Spontaneous symmetry breaking in thermalization and anti-thermalization

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The phenomenon of spontaneous symmetry breaking is investigated in the dynamic thermalization of a degenerate quantum system. A three-level system interacting with a heat bath is carefully studied to this end. It is shown that the three-level system with degenerate ground states might have different behaviors depending on the details of the interaction with the heat bath when the temperature approaches zero. If we introduce an external field to break the degeneracy of the ground states and let it approach zero after letting the temperature approach zero, then two possibilities will arise: the steady state is a definite one of the degenerate states independent of the initial state, or the steady state is dependent on the initial state in a complicated way. The first possibility corresponds to a spontaneous symmetry breaking of the system and the second one implies that the heat bath could not totally erase the initial information in certain cases.

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Introduction.—Conventionally, thermalization is understood as a dynamic process in which an open quantum system (OQS) approaches an equilibrium state with the same temperature \( T \) as that of its heat bath [1]. According to the third law of thermodynamics (the generic version), the entropy of a non-degenerate system will vanish at the absolute zero temperature. That is to say, at the absolute zero temperature, the system will reach a steady pure state. Is it still the case when the system has degenerate ground states? This turns out to be a subtle problem related to the process of thermalization. In quantum physics, thermalization seems to be a much more complex concept than in classical physics. In fact, most recently a new kind of thermalization, called canonical thermalization [2, 3, 4, 5], has been proposed.

At zero temperature a system with degenerate ground states might have a finite entropy depending on the degree of degeneracy \( d \): \( S = k_B \ln d \) [6]. Roughly speaking, this can be understood by studying the following two non-commutative limit processes: letting the perturbation introduced to break the degeneracy approach zero and letting the temperature of the heat bath approach zero. Actually, in the thermal equilibrium case (the system is thermalized to reach a thermal equilibrium state), if we first take the second limit and then take the first limit, the OQS will reach a definite pure state and thus have a vanishing entropy. This is a phenomenon of spontaneous symmetry breaking (SSB) [6, 7]. On the other hand, if we reverse the order of these two limit processes, the OQS will reach a maximally mixing state of all the degenerate ground states and thus possess a non-vanishing entropy.

Unfortunately, the above discussion about the thermalization of a system with degenerate ground states proves to be overly simplified. In the study of the dynamic thermalization of a simple system, we find that the above mentioned SSB in the thermalization can only happen when bath induced transition is not forbidden by some selection rule. If there is a selection rule to forbid the bath induced transition between the degenerate ground states, the steady thermalized state will depend on the initial state and thus the SSB will not appear.

In this case, the OQS enjoys the so called anti-thermalization effect: some information of the initial state is kept after the OQS is thermalized to a steady state.

We will study a three-level system interacting with a heat bath. The two lower (or higher) energy states \( |g_1\rangle \) and \( |g_2\rangle \) of this three-level system are degenerate and can be split by applying an external field. The heat bath is modeled as the bath of harmonic oscillators. The dynamic process of the system’s approaching the steady state at zero temperature will be carefully analyzed from the master equation approach. We will prove that if there exists a non-vanishing coupling to the bath for arbitrary two energy levels of the three-level system, then the third law of thermodynamics is valid thanks to the SSB. On the other hand, for the conventional A- and V-type atoms, we will reveal the exotic anti-thermalization effect. This effect happens as a result of the absence of the bath coupling induced quantum transition between \( |g_1\rangle \) and \( |g_2\rangle \) and the occurrence of the quantum interference between the transition to \( |g_1\rangle \) and the transition from \( |g_2\rangle \). At zero temperature, these

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FIG. 1: (Color online). The schematic illustration of spontaneous symmetry breaking (SSB) in thermalization. (a) The heat bath usually does not single out a particular state from the degenerate ground states at zero temperature; (b) Breaking the symmetry of the potential will cause a preference of the system to a particular ground state at zero temperature; (c) After the symmetry is recovered at zero temperature, the system will remain in the preferred state.
conclusions coincide with those reached in the context of the spontaneous emission of $V$-type atom in vacuum [3].

