Zeroth law of thermodynamics for thermalized open quantum systems having constants of motion

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We study the evolution of an open quantum system described by a dynamical semigroup having the Lindblad superoperator as a generator. This generator may have an eigenfunction with a zero eigenvalue referred to as a constant of motion (COM). An open quantum system has a unique stationary state if and only if it has no COMs. A system with multiple stationary states has a basis of COMs, any COM of the system is a linear combination of the basis COMs. The basis divides the space of system states into subspaces. In each subspace, its own stationary state is formed, and any stationary state of the system is a linear combination of these states. Usually, neither the basis of COMs nor even their number is known. We demonstrate that finding the stationary state of the system does not require looking for COMs. Instead, one can construct a set of "invariant" subspaces. If the system evolution begins from one of these subspaces, the system will remain in it, arriving at a stationary state independent of evolution in other subspaces. We suggest a direct way of finding the invariant subspaces by studying the evolution of the system. We show that the sets of invariant subspaces and subspaces generated by the basis of COMs are equivalent. A stationary state of the system is a weighted sum of stationary states in each invariant subspace; weighting factors are determined by the initial state of the system.

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I. INTRODUCTION

Recently, the applicability of the laws of thermodynamics to open quantum systems interacting with reservoirs has been actively discussed [1–13]. This issue is interesting not only from a fundamental point of view but is also important for practical purposes. Many applications require creating a system state with desired properties, e.g., quantum entanglement of a large array of qubits for quantum computer elements [14–16], antibunched photons for quantum cryptography [17,18], and a coherent state of an electromagnetic field for nanoscale radiation sources [19–22]. Attaining, as well as retaining, desired states of an open system is a difficult problem because the system interacts with an external reservoir, and the outcome of this interaction is constrained by the laws of thermodynamics. First, the laws of thermodynamics determine possible system states. Second, according to thermodynamics, any state should relax to the stationary state determined by coupling with the reservoir. This significantly limits the number of desirable states.

However, the applicability of the laws of thermodynamics to quantum systems is still not clear. Under the assumption that the density operators of the system and the reservoir are always separable, that the reservoir state does not change in time (the Born approximation), and that the system dynamics is local in time (the Markov approximation), one can obtain the master equation for the density matrix $\hat{\rho}_S(t)$ of the system in the Lindblad-Gorini-Kossakowski-Sudarshan (LGKS) form [23–27]:

$$\partial\hat{\rho}_S(t)/\partial t = L[\hat{\rho}_S(t)]. \tag{1}$$

For any Hamiltonians of the system $\hat{H}_S$, the reservoir $\hat{H}_R$, and the interaction between them $\hat{H}_{SR}$, the Lindblad superoperator $\hat{L}$ should preserve the norm and positive definiteness of the operator $\hat{\rho}_S(t)$. It has been shown [25] (see also [28,29]) that these requirements are satisfied if the Lindblad superoperator $\hat{L}$ has the following form:

$$\hat{L}(\hat{A}(t)) = -i[\hat{H}_S, \hat{A}(t)] + \frac{1}{2}\sum_{i_1,i_2=1}^{N}\left(\left[\hat{F}_{i_1i_2}, \hat{A}(t)\hat{F}_{i_1i_2}^{\dagger}\right] + \left[\hat{F}_{i_1i_2}\hat{A}(t), \hat{F}_{i_1i_2}^{\dagger}\right]\right), \tag{2}$$

where $\hat{A}$ is a positively defined operator, [,] denotes a commutator, and $\hat{F}_{i_1i_2}$ are arbitrary operators. For a physical system, these operators are determined by the Hamiltonians $\hat{H}_S$ and $\hat{H}_{SR}$. We consider N-dimensional Hilbert space, where N can be arbitrarily large. This is a good approximation for interacting quantum systems (see, e.g., Ref. [30]). Examples of such systems are interacting molecules that include two-, three-, or four-level subsystems and systems or interacting qubits [26,31,32].

Usually, it is assumed that the Hamiltonian of the interaction between the system and the reservoir has the form $\hat{H}_{SR} = \hbar\lambda\hat{S}\hat{R}$ [26,33,34], where $\hat{S}$ and $\hat{R}$ are dimensionless operators that only depend on dynamical variables of the system and the reservoir, respectively, and the interaction parameter λ has the dimension of frequency. In such a case, the operators $\hat{F}_{i_1i_2}$ are determined by the operator $\hat{S}$ through the equality $\hat{F}_{i_1i_2} = \sqrt{G(\omega_{i_1i_2})}\langle k_{i_1}|\hat{S}|k_{i_2}\rangle|k_{i_1}\rangle\langle k_{i_2}|$, where $|k_i\rangle$ are the eigenstates of the system Hamiltonian $\hat{H}_S$, $\omega_{i_1i_2} = \omega_{k_{i2}} - \omega_{k_{i1}}$, and $G(\omega)$ is

the reservoir correlation function. In Eq. (2), the summation is taken over all couples of eigenstates $\{|k_{i_1}\rangle, |k_{i_2}\rangle\}$. For such a form of the interaction Hamiltonian, the first law and the second law in the Clausius form follow from Eq. (1) [6,26,28], whereas the zeroth law, which affirms that the stationary state of the system has a unique Gibbs distribution with the reservoir temperature (system thermalization), follows from LGKS Eq. (1), if and only if the system does not have constants of motion (COMs) [28,29,35].

A COM $\hat{I}(t)$ is an eigenoperator of the evolution generator $\exp(\hat{L}t)$, for which the eigenvalue is equal to unity (the eigenvalue of the generator $\hat{L}$ is zero). It has been shown [29] that $\hat{I}(t)$ should be invariant under the action of the Lindblad superoperator (2). We assume that the dimension of the Hilbert space of the problem is finite. The interaction parameter λ has the dimension of frequency. An operator $\hat{I}(t)$ is a COM, if $\hat{L}[\hat{I}(t)] = 0$. Below we show that in the model of evolution considered here, $\hat{I}(t)$ commutes with both the system Hamiltonian and the operator $\hat{S}$.

Since a COM $\hat{I}(t)$ commutes with H_S, these two operators have a common set of eigenvectors, referred to below as basis vectors. Following the general theory [29], we need to find a basis of COMs, the linear combinations of which generate all possible COMs of the system. In Ref. [29], it has also been shown that the basis of COMs is mapped into the family of projection operators that divides the space of system state into subspaces. The existence theorem (see Ref. [29]) establishes that in each subspace, its own stationary state is formed and that any stationary state of the system is a linear combination of these states. In other words, the determination of stationary states requires knowledge of the COMs. However, there are no general recipes for finding COMs or even for determining their total number [36–41].

