

Quantum thermalization with couplings

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We present an exactly solvable model to study the role of the system-bath coupling for the generalized canonical thermalization, which reduces almost all the pure states of the “universe” (formed by a system S plus its surrounding heat bath B) to a canonical equilibrium state of S . It is found that, for the overwhelming majority of the “universe” states (they are entangled at least), the diagonal canonical typicality remains robust with respect to finite interactions between S and B . Particularly, a decoherence mechanism is utilized here to account for the vanishing of the off-diagonal elements of the reduced density matrix of S . The nonvanishing off-diagonal elements due to the finite size of the bath and the stronger system-bath interaction might offer more to quantum thermalization.

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Recently a quantum entanglement based mechanism for universal canonical thermalization has been found in the following meaning: almost all the pure states of the “universe” can be reduced into a generalized canonical state of the system S by tracing over the bath [1]. Here, the allowed “universe” states are in a subspace defined by a general constraint R , which limits the number of the states to be finite, yet very large. It is noticed that in such generalized thermalization, the constraint R is rather general and does not need to be the energy shell of the “universe,” and generally speaking, it does not lead to the usual canonical state in thermal equilibrium.

When the constraint R is specialized as a total energy shell, the generalized canonical state becomes a usual canonical thermal state. Such a thermalization was described by the canonical typicality in Ref. [2] associated with the so-called overwhelming majority rule, based on the law of large numbers. Significant results concerning such canonical typicality have been obtained by several authors for different purposes [3–8]. Actually, to derive the canonical distribution of S from the microcanonical density matrix [9] or an entangled pure state [2] of the “universe” $U=S+B$, the interaction between S and B should be weak enough to allow a physical partition for the “universe.”

In this paper, we will quantitatively consider the effect of system-bath coupling in the canonical thermalization leading to the equilibrium canonical state mentioned above. The present investigation only concerns the usual canonical state. In the weak interaction limit, the inverse temperature $\beta = \partial S(E)/\partial E$ emerges from the thermodynamic entropy $S(E) = \ln \Omega(E, \delta)$, where $\Omega(E, \delta)$ is the microstate number of the bath in the energy shell $[E, E + \delta]$. Since the interaction between S and B deforms the geometry of the energy shell, we will reexamine the validity of the temperature definition from the new perspective offered by the generalized thermalization [1,2]. We understand how the off-diagonal elements of the reduced density matrix of S vanish due to the factorization structure, in association with the random phase expla-

nation [10,11]. We find that if the number of modes of the bath is not large enough and the system-bath coupling is strong enough, generally there exist nonzero off-diagonal elements in the reduced density matrix. Notice that these nonzero off-diagonal elements introduce quantum coherence into the usual thermal equilibrium state and thus result in thermodynamic features.

We begin with a simple model: the system S we consider is an M -level system with the Hamiltonian $H_S = \sum_n \epsilon_n |n\rangle\langle n|$, where $|n\rangle$ is the eigenstate with eigenvalue ϵ_n , $n = 1, 2, \dots, M$; and the bath B is modeled as a collection of N harmonic oscillators of frequencies ω_j ($j=1, 2, \dots, N$) with the Hamiltonian $H_B = \sum_j \omega_j a_j^\dagger a_j$. This model can be regarded as a universal approach, because in the weak coupling limit, any heat bath could be universally modeled as a collection of harmonic oscillators with linear couplings to the surrounded system according to the proofs in Ref. [13]. For this reason, the interaction H_I between B and S should be modeled to be linear with respect to the bath variables a_j^\dagger and a_j . So we assume a simplest system-bath coupling

$$H_I = \sum_{j,n} \lambda_n |n\rangle\langle n| (g_j a_j^\dagger + \text{H.c.}), \quad (1)$$

where λ_n are real numbers. Note that H_I is of nondemolition character since $[H_S, H_I] = 0$. Thus, the interaction only causes the dephasing of S , and the energy dissipation of S will not appear [11,12].

