy shell in the phase space. In a N-dimensional space, the volume confined in an isoenergic surface of energy E can be considered as the volume of a N-dimensional polyhedron with effective radius E, which is proportional to $E^{\zeta N}$, where ζ is a dimensionless real number independent of N and is usually related to the degeneracy of the system. Therefore, the volume of the energy shell is given by

$$\Omega(E) \propto (E + \delta)^{\zeta N} - E^{\zeta N}, \qquad (18)$$

which leads to

$$\beta(E) = \frac{\partial S(E)}{\partial E} = \frac{k_B(\zeta N - 1)}{E}. \qquad (19)$$

With the thermodynamic relations, $\beta = (k_B T)^{-1}$ and T is the temperature of the system in equilibrium. Obviously, Eq. (19) recovers the equipartition theorem $E \approx \zeta N k_B T$, i.e., each degree of freedom contributes $\zeta k_B T$ to the total energy. Therefore, the noncanonical distribution reads

$$\tilde{P}_n(E) = \frac{1}{\tilde{\mathcal{Z}}}e^{-\beta E_n + \phi_n/k_B}, \qquad (20)$$

where $\tilde{\mathcal{Z}} = \sum \exp(-\beta E_n + \phi_n/k_B)$ is the partition function.

If the interaction energy could be neglected compared with the total energy E, the variation terms ϕ_n containing $\delta_n S(E)$ in Eq. (20) can be dropped and thus naturally lead to the usual canonical form,

$$P_n(E) = \frac{1}{\mathcal{Z}}e^{-\beta E_n}. \qquad (21)$$

Otherwise, the deformation of energy shell which leads to ϕ_n will shift the system energy level and thus modify $P_n(E)$. Usually ϕ_n cannot be calculated easily; however, for some special models (one of which will be introduced in the next section), we can find a simple expression for ϕ_n.

III. ILLUSTRATION WITH HARMONIC OSCILLATORS SYSTEM

Now we consider a coupled harmonic oscillators system as an example to illustrate the statistical thermodynamic properties of a finite system. The system S is a single harmonic oscillator with eigenfrequency ω and $a^\dagger(a)$ as its creation (annihilation) operator. The heat bath is generally modeled as a collection of harmonic oscillators with Hamiltonian $H_B = \sum_{j=1}^{N} \omega_j b_j^\dagger b_j$. Here $b_j^\dagger(b_j)$ is the creation (annihilation) operator of the oscillator with frequency ω_j. In the weak-coupling limit, we can assume the effective system-bath interaction as

$$H_I = \sum_{j=1}^{N} \lambda_j a^\dagger a(b_j^\dagger + b_j). \qquad (22)$$

This Hamiltonian is usually used to describe the interaction between a single mode light field and mechanical oscillators in opticalmechanical system [19–21].

In this model, the eigenvalues of the total Hamiltonian are

$$E(n,\vec{m}(n)) = n\omega + \Delta_n + \sum_{\{m_j\}} m_j \omega_j, \qquad (23)$$

which corresponding to the eigenstates $|n,\vec{m}(n)\rangle = |n\rangle \otimes \prod_{j=1}^{N} |m_j(n)\rangle$. The eigenstate of the heat bath $|m_j(n)\rangle$ is defined as a displaced Fock state $|m_j(n)\rangle = D(-\lambda_j n/\omega_j)|m_j\rangle$, with the displacement operator $D(\alpha_j) = \exp(\alpha a_j^\dagger - \alpha^* a_j)$. Here the deformation of the energy shell is described by an n-dependent factor,

$$\Delta_n = -\sum_{j=1}^{N} \frac{\lambda_j^2 n^2}{\omega_j} \equiv -\kappa n^2. \qquad (24)$$