**SSB in thermalization.**—In general, the Hamiltonian $\hat{H}_S$ of an OQS to be thermalized can be written as $\hat{H}_S = \sum_{n,a} E_n |n,\alpha\rangle \langle n,\alpha|$, where $|n,\alpha\rangle (\alpha = 1,2,\cdots,d_n)$ are degenerate states correspond to the same eigenvalue $E_n$ ($n = 1,2,3,\cdots$) and $d_n$ is the degree of degeneracy. Let an external field be applied to break the energy level degeneracy as $E_n \rightarrow E_n + \Delta_n$ and then let this degeneracy split system contact with a heat bath temperature $T$ for a time longer than the conventional relaxation time. Then the system is supposed to be thermalized to the thermal equilibrium state $\hat{\rho}_S (\Delta_n,\beta) = \sum_{n,a} \exp[-\beta (E_n + \Delta_n)] Z^{-1} |n,\alpha\rangle \langle n,\alpha|$, where $\beta = 1/(k_B T)$ is the inverse temperature (hereafter, we set $k_B = 1, \hbar = 1$) and $Z = \text{Tr}[\exp(-\beta \hat{H}_S)]$ is the partition function of the OQS.

We observe that for $\hat{\rho}_S (\Delta_n,\beta)$, there exist the following two limit processes:

\[
\lim_{\Delta_n \rightarrow 0} \lim_{\beta \rightarrow +\infty} \hat{\rho}_S (\Delta_n,\beta) = |1,1\rangle \langle 1,1|, \quad (1)
\]

\[
\lim_{\beta \rightarrow +\infty} \lim_{\Delta_n \rightarrow 0} \hat{\rho}_S (\Delta_n,\beta) = \frac{1}{d} \sum_{\alpha=1}^{d} |1,\alpha\rangle \langle 1,\alpha|, \quad (2)
\]

where $|1,1\rangle$ denotes the ground state with vanishing energy in the presence of the external field. Note that taking the two limits in different orders leads to completely different results, the former being a reflection of the SSB phenomenon.

We would like to remark that though both of the two results are correct in the mathematical sense, the former is physically more acceptable than the latter, which is in accordance with the generic version of the third law of thermodynamics. Indeed, in view of the existence of the perturbation breaking the degeneracy, it seems reasonable to let the temperature approach zero first in the calculation. However, things are not so simple. In fact, due to quantum interference effect, even if we let the temperature approach zero first in the calculation, the happening of SSB is not unconditional. This is the main conclusion of this letter.

**Dynamic thermalization of a three-level system.**— Generally, the process of dynamic thermalization begins from a factorized initial state $\hat{\rho}(0) = \hat{\rho}_S (0) \otimes \hat{\rho}_B (\beta)$, where $\hat{\rho}_B (\beta)$ is the thermal state of the heat bath. Let the heat bath be modeled as the harmonic oscillator system with the Hamiltonian $\hat{H}_B = \sum_j \omega_j \hat{a}_j^\dagger \hat{a}_j$. Then we have $\hat{\rho}_B (\beta) = \exp(-\beta \hat{H}_B)/Z_B$ where $Z_B = \text{Tr}[\exp(-\beta \hat{H}_B)]$ is the partition function. The time evolution of the total system driven by the coupling $\hat{H}_t$ between the system and the heat bath is determined by $\hat{H}(t) = \exp[-i(\hat{H}_S + \hat{H}_B + \hat{H}_t)]$. The steady state of the system, as $t \rightarrow \infty$ at $T = 0$, can then be obtained by calculating the reduced density matrix $\hat{\rho}_S (t,\beta) = \text{Tr}_B [\hat{U}(t) \hat{\rho}(0) \otimes \hat{\rho}_B \hat{U}^\dagger(t)]$ of the OQS ($\text{Tr}_B$ stands for tracing over the heat bath).

To be specific, let us study the dynamic thermalization of a simple three-level system. The Hamiltonian $\hat{H}_S = \omega_2 \hat{\sigma}_{ee} + \Delta \hat{\sigma}_{g,e}$ of the three-level system (as illustrated in Fig. 2) is written in terms of the flip operators $\hat{\sigma}_{\alpha\beta} = |\alpha\rangle \langle \beta| (\alpha,\beta = e,g_1,g_2)$, where $\omega_1 = \omega_e - \omega_g$ ($l = 1,2$) and $\Delta = \omega_e - \omega_1$. Here, we choose the eigen-energy of the state $|g_2\rangle$ as the energy zero point. The interaction Hamiltonian of the three-level system with its heat bath reads

\[
\hat{H}_I = \sum_{l=1,2} \hat{\sigma}_{gel} \hat{B}_l + \hat{\sigma}_{gel} \hat{B}_3 + h.c.,
\]

where $\hat{B}_l = \sum_j \eta_j (\omega_l) \hat{a}_j$ ($l = 1,2,3$). For simplicity, we assume $\eta_j (\omega_l)$ to be real below.