Obviously, the eigenvalues of the “universe” formed by B and S are $E(n, \{n_j\}) = \epsilon_n(\kappa) + \sum_{j=1}^N n_j \omega_j$, corresponding to the eigenstates $|n, \{n_j\}\rangle = |n\rangle \otimes \prod_{j=1}^N |n_j(n)\rangle$, where $\epsilon_n(\kappa) = \epsilon_n - \kappa \lambda_n^2$ and the displaced Fock state $|n_j(n)\rangle = D(\alpha_{jn}) |n_j\rangle$ is defined in terms of the Fock states $|n_j\rangle$ of B and the coherent-state-generate operator $D(\alpha_{jn}) = \exp(\alpha_{jn} a_j^\dagger - \text{H.c.})$ with the displacement parameters $\alpha_{jn} = -\lambda_n g_j / (2\omega_j)$; especially, the parameter $\kappa = \sum_j |g_j|^2 / (4\omega_j)$ reflects the role of the interaction between S and B .

Note that the system-bath coupling deforms the energy shell of thickness δ defined by the total constraint $E \leq E(n, \{n_j\}) \leq E + \delta$. This energy shell determines a subset of the “universe” states. For convenience, we denote by $V(E, \delta)$

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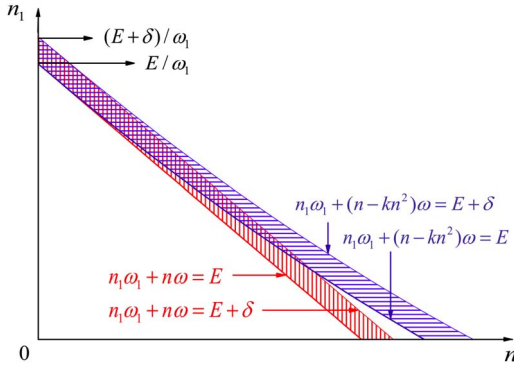


FIG. 1. (Color online) Geometrical deformation of the energy shell. Here we show explicitly the deformation, when S is a harmonic oscillator. (a) Without the interaction, the energy shell is the red area (vertical stripes); (b) the interaction deforms the red area (vertical stripes) into the blue area (horizontal stripes).

the subspace spanned by this subset. We consider the following simple example: the system S is a harmonic oscillator with frequency ω and $\lambda_n = n$. In this case, the renormalized energy of S is $E_s(n) = n\omega - \kappa n^2$. In Fig. 1, we illustrate the deformation of the energy shell when $N=1$. If there were no interaction, the above constraint would produce the red area (vertical stripes). The interaction introduces the nonlinear term κn^2 to deform it into the blue area (horizontal stripes).

Generally, in order to derive the canonical distribution of S from an entangled pure state of the “universe,” we need to calculate the dimension $\mathcal{H}_N(E, \delta, \kappa)$ of $V(E, \delta)$ and the dimension $\Omega_N(E - \epsilon_n, \delta, \kappa)$ of the subspace $V^B(n, \kappa)$ spanned by the states with the constraint

$$E - \epsilon_n(\kappa) \leq \sum_j n_j \omega_j \leq E + \delta - \epsilon_n(\kappa). \quad (2)$$

Let us start with a pure entanglement state

$$|\psi\rangle = \sum' C(n, \{n_j\}) |n, \{n_j\}\rangle \quad (3)$$

of the constrained “universe,” where \sum' denotes the summation under the total constraint. By tracing over the variables of B , the reduced density matrix $\rho_S = \text{Tr}_B(|\psi\rangle\langle\psi|)$ of S is obtained as

$$\rho_S = \sum_n P_n |n\rangle\langle n| + \sum_{n \neq m} F_{nm} |n\rangle\langle m|, \quad (4)$$

where the diagonal elements are $P_n = P_n(E, \kappa) = \sum'' |C(n, n_j)|^2$ and \sum'' stands for the summation under the constraint (2). We represent this summation by the summation over the constrained indices $[n_j]_{E, \kappa}$, then the off-diagonal elements can be written as

$$F_{nm} = \sum_{[m_j]_{E, \kappa}} \sum_{[n_j]_{E, \kappa}} C(n, n_j) C^*(m, m_j) D_{m(m_j)}^{n(n_j)}, \quad (5)$$