Therefore, in this model the deformation of each subenergy shell is only related to Δ_n, which is independent of the specific state of the heat bath. Then the deformed energy shell is simply related with the original energy shell without considering H_I by

$$\tilde{V}_n(E - E_n,\delta) = V_n(E - \Delta_n - E_n,\delta). \qquad (25)$$

Further, the function form of $\tilde{S}(E - E_n)$ is the same as $S(E - E_n)$ by only substituting E with $E - \Delta_n$:

$$\tilde{S}(E - E_n) = S(E - \Delta_n - E_n). \qquad (26)$$

Then the functional variation $\delta_n S(E)$ can be calculated by the usual differential to the first order,

$$\delta_n S(E) \approx \frac{\partial S(E)}{\partial E}\Delta_n. \qquad (27)$$

Together with the results in Eq. (20), the noncanonical distribution is given by

$$\tilde{P}_n(E) = \frac{1}{\tilde{\mathcal{Z}}}e^{-\beta(n\omega - n^2\kappa) - \xi \omega \kappa n^3}, \qquad (28)$$

where

$$\xi = \frac{\partial^2 S(E)}{\partial E^2} = -\frac{k_B(\zeta N - 1)}{E^2}. \qquad (29)$$

The square and cubic terms of n in the exponent of $\tilde{P}_n(E)$ greatly change the statistical distribution from the canonical
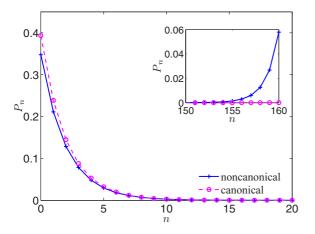
FIG. 3. (Color online) The noncanonical (blue solid line) and canonical (pink dashed line) distribution functions for coupled oscillators system. We choose $\omega = 1$, $E = 100$, $\beta = 0.5$, and $\kappa = 0.00235$. The highest energy level is $n_{\max} = 160$. The noncanonical and canonical distributions are similar for low energy levels while they differ greatly for high energy levels.

distribution $P_n(E) = \mathcal{Z}^{-1} \exp(-\beta n\omega)$, especially for large n. However, Eq. (28) does not apply to very large N for the following reason: The total energy E of the system and the heat bath is conserved, and the heat bath energy should always be non-negative $\sum_{\{m_j\}} m_j \omega_j > 0$. Thus, the energy shell of $V_n(E - \Delta_n - E_n, \delta)$ constrains the system energy level by $E \geqslant E_n$, which implies $n < (\omega - \sqrt{\omega^2 - 4\kappa E})/(2\kappa)$. Therefore, for such coupled system, the maximum energy level for the system is

$$ n_{\max} = \left\lfloor \frac{\omega - \sqrt{\omega^2 - 4\kappa E}}{2\kappa} \right\rfloor, \tag{30} $$
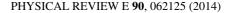
where $\lfloor x \rfloor$ represents the maximum integer below x.

Usually κ is much smaller than ω, thus the noncanonical statistics distribution $\tilde{P}_n(E)$ for low energy levels does not differ much from the canonical one, as shown in Fig. 3. However, as $|\Delta_n|$ grows with n^2, the high energy levels have more populations than those in the canonical distribution, which can be seen from the inset of Fig. 3. We choose the system eigenfrequency as unit $\omega = 1$, the total energy $E = 100$, and $\kappa = 0.00235$. According to Eq. (30), the highest energy level is $n_{\max} = 160$ in this situation. The canonical distribution is plotted by set $\kappa = 0$ in $\tilde{P}_n(E)$. A numerical research also gave the similar noncanonical distribution for coupled spin systems [22].