Under the Born-Markov approximation, the evolution of the reduced density matrix of the three-level system is governed by the master equation,

\[
\dot{\hat{\rho}}_S = -i [\hat{\rho}_S, \Delta \hat{\sigma}_{g,e}^\dagger] + \sum_{l=1}^{3} L_l[\hat{\rho}_S] + L_x[\hat{\rho}_S],
\]

where

\[
L_l[\hat{\rho}_S] = \gamma_{2l} \left( \bar{n}(\omega_l) + 1 \right) \left( 2 \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} - \hat{\sigma}_{gel} \hat{\sigma}_{gel} \hat{\rho}_S - \hat{\rho}_S \hat{\sigma}_{gel} \right) + \gamma_{2l} \left( \bar{n}(\omega_l) + 1 \right) \left( 2 \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} - \hat{\sigma}_{gel} \hat{\sigma}_{gel} \hat{\rho}_S - \hat{\rho}_S \hat{\sigma}_{gel} \right),
\]

\[
L_x[\hat{\rho}_S] = \frac{\gamma_1}{2} \left( \bar{n}(\Lambda) + 1 \right) \left( 2 \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} - \hat{\sigma}_{gel} \hat{\sigma}_{gel} \hat{\rho}_S - \hat{\rho}_S \hat{\sigma}_{gel} \right) + \gamma_1 \left( \bar{n}(\Lambda) + 1 \right) \left( 2 \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} - \hat{\sigma}_{gel} \hat{\sigma}_{gel} \hat{\rho}_S - \hat{\rho}_S \hat{\sigma}_{gel} \right),
\]

\[
L_{x}[\hat{\rho}_S] = \frac{\gamma_1}{2} \left( \bar{n}(\omega_1) + 1 \right) + \frac{\gamma_1}{2} \left( \bar{n}(\omega_2) + 1 \right) \left( \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} + \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} \right) + \frac{\gamma_1}{2} \left( \bar{n}(\omega_2) + 1 \right) \left( \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} + \hat{\sigma}_{gel} \hat{\rho}_S \hat{\sigma}_{gel} \right),
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Here, the decay rates $\gamma_l = 2\pi \rho(\omega_l)\eta(\omega_l)^2$ and $\gamma_{lm} = 2\pi \rho(\omega_l)\eta_l(\omega_m)$, for $\omega_3 = \Delta$ and $l \neq m, m = 1, 2$, depend on the mode density $\rho(\omega)$ of the heat bath; $\tilde{n}(\omega) = 1/\{\exp(\beta \omega) - 1\}$ is the thermal average excitation number for the boson mode of frequency $\omega$ at temperature $T$. Note that in the master equation \ref{eq:master}, we have neglected the Lamb shifts.

The evolution of the density matrix elements governed by the master equation \ref{eq:master} can be described with the optical Bloch equation $\dot{X} = MX$, where the state vector $X = X(t)$ and the coefficient matrix $M$ are respectively defined as $X = X_R \otimes X_S$ and $M = R \otimes S$, with $X_S = (\langle \sigma_{E1} \rangle, \langle \sigma_{E2} \rangle)^T$ and $R = \begin{pmatrix} \gamma_1(2\tilde{n}(\omega_1) + 1) & \gamma_2(\tilde{n}(\omega_1) + 1) & 0 & 0 \\ \gamma_1(\tilde{n}(\omega_2) + 1) & \gamma_2(2\tilde{n}(\omega_2) + 1) & \gamma_3(2\tilde{n}(\omega_2) + 1) & 0 \\ \gamma_1(\tilde{n}(\Delta) + 1) & -\gamma_2(\tilde{n}(\Delta)) & -\gamma_3(2\tilde{n}(\Delta)) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$, $S = \begin{pmatrix} \gamma_1(2\tilde{n}(\omega_1) + 1) + \gamma_2(\tilde{n}(\omega_2) + 1) + \gamma_3(2\tilde{n}(\Delta) + 1)/2 & 0 & 0 & 0 \\ i\Delta - \frac{1}{2}[\gamma_2(2\tilde{n}(\omega_2) + 1) + \gamma_1(\tilde{n}(\omega_1) + 1) + \gamma_3(\tilde{n}(\Delta))] & \gamma_1(\tilde{n}(\omega_1) + 1) & \gamma_2(\tilde{n}(\omega_2) + 1) & 0 \\ \gamma_1(\tilde{n}(\omega_1) + 1) & \gamma_2(\tilde{n}(\omega_2) + 1) & \gamma_3(2\tilde{n}(\omega_2) + 1) & 0 \\ \gamma_1(\tilde{n}(\Delta) + 1) & -\gamma_2(\tilde{n}(\Delta)) & -\gamma_3(2\tilde{n}(\Delta)) & 0 \end{pmatrix}$.