where

$$D_{m(m_j)}^{n(n_j)} = \prod_{j=1}^N d_{m_j(m)}^{n_j(n)} = \prod_{j=1}^N \langle m_j(m) | n_j(n) \rangle \quad (6)$$

are decoherence factors with a factorized structure and for $m \neq n, m_j \geq n_j$, each factor

$$d_{m_j(m)}^{n_j(n)} = \Delta_\alpha^{(m_j - n_j)} e^{-\Delta_\alpha^2/2} L_{n_j}^{(m_j - n_j)}(\Delta_\alpha^2) \sqrt{\frac{n_j!}{m_j!}} \quad (7)$$

is expressed in terms of the associated Laguerre polynomials $L_n^m(x)$ with the variable $\Delta_\alpha = -g_j(n-m)/2\omega_j$. In the reduced density matrix of the system, there exists a “Franck-Condon” suppression of decoherence factors in F_{nm} , however, F_{nm} is a infinite sum and thus the decoherence cannot automatically happen so that the off-diagonal elements ρ_S vanishes. There would be an effect due to the off-diagonal elements induced by the finite size of the environment.

In order to show the generalized quantum thermalization, we need to study how the diagonal elements of ρ_S approach the Gibbs distribution $P_n \propto p_n^G = \exp(-\beta \epsilon_n)$, while the off-diagonal elements F_{nm} vanish as a quantum decoherence effect. To this end, we use the basic assumptions for statistical mechanics that $\delta \ll \omega$, but $\delta \gg \omega_j$ and $N \rightarrow \infty$.

First, we consider the diagonal elements. Let us establish the formula

$$P_n(E, \kappa) = \frac{\Omega_N(E - \epsilon_n, \delta, \kappa)}{\mathcal{H}_N(E, \delta, \kappa)} \quad (8)$$

in some sense under the reasonable assumption that $|C(n, \{n_j\})|^2$ are random variables with an identical distribution. In fact, if this condition is satisfied, the random variables have the same mathematical expectation value $[\Omega_{N+1}(E, \delta, \kappa)]^{-1}$ due to the restriction $\sum' |C(n, \{n_j\})|^2 = 1$. It then follows from the law of large numbers that $\sum'' |C(n, \{n_j\})|^2$ approaches to $\Omega_N(E - \epsilon_n, \delta, \kappa) / \mathcal{H}_N(E, \delta, \kappa)$ with high probability. Here we remark that with a straightforward calculation (e.g., in Ref. [2]), this formula can be obtained from the microcanonical state $\rho_{MC} = \sum' [1/\mathcal{H}_N(E, \delta, \kappa)] |n, \{n_j\}\rangle \langle n, \{n_j\}|$ of the “universe.”

We are now in a position to consider how $P_n(E, \kappa)$ leads to the canonical distribution. According to Refs. [1,2], when there is no interaction, $P_n(E, \kappa=0)$ does give rise to the canonical distribution for almost all the pure states $|\psi\rangle$ of the constrained “universe.” But when there exists an interaction between S and B , is it still the case? The answer seems to be positive when the interaction is weak. We will attack this problem by theoretical analysis and numerical simulation.

If we can show that $P_n(E, \kappa)$ possesses a “conformal invariance” with respect to the geometrical deformation of the energy shell caused by the interaction, i.e., $P_n(E, \kappa) \sim P_n(E, \kappa=0)$, then the problem is solved. We try to justify this “conformal invariance” for weak interaction ($\kappa \neq 0$). It follows from the direct sum decomposition $V(E, \delta) = \sum_n \oplus V^B(n, \kappa)$ of the Hilbert space $V(E, \delta)$ that the dimension of $V(E, \delta)$ can be written as $\mathcal{H}_N(E, \delta, \kappa) = \sum_{n=1}^M \Omega_N(n)$. Here, $\Omega_N(n)$ stands for the number of states in the area defined by Eq. (2), and M is an upper bound of the summation range,

which is determined by the positiveness of both the bath energy and the system energy. By straightforward calculation we obtain

$$\Omega_N(n) \simeq \frac{[E - \epsilon_n(\kappa)]^{N-1} \delta}{(N-1)! \prod_{j=1}^2 \omega_j^2} \quad (9)$$

for very small δ . Thus the diagonal elements of ρ_S take the form

$$P_n = \frac{[E - \epsilon_n(\kappa)]^{N-1}}{\sum_{n=1} [E - \epsilon_n(\kappa)]^{N-1}} \quad (10)$$

with a large N . Since the eigenenergy ϵ_n of the system is much smaller than the total energy of the energy shell, β is defined as

$$\beta = \frac{dS(E)}{dE} = \frac{(N-1) \sum_n [E - \epsilon_n(\kappa)]^{N-2}}{\sum_n [E - \epsilon_n(\kappa)]^{N-1}}. \quad (11)$$