Because the high-energy states have relatively larger populations, the internal energy of the system

$$ U = \sum_{n=0}^{n_{\max}} n\omega \tilde{P}_n(E) \tag{31} $$

under the noncanonical statistics is larger than that under the canonical one. This fact is illustrated in Fig. 4, where the internal energy U is plotted with respect to β. The distinction between the noncanonical and canonical statistics for U evidently appears when the inverse temperature β decreases and the interaction energy strength κ grows. As β approaches
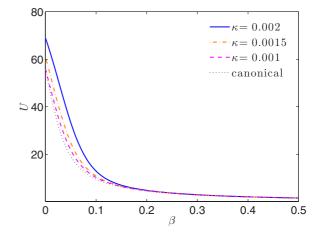

FIG. 4. (Color online) The internal energy U of the system with respect to β for noncanonical and canonical statistics. We plot the cases of $\kappa = 0.002$, $n_{\max} = 138$ (blue solid line); $\kappa = 0.0015$, $n_{\max} = 122$ (orange dotted-dash line); $\kappa = 0.001$, $n_{\max} = 112$ (pink dashed line); and the canonical case for $\kappa = 0$, $n_{\max} = 112$. For small β, the internal energy U is explicitly larger than that given by canonical statistics.

zero, the high-temperature limit of the internal energy U arrives at $n_{\max}\omega/2$, which is finite as the total energy is up-bounded by E for small heat bath. This differs substantially from the case in the thermodynamic limit: The average energy of a harmonic oscillator which contacts with an infinite heat bath will diverge when β decreases to zero.

Another feature reflecting the nonmonotony of the non-canonical distribution is the relative fluctuation of the system internal energy

$$ (\Delta U)^2 = \frac{1}{U^2} \sum_{n=0}^{n_{\max}} (n\omega - U)^2 \tilde{P}_n(E). \tag{32} $$
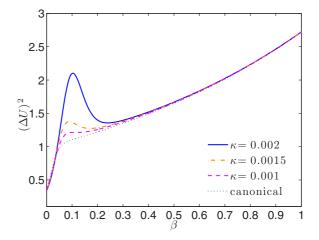

FIG. 5. (Color online) The internal energy relative fluctuation $(\Delta U)^2$ of the system with respect to β for noncanonical and canonical statistics. The parameters are chosen the same as Fig. 4. A local maximum appears in the energy fluctuation for small β which results of the noncanonical statistics.

As shown in Fig. 5, at both the low- and high-temperature limits, the noncanonical and canonical statistics of the system present similar fluctuation behavior. To characterize these two limits, we consider the system as a harmonic oscillator with truncated energy levels (the highest energy level is labeled by $n_{\max}$) under canonical statistics ($\kappa = 0$), whose energy fluctuation is denoted as $(\Delta U_C)^2$. It is analytically calculated that in the low-temperature limits, the fluctuation $(\Delta U_C)^2 \approx \exp(\beta\omega)$ is exactly the same as the result when $n_{\max} \to \infty$. Because the populations of the high-energy levels decrease significantly in the low temperature, only the several low-energy levels determine the thermodynamic behavior. In the high-temperature limit, the energy fluctuation behaves as

$$(\Delta U_C)^2 \approx \frac{1}{3} + \frac{2}{3n_{\max}} + \frac{n_{\max}}{9}\beta, \qquad (33)$$

which is a linear function of β. We remark here that the high-temperature limit and thermodynamic limit cannot commute with each other, as

$$\lim_{n_{\max}\to\infty}\lim_{\beta\to 0}(\Delta U_C)^2 = \tfrac{1}{3}, \qquad (34)$$

while

$$\lim_{\beta\to 0}\lim_{n_{\max}\to\infty}(\Delta U_C)^2 = 1. \qquad (35)$$

However, in the intermediate range of β, a local maximum in energy fluctuation distinguishes the noncanonical distribution from the canonical one, especially for strong system-bath interaction κ. This maximum can be qualitatively understood as follows: we can rewrite the noncanonical distribution as $\tilde{P}_n(E) = \mathcal{Z}^{-1}\exp(-\beta\eta_n n\omega)$, where $\eta_n = 1 - \kappa n/\omega - \kappa n^2/E$ is a positive factor for $n \leqslant n_{\max}$. As $\eta_n \leqslant 1$, the reverse temperature β can be considered as effectively reduced by η_n, thus the linear region for small β is enlarged in the noncanonical statistics. Based on the above observations, we know that the noncanonical statistics exhibits obviously novel effects when the interaction energy strength κ is large and the temperature is high.