It seems that the only way for the implementation of this highly abstract theory is to run over all possible operators to find COMs. Since a COM is diagonal in the basis of eigenvectors of H_S, a general form of a COM is a diagonal matrix containing n ones and $N - n$ zeros that occupy arbitrary places, where N is the rank of system state space. The total number of such matrices is 2^N. To choose COMs of 2^N matrices, one needs to make sure that they satisfy the equation $L[\hat{I}(t)] = 0$.

The next step is to determine the basis COMs. If there is only one COM, then the states with a certain eigenvalue of this COM can be separated as a subspace. Thus, each COM leads to a division of the state space into subspaces. The division that corresponds to the basis COMs is the intersection of all subspaces of all COMs. Finally, the eigenvalues of H_S, which correspond to the eigenvectors belonging to one of such subspaces, determine the partition function and the Gibbs distribution in the subspace.

In this paper, we propose a way of determining stationary states of an open system of finite dimension. The developed approach only requires the knowledge of the Hamiltonians of the system and the system-reservoir interaction; it does not require knowing either COMs or their number. Moreover, the proposed method enables one to find all basis COMs. The method is based on the determination of invariant subspaces. These are such subspaces that if the system evolution begins from one of them, the system remains in this subspace reaching the stationary state. We also show that the sets of invariant and basis subspaces are equivalent. The behavior of the system inside a subspace is equivalent to the behavior of the system without COMs, and according to Ref. [29], its stationary state would be described by the Gibbs distribution. The stationary state of the whole system depends on the projection of the initial state onto the subspaces. It is a weighted sum of the stationary states in each invariant subspace. The weighting factors are determined by the initial state of the system.

II. MASTER EQUATION FOR OPEN QUANTUM SYSTEM

Let us consider the finite-dimension system S with non-degenerate spectrum described by the Hamiltonian $\hat{H}_S$. The system interacts with the reservoir R having the Hamiltonian $\hat{H}_R$ via the interaction Hamiltonian $\hat{H}_{SR} = \hbar\lambda\hat{S}\hat{R}$ discussed above. The dynamics of the system and the reservoir is described by the von Neumann equation for the density matrix $\hat{\rho}$:

$$\frac{d\hat{\rho}(t)}{dt} = \frac{i}{\hbar}[\hat{\rho}(t), \hat{H}_S + \hat{H}_R + \hat{H}_{SR}]. \tag{3}$$

One can eliminate the reservoir degrees of freedom and reduce Eq. (3) to the master LGKS Eq. (1) that describes the dynamics of the system density matrix $\hat{\rho}_S = \mathrm{Tr}_R\hat{\rho}$ [6,23,26,28]. The operator $L[\hat{\rho}_S(t)]$ from Eq. (1) may be presented in the following form:

$$L[\hat{\rho}_S(t)] = -\frac{i}{\hbar}[\hat{H}_S, \hat{\rho}_S] + \lambda^2 \sum_{k_1,k_2} G\left(\omega_{k_1} - \omega_{k_2}\right) \times \left(\left[\hat{S}_{k_1k_2}, \hat{\rho}_S(t)\hat{S}^\dagger_{k_1k_2}\right] + \left[\hat{S}_{k_1k_2}\hat{\rho}_S(t), \hat{S}^\dagger_{k_1k_2}\right]\right). \tag{4}$$

In Eq. (4), the operators $\hat{S}_{k_1k_2} = S_{k_1k_2}|k_1\rangle\langle k_2|$ are connected to operator $\hat{S}$ as,

$$\hat{S} = \sum_{k_1,k_2} S_{k_1k_2}|k_1\rangle\langle k_2|, \tag{5}$$

where $|k_i\rangle$ $(i = 1, ..., N)$ are nondegenerate eigenstates of the system Hamiltonian $\hat{H}_S$, ω_{k_i} are eigenfrequencies corresponding to these states, and the function

$$G(\omega) = \int_{-\infty}^{\infty} \exp(i\omega\tau)\mathrm{Tr}_R(\hat{\tilde{R}}(t)\hat{\tilde{R}}(t+\tau)\hat{\rho}_R)d\tau$$

is the Fourier transform of the reservoir correlation function

$$\hat{\tilde{R}}(t) = \exp(i\hat{H}_R t/\hbar)\hat{R}\exp(-i\hat{H}_R t/\hbar).$$

Note that if the reservoir has the temperature T, i.e.,

$$\hat{\rho}_R = \exp(-\hat{H}_R/kT)/\mathrm{Tr}\exp(-\hat{H}_R/kT),$$

then the Kubo-Martin-Schwinger condition,

$$G(\omega) = \exp(\hbar\omega/kT)G(-\omega), \tag{6}$$

is satisfied.

Now we show that a COM commutes with both $\hat{H}_S$ and $\hat{S}$. By definition, a COM, such as $\hat{I}$, should stay invariant under the action of the Lindblad superoperator, i.e.,$\hat{L}[\hat{I}] = 0$. This means that $d\langle\hat{I}\rangle/dt$ should be equal to zero.

The dynamics of the expected value of the operator $\hat{I}$ is governed by the equation

$$\frac{d}{dt}\langle\hat{I}\rangle = \mathrm{Tr}_S\left(\frac{d}{dt}\hat{\rho}_S\hat{I}\right) = \sum_{k_1k_2}\mathrm{Tr}_S\left(iI_{k_1k_2}(\omega_{k_1}-\omega_{k_2})|k_1\rangle\langle k_2|\hat{\rho}_S\right)$$
$$+\frac{1}{2}\sum_{k_1,k_2}\gamma_{k_1k_2}\left|S_{k_1k_2}\right|^2\mathrm{Tr}_S\left(\left(2I_{k_1k_1}|k_2\rangle\langle k_2| - \sum_k I_{k_2k}|k_2\rangle\langle k| - \sum_k I_{kk_2}|k\rangle\langle k_2|\right)\hat{\rho}_S\right), \tag{7}$$

where $\gamma_{k_1k_2} = \lambda^2 G(\omega_{k_1}-\omega_{k_2}) \geqslant 0$ and time evolution of the density matrix is governed by Eq. (1). Since $\hat{I}$ is a COM, we have $d\langle\hat{I}\rangle/dt = 0$ at any moment, including the initial moment. At the initial moment, we may arbitrarily choose $\hat{\rho}_S$. In particular, at the initial moment, we choose the system to be in a pure state $|k_\alpha\rangle$, then the density matrix has a form $\hat{\rho}_S = |k_\alpha\rangle\langle k_\alpha|$ and the equality of the right-hand side of Eq. (7) to zero reduces to

$$\sum_{k_1}\gamma_{k_1k_\alpha}\left|S_{k_1k_\alpha}\right|^2\left(I_{k_1k_1} - I_{k_\alpha k_\alpha}\right) = 0, \quad \alpha = 1, ..., N. \tag{8}$$