Usually the energy correction

$$\kappa \lambda_n^2 = \lambda_n^2 \sum_j \frac{|g_j|^2}{4\omega_j} \quad (12)$$

is much smaller than the shell energy E , thus the temperature becomes independent of κ , $\beta \approx (N-1) [\sum_n (E - \epsilon_n)^{N-2}] / [\sum_n (E - \epsilon_n)^{N-1}]$. Therefore, P_n is ‘‘conformably invariant’’ with respect to κ , and for this reason we can expect the Gibbs distribution $P_n \approx \exp(-\beta \epsilon_n) / \sum_{n=1} \exp(-\beta \epsilon_n)$.

It should be pointed out that the above argument is only heuristic since neither the sum $\sum \Omega_N(n)$ nor the distribution P_n is calculated analytically. Thus we will resort to numerical simulation to support our expectation. Let us assume the system is a harmonic oscillator. In this case, $\lambda_n = n$ and the temperature of the system is exactly

$$\beta = \frac{(N-1) \sum_n [E - n\omega + \kappa n^2]^{N-2}}{\sum_n [E - n\omega + \kappa n^2]^{N-1}}.$$

We choose $E=0.5$ and $\omega=10^{-3}$ and display in Fig. 2 the relationship between the distribution P_n and n for different κ when $N=50$. It is clearly shown that P_n indeed decays exponentially as Gibbs distribution as n increases. Table I gives the inverse temperature of the system for different coupling parameters κ . These numerical results demonstrate that the state obtained by tracing over the bath is just the Gibbs canonical state under some conditions.

Now we consider the bath-induced decoherence effect, which causes the off-diagonal elements of ρ_S to approach zero. When the system-bath couplings can be ignored in comparison with the energy level spacing and the total energy of the bath, any two subspaces defined by the constraint (2) cannot overlap each other and then the decoherence factor vanishes. In the present situation, the system-bath cou-

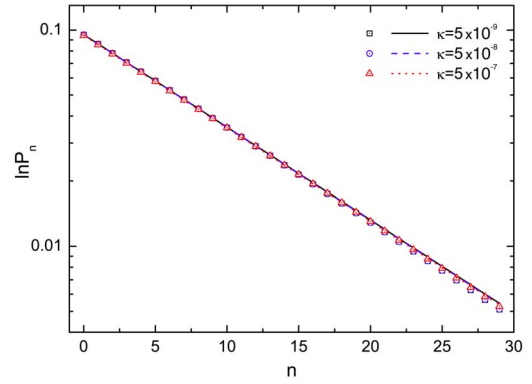


FIG. 2. (Color online) Plot of $\ln P_n$ as a function of the number n of the system, when $N=50$ with different κ : 5×10^{-9} (\square), 5×10^{-8} (\circ), and 5×10^{-7} (\triangle). The fitting of the Gibbs distribution is shown by the corresponding lines.

pling will weaken this decoherence for thermalization since the positive terms $\lambda_{n+1}^2 - \lambda_n^2$ reduce the effective system’s energy spacings

$$\epsilon_{n+1}(\kappa) - \epsilon_n(\kappa) = \epsilon_{n+1} - \epsilon_n - \kappa(\lambda_{n+1}^2 - \lambda_n^2) \quad (13)$$

to make them comparable to the thickness δ of the energy shell. Then two subspaces $V^B(n, \kappa)$ and $V^B(m, \kappa)$ of B can overlap each other and the off-diagonal elements F_{nm} will not vanish. However, notice that the norm of each component $d_{m_j(n)}$ in the decoherence factor is less than unity. Thus, the decoherence factor D still vanishes in the thermodynamic limit $N \rightarrow \infty$. So we conclude that the factorized structure of D enhances the decoherence [10,11], and to some extent compensates the negative effect of interaction in thermalization.