Besides the high distribution tail for a single system, the noncanonical statistics provides other new characters when the system is a composite of two independent subsystems l_1 and l_2. Even if these two subsystems do not directly interact with each other, the deformation of the energy shell can effectively result in a correlation between them. Here we still use harmonic oscillator (HO) systems for illustration. The system consists of two single-mode HOs with the Hamiltonian $H_S = \sum_{k=1,2}\omega_k a_k^\dagger a_k$. The system interacts with a common small heat bath, which can be modeled by the Hamiltonian $H_B = \sum_{j=1}^{N}\omega_j b_j^\dagger b_j$. The interaction term reads

$$H_I = \sum_{k=1,2}\sum_{j=1}^{N}\lambda_{kj}a_k^\dagger a_k(b_j^\dagger + b_j). \qquad (36)$$

Following the same discussion about the energy shell deformation for a single system, we can straightforwardly obtain the joint distribution of the composite system as

$$\tilde{P}\big(E,E_n^{(1)},E_m^{(2)}\big) = \frac{1}{\mathcal{Z}_t}e^{-\beta(E_{nm}+\Delta_{nm})+\xi\Delta_{nm}E_{nm}}, \qquad (37)$$
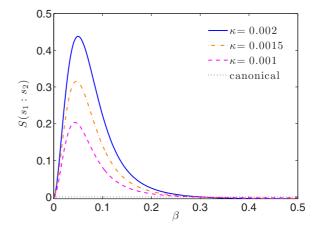

FIG. 6. (Color online) The mutual entropy of two identical harmonic oscillators (HOs) by noncanonical and canonical statistics. The eigenfrequency of two identical HOs is $\omega = 1$, and $\kappa = 0.002$, $n_{\max} = 138$ (blue solid line); $\kappa = 0.0015$, $n_{\max} = 122$ (orange dotted-dash line); $\kappa = 0.001$, $n_{\max} = 112$ (pink dashed line); and the canonical case for $\kappa = 0$, $n_{\max} = 112$.

where $E_{nm} = n\omega_1 + m\omega_2$ and

$$\Delta_{nm} = -\sum_{j=1}^{N}\frac{(\lambda_{1j}n + \lambda_{2j}m)^2}{\omega_j}$$

$$\mathcal{Z}_t = {\sum_{n,m}}'e^{-\beta(E_{nm}+\Delta_{nm})+\xi\Delta_{nm}E_{nm}}.$$

Here $\sum'_{n,m}$ means the summation of the system energy levels should satisfy the constrain $0 \leqslant E_{nm} + \Delta_{nm} \leqslant E$. It can be seen from Eq. (37) that the statistics of two subsystems are not independent with each other due to the cross-term in Δ_{nm}. This statistical correlation can be described by mutual information defined as

$$S(l_1 : l_2) = S(l_1) + S(l_2) - S(l_1 + l_2), \qquad (38)$$

where the entropy

$$S(l_k) = -\sum_{n=0}^{n_{\max}}\tilde{P}\big(E,E_n^{(k)}\big)\ln\tilde{P}\big(E,E_n^{(k)}\big) \qquad (39)$$

and

$$S(l_1 + l_2) = -{\sum_{n,m}}'\tilde{P}\big(E,E_n^{(1)},E_m^{(2)}\big)\ln\tilde{P}\big(E,E_n^{(1)},E_m^{(2)}\big). \quad (40)$$

For simplicity, we assume the two HOs are identical with $\omega_1 = \omega_2 \equiv \omega$, $\lambda_{1j} = \lambda_{2j} \equiv \lambda_j$, and κ is defined the same as Eq. (24). As shown in Fig. 6, there appears to be a nonzero mutual entropy if we use noncanonical statistics to describe the composite system in a common small heat bath. In contrast, if the interaction energy is too small to be considered compared with the total energy, we can use the canonical distribution to calculate the mutual entropy, which naturally gives $S(l_1 : l_2) = 0$, i.e., the two subsystems are not correlated with each other.