Equations (8) holds for arbitrary k_α. Thus, we have a system of N equations. Since the operators in Eqs. (8) do not depend on time, this system is valid at any time.

Now we prove that the term in the sum in each equation of system (8) is zero. Since N is finite, quantities $I_{k_\alpha k_\alpha}$ can be ordered as $I_{k_{\alpha_1}k_{\alpha_1}} \leqslant I_{k_{\alpha_2}k_{\alpha_2}} \leqslant \ldots \leqslant I_{k_{\alpha_N}k_{\alpha_N}}$. First, we consider the equation from system (8) for $\alpha = \alpha_1$, i.e., $I_{k_{\alpha_1}k_{\alpha_1}}$ is the smallest. Because $\gamma_{k_1k_\alpha} \geqslant 0$, all the terms in Eq. (8) are non-negative and this equation is valid only if each term is equal to zero

$$\left|S_{k_1k_{\alpha_1}}\right|^2\left(I_{k_1k_1} - I_{k_{\alpha_1}k_{\alpha_1}}\right) = 0 \tag{9}$$

for arbitrary k_1. As a result, all the terms with $\alpha = \alpha_1$ drop out from system (8). Then, we repeat the procedure for $I_{k_{\alpha_2}k_{\alpha_2}}$. This excludes terms with $k_1 = \alpha_2$. After N iterations, we obtain that for all diagonal terms $|S_{k_{\alpha_2}k_{\alpha_1}}|^2(I_{k_{\alpha_2}k_{\alpha_2}} - I_{k_{\alpha_1}k_{\alpha_1}}) = 0$.

Now we show that all nondiagonal $I_{k_\beta k_\alpha}$ are zero. If at the initial moment we choose $\hat{\rho} = (a|k_\alpha\rangle + b|k_\beta\rangle)(a^*\langle k_\alpha| + b^*\langle k_\beta|)$, then from Eqs. (7) and (8) we obtain

$$ab^*I_{k_\beta k_\alpha}\left(i\left(\omega_{k_\alpha}-\omega_{k_\beta}\right) - \sum_{k_1}\gamma_{k_1k_\beta}\left|S_{k_1k_\beta}\right|^2 - \sum_{k_1}\gamma_{k_1k_\alpha}\left|S_{k_1k_\alpha}\right|^2\right)$$
$$+a^*bI_{k_\alpha k_\beta}\left(i\left(\omega_{k_\beta}-\omega_{k_\alpha}\right) - \sum_{k_1}\gamma_{k_1k_\beta}\left|S_{k_1k_\beta}\right|^2 - \sum_{k_1}\gamma_{k_1k_\alpha}\left|S_{k_1k_\alpha}\right|^2\right) = 0. \tag{10}$$

Because the coefficients a and b and the eigenstates $|k_\alpha\rangle$ and $|k_\beta\rangle$ are arbitrary, it follows from Eq. (10) that

$$I_{k_\beta k_\alpha}\left[i\left(\omega_{k_\alpha}-\omega_{k_\beta}\right) - \sum_{k_1}\gamma_{k_1k_\beta}\left|S_{k_1k_\beta}\right|^2 - \sum_{k_1}\gamma_{k_1k_\alpha}\left|S_{k_1k_\alpha}\right|^2\right] = 0 \tag{11}$$

for any nondiagonal element $I_{k_\beta k_\alpha}$ of the operator $\hat{I}$. Note, that each term, $\gamma_{k_1k_\beta}|S_{k_1k_\beta}|^2$, in the sums in Eq. (11) is real. Since we consider the Hamiltonian $\hat{H}_S$, for which the spectrum is nondegenerate, then $i(\omega_{k_\alpha}-\omega_{k_\beta}) \neq 0$. Thus, in Eq. (11), the expression in the brackets has a nonzero imaginary part and, consequently, Eq. (11) holds only if $I_{k_\beta k_\alpha} = 0$. This means that the operator $\hat{I}$ is diagonal in the basis of the eigenvectors of $\hat{H}_S$, $\hat{I} = \sum_k I_{kk}|k\rangle\langle k|$. Thus $\hat{I}$ and $\hat{H}_S$ commute.

Using the diagonal representation of the operator $\hat{I}$, $\hat{I} = \sum_k I_{kk}|k\rangle\langle k|$, the commutator of $\hat{I}$ and $\hat{S}$ may be expressed as

$$[\hat{I},\hat{S}] = \sum_k I_{kk}|k\rangle\langle k|\sum_{k_1,k_2}S_{k_1k_2}|k_1\rangle\langle k_2|$$
$$-\sum_{k_1,k_2}S_{k_1k_2}|k_1\rangle\langle k_2|\sum_k I_{kk}|k\rangle\langle k|$$
$$=\sum_{k_1,k_2}S_{k_1k_2}\left(I_{k_1k_1} - I_{k_2k_2}\right)|k_1\rangle\langle k_2|. \tag{12}$$

Using Eq. (9) we arrive at the commutativity of the operators $\hat{I}$ and $\hat{S}$, $[\hat{I},\hat{S}] = 0$. Thereby, the COM $\hat{I}$ commutes with both $\hat{H}_S$ and $\hat{S}$; analogously, one can obtain that any operator that commutes with $\hat{H}_S$ and $\hat{S}$ is a COM.

It can be shown that Eqs. (1) and (4) ensure that the first and the second laws of thermodynamics are satisfied [6,23,26,28]. Usually, it is assumed that if a system has a COM, the zeroth law of thermodynamics is violated. It implies that there are many stationary states of the system. Below we show how to construct these stationary states.