Next, we wish to point out that in the mesoscopic case, that is to say, N is not large enough, effects may arise. In this case, if the system-bath coupling is strong, there will exist finite off-diagonal elements F_{nm} in the reduced density matrix. This means quantum coherence is introduced into the usual thermal equilibrium state. Such a state is called a quasithermal state.

For a two-level system with single energy spacing Δ , the quasithermal state can be described by the reduced density matrix

$$\rho_S = \begin{bmatrix} p_+ & F \\ F^* & p_- \end{bmatrix}. \quad (14)$$

The diagonal elements $p_{\pm} = 1/[1 + \exp(\pm \beta \Delta)]$ approach the standard Gibbs distributions while the off-diagonal elements are nonvanishing, $F = F_{12}$. We can diagonalize the above reduced density matrix to obtain the two effective probabilities

TABLE I. Inverse temperature vs interaction.

κ	5×10^{-9}	5×10^{-8}	5×10^{-7}
β	98.94	98.85	98.69

$P_{\pm}(F)$ exactly. For small F , $P_{\pm}(F)$ can be approximated as

$$P_{\pm}(F) \approx p_{\pm} \mp \coth\left(\frac{\beta\Delta}{2}\right)|F|^2. \quad (15)$$

Then, the von Neumann entropy $S_{\text{VN}} = -\sum_{\alpha=\pm} P_{\alpha}(F) \ln P_{\alpha}(F)$ is approximated as

$$S_{\text{VN}} \approx S(E) - \beta\Delta|F|^2 \coth\left(\frac{\beta\Delta}{2}\right). \quad (16)$$

It is observed that due to the system-bath interaction the von Neumann entropy explicitly deviates from the thermodynamic entropy

$$S(E) \approx \frac{\beta\Delta}{e^{\beta\Delta} + 1} + \ln(e^{-\beta\Delta} + 1),$$

which is by definition the entropy of the Gibbs equilibrium state $\rho_G = \text{diag}(p_+, p_-)$. Therefore, generally von Neumann entropy does not relate to the meaningful usual notion of temperature. In fact, there is no good physical notion of temperature for a general nonthermal equilibrium. But the erasure of quantum information by thermalization indicates where temperature enters in this matter.

However, only for the two-level system or a system with homogeneous energy level spacing can we define an effective temperature $T_{\text{eff}} = 1/\beta_{\text{eff}}$ [14] by the ratio

$$r(t) = \frac{P_+(F)}{P_-(F)} = e^{-\beta_{\text{eff}}\Delta} \quad (17)$$

and the level spacing Δ . For such a system interacting with a finite heat bath, even in a nonequilibrium state, we can imagine

that it is in a virtual equilibrium state with the effective inverse temperature

$$\beta_{\text{eff}} \approx \beta + \frac{4|F|^2}{\Delta} \cosh^2\left(\frac{\beta\Delta}{2}\right) \coth\left(\frac{\beta\Delta}{2}\right).$$

This effective inverse temperature in the quasithermal state is higher than the usual equilibrium inverse temperature. Such kind of quasithermal state with a bit of quantum coherence can demonstrate various exotic natures in thermodynamical processes. Scully *et al.* [15] have proposed a quantum Carnot engine in which the bath atoms are given with some quantum coherence, which can increase the effective temperature of the radiation field. In this case, though the second law of thermodynamics is not violated, the quantum Carnot engine possesses some features that are not possible in a classical case.

In summary, based on an exactly solvable model, the quantum kinetic thermalization of the system is explored for the case with weak interaction between system and bath. The effect of finite interaction is demonstrated as the deformation of the energy shell. Here, a decoherence mechanism is used to account for the disappearance of the off-diagonal elements of the reduced density matrix of the system in contact with a bath of infinitely large particle number in the weak coupling limit. Moreover, we emphasize the thermodynamic effects that can result from the nonvanishing off-diagonal elements of the reduced density matrix when the bath is mesoscopic.

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