For $l = 1, 2$. Here $\langle \hat{A} \rangle_{\tilde{S}} = \text{Tr}_S[A \hat{\rho}_{\tilde{S}}(\infty)]$, $\hat{A}$ being the operator concerned. Considering the normalization conditions $\langle \hat{\sigma}_{E1} \rangle_{\tilde{S}} + \langle \hat{\sigma}_{E2} \rangle_{\tilde{S}} + \langle \hat{\sigma}_{ee} \rangle_{\tilde{S}} = 1$, from Eq. \ref{eq:master} we then have

$$\langle \hat{\sigma}_{E1} \rangle_{\tilde{S}} = \frac{e^{\beta \omega_1}}{1 + e^{\beta \omega_1} + e^{\beta \omega_2}}, \quad \langle \hat{\sigma}_{E2} \rangle_{\tilde{S}} = \frac{e^{\beta \omega_2}}{1 + e^{\beta \omega_1} + e^{\beta \omega_2}}, \quad \langle \hat{\sigma}_{ee} \rangle_{\tilde{S}} = 0$$

for $l = 1, 2$.

Next, we consider the case with vanishing bath temperature. In this case, we have $\tilde{n}(\omega_1) = \tilde{n}(\omega_2) = \tilde{n}(\Delta) = 0$ and thus det($M$) = 0. We thus cannot obtain the steady state solution of the optical Bloch equation by simply setting $X = 0$ as the resulted equation $0 = MX$ would not have a unique solution. Instead, we have to turn to the transient solution first and then consider the time behavior. One can expect that it cannot be determined without regard to the details of the interaction or the initial state. Indeed, complexity will arise here. Let us focus on the case with $\gamma_3 \neq 0$ in this section, and leave the case with $\gamma_3 = 0$ to the next section.

When $\gamma_3 \neq 0$, namely, there exists a bath induced coupling between the states $|g_1\rangle$ and $|g_2\rangle$, the transient solution, which is not presented here for the technicalities, results in $\langle \hat{\sigma}_{ee} \rangle_{SS} = \langle \hat{\sigma}_{E1} \rangle_{SS} = 0$, and $\langle \hat{\sigma}_{ee} \rangle_{SS} = 1$. This implies that whether the three-level system has degenerate ground states or not, the steady state of the master equation \ref{eq:master} is just the thermal equilibrium state ($\propto \exp(-\beta \hat{H}_S)$) of the OQS even at zero temperature. This conforms to the conventional idea. However, when $\gamma_3 = 0$, in the next section we will see an exotic nature of thermalization as $T \to 0$.

Now it is easily seen that taking the limits in different orders leads to the following different results: $\lim_{\Delta \to 0} \lim_{\rho \to +\infty} \langle \hat{\sigma}_{E1} \rangle_{SS} = 0$, $\lim_{\Delta \to 0} \lim_{\rho \to +\infty} \langle \hat{\sigma}_{E2} \rangle_{SS} = 1$, and $\lim_{\rho \to +\infty} \lim_{\Delta \to 0} \langle \hat{\sigma}_{E1} \rangle_{SS} = \lim_{\rho \to +\infty} \lim_{\Delta \to 0} \langle \hat{\sigma}_{E2} \rangle_{SS} = 1/2$. Following the first procedure, we will reach the conclusion that the final steady state is the pure state $|g_2\rangle$ and that there exists SSB effect in the thermalization. But if we adopt the second procedure, we should conclude that the final steady state is the maximally mixing state $\langle g_1 | g_2 \rangle = | g_2 \rangle | g_1 \rangle$. By the way we remark that the SSB can also be seen from the von Neumann entropy $S = -\text{Tr}_S[\hat{\rho}_S(\infty) \ln \hat{\rho}_S(\infty)]$ of the steady state $\hat{\rho}_S(\infty)$ of the three-level system. In Fig. \ref{fig:ent} we plot the von Neumann entropy $S$ as a function of $\Delta$ and $T$. In the figure the character of double values of $S$ at the point $(\Delta, T) = (0, 0)$ is clearly illustrated: along the route $(T = 0, \Delta \to 0)$, the von Neumann entropy $S \to 0$ while along the route $(\Delta = 0, T \to 0)$ the von Neumann entropy $S \to 1$.