III. SUBSPACES GENERATED BY SYSTEM-RESERVOIR INTERACTION AND CONSTANTS OF MOTION

If in the basis vectors $|k_s\rangle$, the matrix $\hat{S}$ defined by Eq. (5) has a block-diagonal form, then the whole space of the system states is a direct sum of subspaces corresponding to blocks of the matrix $\hat{S}$. If the initial system state belongs to one of such a subspace, then the system does not leave this subspace during

the evolution. Indeed, using Eqs. (1) and (4) for diagonal and nondiagonal elements of the density matrix, we obtain

$$\dot{\rho}_S^{(k_1k_1)} = \sum_{k_2=1}^{N} \gamma_{k_2k_1} \left|S_{k_2k_1}\right|^2 \rho_S^{(k_2k_2)} - \rho_S^{(k_1k_1)} \sum_{k_2=1}^{N} \gamma_{k_1k_2} \left|S_{k_1k_2}\right|^2, \tag{13}$$

$$\dot{\rho}_S^{(k_1k_2)} = -i\left(\omega_{k_1} - \omega_{k_2}\right)\rho_S^{(k_1k_2)} - \frac{1}{2}\sum_{k=1}^{N}\left(\gamma_{kk_1}\left|S_{kk_1}\right|^2 + \gamma_{kk_2}\left|S_{kk_2}\right|^2\right)\rho_S^{(k_1k_2)}. \tag{14}$$

From Eq. (14) one can see that any nondiagonal element $\rho_S^{(k_1k_2)}$ decays exponentially and does not interact with other elements. Equation (13) shows that diagonal elements $\rho_S^{(k_1k_1)}$ interact only with other diagonal elements $\rho_S^{(k_2k_2)}$ for which $S_{k_2k_1} \neq 0$. This means that only intra-subsystem transitions that are determined by the matrix elements related to a given subspace are possible. Thus, it is the form of the matrix of the operator $\hat{S}$ that determines the subspaces, in which the system evolves.

In 1937, Krylov [42] developed a special algorithm to construct the subspaces generated by an operator $\hat{S}$. A direct application of this algorithm, however, is not suitable for our purpose, because it includes the transition to new basis vectors. Since the LGKS equation implies the use of the basis vectors $|k_s\rangle$ of $\hat{H}_S$, then to reveal the block-diagonal form of the operator $\hat{S}$, we can only rearrange these vectors. Below, we modify Krylov's procedure in a way that the same basis vectors can be retained. This modification rearranges the basis vectors for the matrix of the operator $\hat{S}$ making it block diagonal.

To construct the first subspace, we have to find the set of the basis vectors $B_1 = \{|k_i\rangle\}_1$, forming the first block of the matrix $\hat{S}$. The set B_1 should be constructed in a way that if some basis vector $|k_i\rangle$ belongs to B_1, then $S_{k_ik_j} = 0$ for any $|k_j\rangle \notin B_1$. The number of vectors in B_1 we denote as $N_1 \leqslant N$, where N is the dimension of the whole space. We need to renumber the basis vector to place the vectors of B_1 at the beginning of the basis. This creates the first block in the upper-left corner of the matrix $S_{k_jk_i}$. Then, we have to repeat this procedure for the remaining basis vectors to create the next block and continue doing this until the whole matrix becomes block diagonal.

To implement this recursive procedure, we start with some eigenvector $|k_1\rangle$ of the Hamiltonian $\hat{H}_S$ and construct the vector $\hat{S}|k_1\rangle$. Since $\hat{H}_S$ and $\hat{S}$ do not commute, the vector $\hat{S}|k_1\rangle$ may not be an eigenvector of $\hat{H}_S$. In this case, $\hat{S}|k_1\rangle$ can be represented as $\hat{S}|k_1\rangle = \sum_{i=1}^{n_1<N} S_{k_ik_1}|k_i\rangle$ with $S_{k_ik_1} \neq 0$. This sum is a linear combination of n_1 basis vectors corresponding to nonzero elements in the k_1-th column of the matrix $S_{k_ik_1}$. These $n_1 \leqslant N$ vectors form the set B_1. For the next step, we decompose each vector $|k_i\rangle$ of the set B_1 as $\hat{S}|k_i\rangle = \sum_{j=1}^{N} S_{k_jk_i}|k_j\rangle$. If in the decompositions, vectors $|k_j\rangle$, which do not belong to B_1, arise, then we should add them to B_1. The procedure is repeated until on some step no new vectors arise in the decompositions. This completes the construction of the set B_1 containing N_1 vectors. Then, we should rearrange the basis vectors in a way that all vectors of B_1 take the first N_1 positions in the basis. As a result, in the upper-leftcorner of the matrix $S_{k_jk_i}$, we form a diagonal block.

If $N_1 = N$, then the dimension of this block is equal to the dimension of the whole space. If $N_1 < N$, then the above procedure should be repeated with the vector $|k_{N_1+1}\rangle$ in the rearranged basis. We obtain the next block and so on. This construction ensures that in the rearranged basis, the matrix of the operator $\hat{S}$ has a block-diagonal form. By construction, this decomposition of the system state space is invariant.

Now we show that the constructed subspaces determine all possible COMs. First, we show that for any subspace B_{l_0}, the operator

$$\hat{I} = I^{(l_0)} \sum_{k_i^{(l_0)} \in B_{l_0}} \left|k_i^{(l_0)}\right\rangle\left\langle k_i^{(l_0)}\right| = I^{(l_0)}\hat{P}_{l_0}$$

(where $I^{(l_0)}$ is some c-number) is a COM. For this, we have to prove that $\hat{I}$ commutes with both $\hat{H}_S$ and $\hat{S}$. Note that $\hat{P}_{l_0}$ is the projection operator onto the l_0-th subspace, i.e., it is a unitary operator in B_{l_0} and is zero in other subspaces. Because $\hat{I}$ is diagonal in the basis of eigenvectors of $\hat{H}_S$, then $[\hat{I}, \hat{H}_S] = 0$.