IV. CONCLUSION

We study the statistical thermodynamics of an open system whose interaction with the heat bath cannot be neglected. The interaction modifies the system energy shell and leads to the noncanonical density matrix for such a system. It is shown in a model that noncanonical distribution has a big "tail" for higher energy levels, which is the most significant difference from the canonical distribution. This noncanonical feature results in higher internal energy and energy fluctuation of the system. Moreover, different parts of the composite system are naturally correlated with each other, which is described by mutual entropy. We note that the noncanonical form of distribution may be related to the explanation of the black hole information paradox [23].

[1] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature (London) **440**, 900 (2006).

[2] J. Liphardt, S. Dumont, S. B. Smith, I. Tinoco, Jr., and C. Bustamante, Science **296**, 1832 (2002).

[3] T. L. Hill, J. Chem. Phys. **36**, 3182 (1962).

[4] H. Dong, S. Yang, X. F. Liu, and C. P. Sun, Phys. Rev. A **76**, 044104 (2007).

[5] M. Rigol, V. Dunjko, and M. Olshanii, Nature (London) **452**, 854 (2008).

[6] J. Rau, Phys. Rev. A **84**, 012101 (2011).

[7] H. Hasegawa, Phys. Rev. E **83**, 021104 (2011).

[8] H. Hasegawa, J. Math. Phys. **52**, 123301 (2011).

[9] M. Falcioni, D. Villamaina, A. Vulpiani, A. Puglisi, and A. Sarracino, Am. J. Phys. **79**, 777 (2011).

[10] W. G. Wang, Phys. Rev. E **86**, 011115 (2012).

[11] G. L. Barnes and M. E. Kellman, J. Chem. Phys. **139**, 214108 (2013).

[12] P. Bocchieri and A. Loinger, Phys. Rev. **114**, 948 (1959).

[13] H. Tasaki, Phys. Rev. Lett. **80**, 1373 (1998).

[14] S. Popescu, A. J. Short, and A. Winter, Nat. Phys. **2**, 754 (2006).

[15] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, Phys. Rev. Lett. **96**, 050403 (2006).

[16] H. Dong, X. F. Liu, and C. P. Sun, Chin. Sci. Bull. **55**, 3256 (2010).

[17] C. K. Lee, J. S. Cao, and J. B. Gong, Phys. Rev. E **86**, 021109 (2012).

[18] K. Huang, *Statistical Mechanics* (John Wiley & Sons, New York, 1987).

[19] C. K. Law, Phys. Rev. A **49**, 433 (1994).

[20] C. K. Law, Phys. Rev. A **51**, 2537 (1995).

[21] J. Chan, T. P. M. Alegre, A. H. Safavi-Naeini, J. T. Hill, A. Krause, S. Gröblacher, M. Aspelmeyer, and O. Painter, Nature **478**, 89 (2011); J. D. Teufel, T. Donner, D. Li, J. W. Harlow, M. S. Allman, K. Cicak, A. J. Sirois, J. D. Whittaker, K. W. Lehnert, and R. W. Simmonds, *ibid.* **475**, 359 (2011).

[22] Wenxian Zhang, C. P. Sun, and Franco Nori, Phys. Rev. E **82**, 041127 (2010).

[23] B. Zhang, Q. Y. Cai, L. You, and M. S. Zhan, Phys. Lett. B **675**, 98 (2009); B. Zhang, Q. Y. Cai, M. S. Zhan, and L. You, Ann. Phys. **326**, 350 (2011).