**Anti-thermalization by quantum interference.** We have shown that when $\gamma_3 \neq 0$, in the dynamic thermalization of the three-level system all initial information will finally be erased. As mentioned above, things are not so simple when $\gamma_3 = 0$. In fact, the steady state of the $\Lambda$-type three-level system immersed in a zero temperature bath will depend on its initial state if the bath coupling between the two lower levels is forbidden. This phenomenon is referred to as anti-thermalization.

When $\gamma_3 = 0$, the analysis of the $\Lambda$-type three level system immersed in a heat bath can be made in the same way as presented above. The time evolution is described by the mas-
The two red arrows indicate its multi-value feature as both $T$ and $\Delta$ approach zero.

ter equation (4) with $\gamma_3 = 0$. At zero temperature, we have $\det(M) = 0$. Thus the optical Bloch equation is reduced to

$$\dot{\sigma}_{ee} = -(\gamma_1 + \gamma_2)\sigma_{ee}, \quad \dot{\sigma}_{eg} = \gamma_1\sigma_{ee},$$

$$\text{Re}[\dot{\sigma}_{eg}] = \frac{1}{2}(\gamma_{12} + \gamma_{21})\sigma_{ee} - \Delta \text{Im}[\dot{\sigma}_{eg}],$$

$$\text{Im}[\dot{\sigma}_{eg}] = -\frac{1}{2}(\gamma_1 + \gamma_2)\sigma_{ee},$$

where $l = 1, 2$.

These equations can be solved straightforwardly to obtain the transient solutions for $\langle \sigma_{ee}(t) \rangle$, $\langle \sigma_{eg}(t) \rangle$ and $\langle \sigma_{eg}(t) \rangle$ where $l = 1, 2$. From these transient solutions it follows that

$$\langle \sigma_{ee}(t) \rangle \simeq \langle \sigma_{ee}(0) \rangle + \frac{\gamma_1}{\gamma_1 + \gamma_2} \langle \sigma_{ee}(0) \rangle,$$

and $\langle \sigma_{eg}(t) \rangle \simeq \langle \sigma_{eg}(0) \rangle + \frac{\gamma_{12} + \gamma_{21}}{2(\gamma_1 + \gamma_2)} \langle \sigma_{ee}(0) \rangle$, where $l = 1, 2$. This is just the steady state solution of equation (9).

Equations (11) clearly show that the steady state of the $A$-type three-level system depends on its initial state. In the steady state, the decaying probabilities from the excited state $|e\rangle$ to the ground states $|g_1\rangle$ and $|g_2\rangle$ are respectively $\gamma_1/(\gamma_1 + \gamma_2)$ and $\gamma_2/(\gamma_1 + \gamma_2)$. Moreover, as is shown in Eq. (11), in the present case the dynamic thermalization will preserve or even increase the off-diagonal elements of the density matrix of the initial state while in the previous case with $\gamma_3 \neq 0$, the dynamic thermalization will lead the system to a steady state whose density matrix possesses no off-diagonal elements. It is also noticed that the steady state of the three-level system is independent of the initial off-diagonal elements between $|e\rangle$ and $|g_l\rangle$ ($l = 1, 2$), and when it is initially prepared in the superposition state of the two ground states its final steady state will be the same as the initial state. Finally let us present two simple examples. Take $\gamma_1 = \gamma_2 = \gamma_{12} = \gamma_{21} = \gamma$ and $\Delta = 0$, then for the initial state $|\psi(0)\rangle = |e\rangle$ we have the steady state $|\psi(\infty)\rangle = (|g_1\rangle + |g_2\rangle)/\sqrt{2}$ and for the initial state $|\psi(0)\rangle = |g_1\rangle$ we have the steady state $|\psi(\infty)\rangle = |g_1\rangle$.

**Summary.**—In summary, in this letter the SSB effect in dynamic thermalization is studied through a three-level system immersed in a heat bath inducing cycle transition couplings. Careful calculation is carried out from the master equation approach to examine the thermalization dynamics when the temperature approaches zero. By this investigation it is concluded that when there is no selection rule to forbid any one of the bath induced cycle transition couplings, the canonical thermal state can be reached as a steady state solution of the master equation at zero temperature and if the bath induced transition between the two lower (higher) energy states of $A$-type ($V$-type) atom is forbidden the anti-thermalization phenomenon will happen due to the quantum interference between the transition from the lower state and the transition to the higher state. In this latter case, the final steady state of the three-level system will depend on its initial state, and thus will preserve some of the initial information. This means that the initial information of the system cannot be completely erased by thermalization and the third law of thermodynamics does not work in the conventional fashion.

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