Next, in the rearranged basis, the operator $\hat{S}$ is block diagonal, therefore $\hat{S} = \sum_l \sum_{k_{i1}^{(l)}, k_{i2}^{(l)} \in B_l} S_{i_1,i_2}|k_{i_1}^{(l)}\rangle\langle k_{i_2}^{(l)}|$. Then

$$[\hat{I}, \hat{S}] = I^{(l_0)}\left[\hat{1}_{l_0}, \sum_{k_{i_1}^{(l_0)}, k_{i_2}^{(l_0)} \in B_{l_0}} S_{i_1,i_2}\left|k_{i_1}^{(l_0)}\right\rangle\left\langle k_{i_2}^{(l_0)}\right|\right] = 0. \tag{15}$$

Thus, $\hat{I} = I^{(l_0)}\hat{P}_{l_0}$ is a COM. As a consequence, any operator, which can be decomposed as

$$\hat{I} = \sum_l I^{(l)}\hat{P}_l, \tag{16}$$

where $I^{(l)}$ are arbitrary c numbers, which are fixed for a given subspace, is also a COM as a linear combination of COMs.

Now, we show that there are no other COMs apart from those having the form (16). Let us assume the contrary: a COM $\hat{I}^*$, which cannot be expressed in the form (16), exists. Since $\hat{I}^*$ is a COM, it commutes with $\hat{H}_S$ and $\hat{S}$. Because the operator $\hat{I}^*$ commutes with $\hat{H}_S$, it is diagonal in the basis $|k\rangle$ of $\hat{H}_S$ eigenvectors. Next, due to the commutativity of $\hat{I}^*$ and $\hat{S}$, Eq. (9) must be satisfied. According to our assumption, $\hat{I}^*$ cannot be presented in the form (16). Hence, *in some subspace*, vectors having different eigenvalues, such as $I^{*(k_j)} \neq I^{*(k_i)}$, must exist. From Eq. (9) it follows that if $I^{*(k_j)} \neq I^{*(k_i)}$, then $S_{k_ik_j} = 0$. This means that it is possible to combine the vectors with identical eigenvalues into new subspaces so that the operator $\hat{S}$ takes a block-diagonal form inside the initial block. This contradicts the fact that invariant subspaces constructed above cannot be divided into invariant subspaces of lower dimensions. Therefore, there are no COMs apart from those that have the form (16). Moreover, this means that during the system evolution, no values of COMs change. Thus, this division corresponds to the basis family of COMs. By construction, during evolution, starting at any point in an invariant subspace, the system visits all points of this subspace.

IV. STATIONARY SOLUTIONS OF THE MASTER EQUATION AND CONSTANTS OF MOTION

Now, we can find the stationary solution of the master equation. For Eqs. (1) and (4), along with the Kubo-Martin-Schwinger condition (6), the stationary solution is the Gibbs distribution:

$$\hat{\rho}_S^{th} = \exp(-\hat{H}_S/kT)/\mathrm{Tr}\exp(-\hat{H}_S/kT). \tag{17}$$

This can be verified by the direct substitution of Eq. (17) into Eq. (1). However, this stationary solution may not be unique. If there are invariant subspaces, then the Gibbs distribution over the states of a given invariant subspace is also a stationary solution. Then, any state of the form

$$\hat{\rho}_S^{st} = \sum_j \lambda_j \frac{\exp(-\hat{P}_j \hat{H} \hat{P}_j/kT)}{\mathrm{Tr}\exp(-\hat{P}_j \hat{H} \hat{P}_j/kT)},$$

$$\sum_j \lambda_j = 1, \quad 0 \leqslant \lambda_j \leqslant 1, \tag{18}$$

is stationary. Because LGKS Eq. (1) conserves the trace and $\{|k_i^{(j)}\rangle\}_{i=\sum_{l=1}^{j-1} N_l+1, \sum_{l=1}^{j-1} N_l+N_j}$ are invariant subspaces, and the quantity $\mathrm{Tr}_j \hat{\rho}_S(t)$ does not change in time. Therefore, $\lambda_{N_j} = \mathrm{Tr}_{N_j} \hat{\rho}_S^{st} = \mathrm{Tr}_{N_j} \hat{\rho}_S(0)$. Thus, in each invariant subspace, the system state evolves to the Gibbs distribution over the states of the subspace with the partition function $\mathrm{Tr}\exp(-\hat{P}_{N_j} \hat{H} \hat{P}_{N_j}/kT)$. In each invariant subspaces, there are no nontrivial COMs. As shown in Refs. [28,29,35], this condition is necessary and sufficient for the uniqueness of a stationary solution. Thus, Eq. (18) determines all possible stationary solutions.

In a particular case, when the operator $\hat{S}$ commutes with the Hamiltonian $\hat{H}_S$, *all* the nondiagonal elements of $\hat{S}$ in the basis of the eigenvectors of $\hat{H}_S$ are equal to zero, and each subset B_l includes only one eigenstate ($N_j = 1$ for each j). Then, any operator that is diagonal in the basis of the eigenstates of the Hamiltonian $\hat{H}_S$ is a COM. In particular, the Hamiltonian $\hat{H}_S$ itself is a COM; therefore, the energy of the system does not change in time. The system does not have the Gibbs distribution, and the distribution depends on the initial state. An example of such a situation is a dephasing reservoir (see Ref. [27]).

V. EXAMPLE: INTERACTING TWO-LEVEL SYSTEMS

To illustrate the results obtained above, we apply the developed procedure to a system of two interacting two-level subsystems (TLSs) that relax into a dephasing reservoir. We begin with considering noninteracting TLSs.

A. Noninteracting TLSs

Suppose that the transition frequencies of TLSs are ω_i, then we denote excited and ground states as $|e_i\rangle$ and $|g_i\rangle$ and the transition operators between excited and ground states of each TSL as $\hat{\sigma}_i$, $i = 1, 2$. The total Hamiltonian of the system is

$$\hat{H}_S = \hat{H}_1 + \hat{H}_2 = \hbar\omega_1 \hat{\sigma}_1^\dagger \hat{\sigma}_1 + \hbar\omega_2 \hat{\sigma}_2^\dagger \hat{\sigma}_2, \tag{19}$$

with eigenstates $|e_1, e_2\rangle$, $|e_1, g_2\rangle$, $|g_1, e_2\rangle$, $|g_1, g_2\rangle$ and eigenvalues $\omega_1 + \omega_2$, ω_1, ω_2, 0.

Suppose that the TLSs interact with the reservoir described by the Hamiltonian:

$$\hat{H}_R = \hbar \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k, \tag{20}$$

where ω_k is the frequency of the k-th reservoir mode, and the interaction Hamiltonian is

$$\hat{H}_{SR} = \hbar \sum_k \gamma_1^k \hat{\sigma}_1^z (\hat{a}_k^\dagger + \hat{a}_k) + \hbar \sum_k \gamma_2^k \hat{\sigma}_2^z (\hat{a}_k^\dagger + \hat{a}_k), \tag{21}$$

where γ_1^k and γ_2^k are the interaction constants between the first and the second TLSs and the k-th reservoir mode, respectively, and $\hat{\sigma}_i^z = [\hat{\sigma}_i^\dagger, \hat{\sigma}_i]$ is the operator of the population inversion of the i-th TLS. For simplicity, we assume that $\gamma_2^k = a\gamma_1^k$, where the constant a does not depend on k. Then,

$$\hat{H}_{SR} = \hbar \sum_k \gamma_1^k (\hat{\sigma}_1^z + a\hat{\sigma}_2^z)(\hat{a}_k^\dagger + \hat{a}_k) = \hbar\lambda \hat{S}\hat{R}, \tag{22}$$

where $\lambda = \max\{\gamma_1^k\}$, $\hat{R} = \sum_k \frac{\gamma_1^k}{\max(\gamma_1^k)}(\hat{a}_k^\dagger + \hat{a}_k)$, and $\hat{S} = \hat{\sigma}_1^z + a\hat{\sigma}_2^z$. Such a reservoir describes phase relaxation of the system. Indeed, the operator $\hat{S} = \hat{\sigma}_1^z + a\hat{\sigma}_2^z$ commutes with the system Hamiltonian $\hat{H}_S$, and the energy of the system is conserved; thus, the reservoir is purely dephasing. According to Sec. IV, in this case, each invariant subspace consists of only one system eigenstate.

To show this explicitly, we follow the procedure developed in Sec. III. Acting by the operator $\hat{S}$ on the eigenstates of $\hat{H}_S$, we obtain

$$\hat{S}|e_1, e_2\rangle = (1+a)|e_1, e_2\rangle, \ \ \hat{S}|g_1, g_2\rangle = -(1+a)|g_1, g_2\rangle, \tag{23}$$

$$\hat{S}|g_1, e_2\rangle = (-1+a)|g_1, e_2\rangle, \ \ \hat{S}|e_1, g_2\rangle = (1-a)|e_1, g_2\rangle. \tag{24}$$

In action on each eigenvector, no new eigenvectors appear. Thus, each eigenvector forms an invariant subspace with the dimension one.

The corresponding COMs are projections over each invariant subspace, namely, $\hat{P}_1 = |e_1, e_2\rangle\langle e_1, e_2|$, $\hat{P}_2 = |g_1, g_2\rangle\langle g_1, g_2|$, $\hat{P}_3 = |e_1, g_2\rangle\langle e_1, g_2|$, and $\hat{P}_4 = |g_1, e_2\rangle\langle g_1, e_2|$. These COMs are basis COMs, and any linear combination of them is also a COM. Since $\sum_i \hat{P}_i = \hat{1}$, out of four COMs, only three are linearly independent.

In this simple example, we can construct linear combinations that have clear physical meanings. The first one is

$$\begin{aligned} &2\hat{P}_1 + 1\hat{P}_3 + 1\hat{P}_4 + 0\hat{P}_2 \\ &= 2|e_1, e_2\rangle\langle e_1, e_2| + 1|e_1, g_2\rangle\langle e_1, g_2| \\ &\quad + 1|g_1, e_2\rangle\langle g_1, e_2| + 0|g_1, g_2\rangle\langle g_1, g_2| \\ &= (|e_1, e_2\rangle\langle e_1, e_2| + |e_1, g_2\rangle\langle e_1, g_2|) \\ &\quad + (|e_1, e_2\rangle\langle e_1, e_2| + |g_1, e_2\rangle\langle g_1, e_2|) \\ &= \hat{\sigma}_1^\dagger \hat{\sigma}_1 + \hat{\sigma}_2^\dagger \hat{\sigma}_2 \end{aligned} \tag{25}$$

This operator describes the number of excitations in the system. Indeed, $\hat{P}_1$ corresponds to the state in which both TLSs are in the excited states, and there are two excitations

in the system, $\hat{P}_2$ corresponds to the state in which both TLSs are in the ground state, and there are no excitations in the system. $\hat{P}_3$ and $\hat{P}_4$ correspond to the subspaces in which only one of TLSs is excited, and there is only one excitation. Thus, the operator $2\hat{P}_1 + 1\hat{P}_3 + 1\hat{P}_4 + 0\hat{P}_2 = \hat{\sigma}_1^\dagger\hat{\sigma}_1 + \hat{\sigma}_2^\dagger\hat{\sigma}_2$ has the eigenvalue which is the number of excitations.

The second linear combination is

$$\begin{aligned}
&2\hat{P}_1 - 2\hat{P}_2 + 0\hat{P}_3 + 0\hat{P}_4 \\
&= 2|e_1, e_2\rangle\langle e_1, e_2| - 2|g_1, g_2\rangle\langle g_1, g_2| \\
&= (|e_1, e_2\rangle\langle e_1, e_2| + |e_1, g_2\rangle\langle e_1, g_2|) \\
&\quad - (|g_1, e_2\rangle\langle g_1, e_2| + |g_1, g_2\rangle\langle g_1, g_2|) \\
&\quad + (|e_1, e_2\rangle\langle e_1, e_2| + |g_1, e_2\rangle\langle g_1, e_2|) \\
&\quad - (|e_1, g_2\rangle\langle e_1, g_2| + |g_1, g_2\rangle\langle g_1, g_2|) \\
&= \hat{\sigma}_1^z + \hat{\sigma}_2^z. \qquad (26)
\end{aligned}$$

The operator $\hat{\sigma}_1^z + \hat{\sigma}_2^z$ describes the total population inversion of the system. Indeed, in the first subspace, the state $|e_1, e_2\rangle$ corresponds to two excited TLSs with the population inversion of 2, in the second subspace, the state is $|g_1, g_2\rangle$ and the population inversion is -2, in subspaces $|e_1, g_2\rangle$ and $|g_1, e_2\rangle$, the population inversion is zero.

The third linear combination of basis COMs is the total energy of the system:

$$\begin{aligned}
&(\omega_1 + \omega_2)\hat{P}_1 + \omega_1\hat{P}_2 + \omega_2\hat{P}_3 + 0\hat{P}_4 \\
&= (\omega_1 + \omega_2)|e_1, e_2\rangle\langle e_1, e_2| + \omega_1|e_1, g_2\rangle\langle e_1, g_2| \\
&\quad + \omega_2|g_1, e_2\rangle\langle g_1, e_2| + 0|g_1, g_2\rangle\langle g_1, g_2| \\
&= \omega_1(|e_1, e_2\rangle\langle e_1, e_2| + |e_1, g_2\rangle\langle e_1, g_2|) \\
&\quad + \omega_2(|e_1, e_2\rangle\langle e_1, e_2| + |g_1, e_2\rangle\langle g_1, e_2|) \\
&= \omega_1\hat{\sigma}_1^\dagger\hat{\sigma}_1 + \omega_2\hat{\sigma}_2^\dagger\hat{\sigma}_2 = \hat{H}_S. \qquad (27)
\end{aligned}$$

Note that the total energy of the system, as well as energies of each TLSs, are conserved. For this reason, the reservoir with Hamiltonian (20) and interaction (21) may be called dephasing.

These three COMs, the number of system excitation, the total population inversion, and the total system energy, fully characterize the final state of the system.

B. Interacting TLSs

Now suppose that there is a dipole-dipole interaction between TLSs so that the interaction between them is described by the Hamiltonian $\hat{V} = (\hat{\mathbf{d}}_1 \cdot \hat{\mathbf{d}}_2 - 3(\hat{\mathbf{d}}_1 \cdot \mathbf{n})(\hat{\mathbf{d}}_2 \cdot \mathbf{n}))/r^3$, where r is the distance between TLSs and $\mathbf{n}$ is the normal unit vector directed from one TLS to another. Using the expression for TLS dipole moment, $\hat{\mathbf{d}}_i = \mathbf{d}_i^{eg}(\hat{\sigma}_i + \hat{\sigma}_i^\dagger)$ ($\mathbf{d}_i^{eg}$ is the matrix element of the dipole transition), the interaction Hamiltonian in the rotating-wave approximation can be rewritten as $\hat{V} = \hbar\Omega_R(\sigma_1^\dagger\hat{\sigma}_2 + \hat{\sigma}_2^\dagger\hat{\sigma}_1)$, where $\Omega_R = [\mathbf{d}_1^{eg} \cdot \mathbf{d}_2^{eg} - 3(\mathbf{d}_1^{eg} \cdot \mathbf{n})(\mathbf{d}_2^{eg} \cdot \mathbf{n})]/\hbar r^3$ is the Rabi constant of the interaction. The Hamiltonian of the system may be written as

$$\begin{aligned}
\hat{H}_S = \hat{H}_1 + \hat{H}_2 + \hat{V} &= \hbar\omega_1\hat{\sigma}_1^\dagger\hat{\sigma}_1 + \hbar\omega_2\hat{\sigma}_2^\dagger\hat{\sigma}_2 \\
&\quad + \hbar\Omega_R(\sigma_1^\dagger\hat{\sigma}_2 + \hat{\sigma}_2^\dagger\hat{\sigma}_1). \qquad (28)
\end{aligned}$$

Eigenstates of $\hat{H}_S$ are

$$\begin{aligned}
|\psi_1\rangle &= |e_1, e_2\rangle, \quad |\psi_2\rangle = |g_1, g_2\rangle, \\
|\psi_3\rangle &= \cos\varphi|e_1, g_2\rangle + \sin\varphi|g_1, e_2\rangle, \qquad (29) \\
|\psi_4\rangle &= -\sin\varphi|e_1, g_2\rangle + \cos\varphi|g_1, e_2\rangle,
\end{aligned}$$

where

$$\varphi = \tan^{-1}\left[\left(\sqrt{\Delta\omega^2/4 + \Omega_R^2} - \Delta\omega/2\right)/\Omega_R\right]. \qquad (30)$$

The eigenvalues of eigenstates (29) are

$$\begin{aligned}
E_1 &= \omega_1 + \omega_2, \quad E_2 = 0, \\
E_{3,4} &= (\omega_1 + \omega_2)/2 \pm \sqrt{\Delta\omega^2/4 + \Omega_R^2}. \qquad (31)
\end{aligned}$$

Note that the interaction between TLSs results in mixing of states $|e_1, g_2\rangle$ and $|g_1, e_2\rangle$ [see Eq. (29)].

Now, we follow the procedure developed in Sec. III. Equation (23) holds as before, because the first two eigenvectors, $|\psi_1\rangle$ and $|\psi_2\rangle$, are equal to $|e_1, e_2\rangle$ and $|g_1, g_2\rangle$, respectively. Since the interaction operator $\hat{V}$ mixes the states $|e_1, g_2\rangle$ and $|g_1, e_2\rangle$, instead of Eq. (24), the action of the operator $\hat{S}$ on the states $|\psi_3\rangle$ and $|\psi_4\rangle$ should be considered. As a result, we have

$$\hat{S}|\psi_3\rangle = (\cos^2\varphi + a\sin^2\varphi)|\psi_3\rangle + \cos\varphi\sin\varphi(1 - a)|\psi_4\rangle. \qquad (32)$$

We can see that $|\psi_3\rangle$ is no longer an eigenvector of $\hat{S}$. The result of the action of $\hat{S}$ on $|\psi_3\rangle$, in addition to $|\psi_3\rangle$, contains another basis vector, $|\psi_4\rangle$. Now, we should act by the operator $\hat{S}$ on this vector:

$$\hat{S}|\psi_4\rangle = \cos\varphi\sin\varphi(1 - a)|\psi_3\rangle + (\sin^2\varphi + a\cos^2\varphi)|\psi_4\rangle. \qquad (33)$$

There are no new basis vectors in Eq. (33). Thus, the subspace spanned by the basis vectors $|\psi_3\rangle$ and $|\psi_4\rangle$ is an invariant subspace with a dimension of two. Thus, the number of invariant subspaces is reduced from four to three. The projection operator on the invariant subspace spanned by the basis vectors $|\psi_3\rangle$ and $|\psi_4\rangle$ is

$$\begin{aligned}
\hat{\hat{P}} &= |\psi_3\rangle\langle\psi_3| + |\psi_4\rangle\langle\psi_4| = (\cos\varphi|e_1, g_2\rangle + \sin\varphi|g_1, e_2\rangle)(\cos\varphi\langle e_1, g_2| + \sin\varphi\langle g_1, e_2|) \\
&\quad + (-\sin\varphi|e_1, g_2\rangle + \cos\varphi|g_1, e_2\rangle)(-\sin\varphi\langle e_1, g_2| + \cos\varphi\langle g_1, e_2|) \\
&= (\cos^2\varphi + \sin^2\varphi)|e_1, g_2\rangle\langle e_1, g_2| + (\sin^2\varphi + \cos^2\varphi)|g_1, e_2\rangle\langle g_1, e_2| \\
&\quad + (\cos\varphi\sin\varphi - \sin\varphi\cos\varphi)|e_1, g_2\rangle\langle g_1, e_2| + (\sin\varphi\cos\varphi - \cos\varphi\sin\varphi)|g_1, e_2\rangle\langle e_1, g_2| \\
&= |e_1, g_2\rangle\langle e_1, g_2| + |g_1, e_2\rangle\langle g_1, e_2| = P_3 + P_4. \qquad (34)
\end{aligned}$$

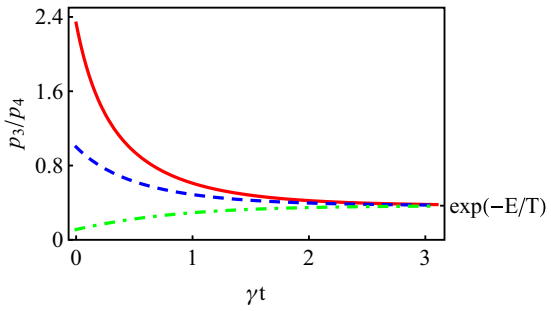

FIG. 1. The dependence of the diagonal matrix elements of the density matrix $p_3 = \rho_{33}$ and $p_4 = \rho_{44}$ on time obtained from LGKS Eq. (13) for the different initial condition: $p_3(0) = 0.7$ and $p_4(0) = 0.3$ (the solid red line), $p_3(0) = 0.7$ and $p_4(0) = 0.3$ (the blue dashed line), $p_3(0) = 0.1$ and $p_4(0) = 0.9$ (the green dot-dashed line); $E = E_3 - E_4 = T = 1$, $\gamma_{34} = 1$, $\gamma_{43} = \gamma_{34}\exp(-E/T)$, t is expressed in the units of γ_{34}.

It should be emphasized that neither $\hat{P}_3$ nor $\hat{P}_4$ is a COM, but their combination $\hat{\tilde{P}}$ is.

In this case, there are two linearly independent COMs. The linear combinations that have physical meaning are the number of excitations, $\hat{\sigma}_1^\dagger\hat{\sigma}_1 + \hat{\sigma}_2^\dagger\hat{\sigma}_2 = 2\hat{P}_1 + 1\hat{\tilde{P}} + 0\hat{P}_2$, and the total population inversion, $2\hat{P}_1 - 2\hat{P}_2 = \hat{\sigma}_1^z + \hat{\sigma}_2^z$. Due to the interaction between TLSs, the system Hamiltonian is no longer a COM. This means that the reservoir ceases to be purely dephasing; now, it causes the energy relaxation in the invariant subspace spanned by the basis vectors $|\psi_3\rangle$ and $|\psi_4\rangle$. It remains dephasing, however, in the subspaces with vectors $|\psi_1\rangle$ and $|\psi_2\rangle$.

Using the obtained COMs and Eq. (18), we may write possible stationary solutions of the corresponding LGKS equation:

$$\hat{\rho}_S^{st} = \lambda_1|\psi_1\rangle\langle\psi_1| + \lambda_2|\psi_2\rangle\langle\psi_2| + \frac{\lambda}{1+\exp\left(-\frac{E_3-E_4}{kT}\right)} \times\left(|\psi_4\rangle\langle\psi_4| + \exp\left(-\frac{E_3-E_4}{kT}\right)|\psi_3\rangle\langle\psi_3|\right), \quad (35)$$

where λ, λ_1, and λ_2 are determined by the initial density matrix $\hat{\rho}(0)$:

$$\lambda_1 = \rho_{11}(0), \quad \lambda_2 = \rho_{22}(0), \quad \lambda = \rho_{33}(0) + \rho_{44}(0). \quad (36)$$

Note that in the invariant subspaces with dimension 1, the stationary and initial states are the same. In the invariant subspace with dimension 2, the stationary solution is the Gibbs distribution.

In Fig. 1, the dependences of the matrix elements $\rho_{33}(t)$ and $\rho_{44}(t)$ on time obtained by computer simulation of the Eq. (13) are shown. One can see that they indeed converge to the Gibbs distribution.

VI. CONCLUSION

In this work, we consider stationary states of an open quantum system interacting with a thermal reservoir in a system that has COMs. We show that stationary states retain the memory of the initial state of the system. To be specific, using the basis of eigenfunctions of the system Hamiltonian H_S, we have shown that the Hamiltonian of the interaction between the system and the reservoir H_{SR} determines the splitting of the space of system states into a set of subspaces. In each of the subspaces, the system behaves as if there are no COMs. This means that, if the initial state of the system belongs to one of these subspaces, the system evolves inside this subspace reaching the Gibbs distribution after thermalization. Hence, each such an invariant subspace can be linked to a COM by assigning some eigenvalue to this COM (such as unity, in one invariant subspace and zeros in the others). Consequently, each subspace determines its own COM that has a fixed eigenvalue in this subspace and zeros in others. If there are N subspaces, then it is possible to define $N-1$ COMs because, in each subspace, COMs with identical values are trivial and do not lead to nonuniqueness of the stationary state. Thus, the algorithm developed in the paper allows one to find *all* invariant subspaces and *all* COMs.

The eigenvalues of existing COMs determine neither the stationary state in each subspace nor the stationary state of the whole system. In any subspace, the Gibbs distribution is determined by the temperature of the reservoir and by the set of eigenfunctions of H_S that construct this subspace. To find the stationary state of the whole system, one must know the initial state of the system. The projection of this state onto subspaces provides the weight factors for Gibbs distributions characterizing each subspace. The weight factors determine the corresponding stationary state of the whole system as a weighted sum of the Gibbs distributions over the subspaces.

Thus, as an open quantum system with COMs interacting with a reservoir evolves, it reaches one of many possible stationary states. Though this state is thermalized with the temperature of the reservoir, it is determined by the initial state of the system.

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