Quantum Equilibration under Constraints and Transport Balance

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For open quantum systems coupled to a thermal bath at inverse temperature β, it is well known that under the Born-, Markov-, and secular approximations the system density matrix will approach the thermal Gibbs state with the bath inverse temperature β. We generalize this to systems where there exists a conserved quantity (e.g., the total particle number), where for a bath characterized by inverse temperature β and chemical potential μ we find equilibration of both temperature and chemical potential. For couplings to multiple baths held at different temperatures and different chemical potentials, we identify a class of systems – providing only a single allowed transition frequency – that equilibrate in a Gibbs state with average temperature and average chemical potential. These results are illustrated by several examples.

Thermalization is a classical phenomenon: Coupling two materials at different temperature will lead to equilibration at some intermediate temperature – depending on the heat capacities of the constituents. Especially when one piece is significantly larger than the other, the temperature of the larger piece will hardly change, such that it may be understood as a heat bath. In contrast, the temperature of the smaller piece will simply approach the bath temperature in that limit.

The dynamics of open quantum systems that are coupled to a thermal bath is however more difficile [1, 2]. A powerful tool to describe the evolution of such systems in various limits is the quantum master equation [3, 4]: A first order differential equation – typically with constant coefficients – describing the evolution of the system part of the density matrix. As the derivation of an exact master equation is impossible in most cases, one has to rely on perturbative schemes. In such schemes, it is often already a challenge to preserve the fundamental properties of the density matrix such as its trace, its self-adjointness, and its positive semidefiniteness. Starting from microscopic models, especially the last property is often hard to fulfill, as for master equations with constant coefficients, preservation of positivity requires the dissipator to be of Lindblad [5] form. Such Lindblad form dissipators are generically derived in the singular coupling limit [6], the weak-coupling limit – also termed Born-Markov-secular [7] (BMS) approximation – and in coarse-graining schemes [8]. Within the BMS approximation, thermalization of the system and equilibration of the systems temperature with that of the bath have been proven [9]. However, some baths are not only described by a temperature, but may also equilibrate under further side constraints – typically modeled by a chemical potential. When we consider couplings to multiple baths held at different temperatures [7, 10] and/or different chemical potentials [11, 12], we have the generic situation for transport [13] from one reservoir through the system to another reservoir, which may be used to generate interesting nonequilibrium stationary states in the system.

This paper is organized as follows: Having introduced the terminology in Sec. I we show how conserved quantities lead to additional properties of the dampening coefficients in Sec. II. The case of a single bath is discussed in Sec. II A, followed by a discussion of multiple baths in Sec. II B. Finally, the results are demonstrated with a number of examples in Sec. III.

I. PRELIMINARIES

We will consider a large closed quantum system with the total Hamiltonian

$$H = H_{\rm S} + H_{\rm B} + H_{\rm SB} \,, \qquad (1)$$

where $H_{\rm S}$ and $H_{\rm B}$ act only on the system and bath parts, respectively, and $H_{\rm SB}$ mediates a coupling. The latter may generally be decomposed as [3]

$$H_{\rm SB} = \sum_{\alpha=1}^{M} A_\alpha \otimes B_\alpha \qquad (2)$$

with M hermitian system ($A_\alpha = A_\alpha^\dagger$) and bath ($B_\alpha = B_\alpha^\dagger$) coupling operators. By convention, the system coupling operators may be chosen traceless and orthonormal ${\rm Tr}\{A_\alpha A_\beta\} = \delta_{\alpha\beta}$. For example, for an N-dimensional system Hilbert space one may use the $M = N^2 - 1$ generators of the $SU(N)$.

Under the Born, Markov, and secular (BMS) approximations [3], and assuming that the bath is kept in an equilibrium state $\bar\rho_{\rm B}$ with the properties ${\rm Tr}_{\rm B}\{B_\alpha\bar\rho_{\rm B}\} = 0$ as well as $[H_{\rm B}, \bar\rho_{\rm B}] = 0$, one derives a master equation of Lindblad form. In the system energy eigenbasis

$H_\text{S} \ket{a} \equiv E_a \ket{a}$, the master equation has the form [14]

$$
\begin{aligned}
\dot{\rho}_\text{S} = {} & -i \left[H_\text{S} + \sum_{ab} \tilde{\sigma}_{ab} \ket{a}\bra{b}, \rho_\text{S}(t) \right] \\
& + \sum_{abcd} \tilde{\gamma}_{ab,cd} \Big[\big(\ket{a}\bra{b} \big) \rho_\text{S}(t) \big(\ket{c}\bra{d} \big)^\dagger \\
& - \frac{1}{2} \left\{ \big(\ket{c}\bra{d} \big)^\dagger \big(\ket{a}\bra{b} \big), \rho_\text{S}(t) \right\} \Big],
\end{aligned} \qquad (3)
$$

where $\tilde{\sigma}_{ab} = \sigma^*_{ba}$ denotes the Lamb-shift and $\gamma_{ab,cd}$ includes the dissipative terms. These coefficients may vanish when some transition frequencies are not matched

$$
\begin{aligned}
\tilde{\sigma}_{ab} = {} & \frac{1}{2i} \sum_c \sum_{\alpha\beta} \sigma_{\alpha\beta}(E_a - E_c)\delta_{E_b,E_a} \times \\
& \times \bra{c} A_\alpha \ket{a}^* \bra{c} A_\beta \ket{b}, \\
\tilde{\gamma}_{ab,cd} = {} & \sum_{\alpha\beta} \gamma_{\alpha\beta}(E_b - E_a)\delta_{E_d-E_c,E_b-E_a} \times \\
& \times \bra{a} A_\beta \ket{b} \bra{c} A_\alpha \ket{d}^*,
\end{aligned} \qquad (4)
$$

which is formally expressed by the Kronecker-δ symbols. In these dampening coefficients, the functions

$$
\begin{aligned}
\gamma_{\alpha\beta}(\omega) &\equiv \int_{-\infty}^{+\infty} C_{\alpha\beta}(\tau)e^{+i\omega\tau}d\tau, \\
\sigma_{\alpha\beta}(\omega) &\equiv \int_{-\infty}^{+\infty} C_{\alpha\beta}(\tau)\text{sgn}(\tau)e^{+i\omega\tau}d\tau
\end{aligned} \qquad (5)
$$

are even ($\gamma_{\alpha\beta}$) and odd ($\sigma_{\alpha\beta}$) Fourier transforms of the bath correlation functions

$$
\mathcal{C}_{\alpha\beta}(\tau) \equiv \text{Tr}_\text{B} \left\{ e^{+i\tau H_\text{B}} B_\alpha e^{-i\tau H_\text{B}} B_\beta \bar{\rho}_\text{B} \right\}. \qquad (6)
$$

The bath correlation functions have many interesting analytic properties [3]. For example, when the bath is held at a thermal equilibrium state

$$
\bar{\rho}_\text{B} = \frac{e^{-\beta H_\text{B}}}{\text{Tr}_\text{B} \{ e^{-\beta H_\text{B}} \}}, \qquad (7)
$$

one can easily verify [3] the Kubo-Martin-Schwinger [15–17] (KMS) condition $\mathcal{C}_{\alpha\beta}(\tau) = \mathcal{C}_{\beta\alpha}(-\tau - i\beta)$. When the bath correlation functions are analytic in the lower complex half plane, the Fourier transform of the KMS condition reads

$$
\gamma_{\alpha\beta}(-\omega) = e^{-\beta\omega}\gamma_{\beta\alpha}(+\omega), \qquad (8)
$$

and can be used to prove [9] that the equilibrated Gibbs state

$$
\bar{\rho}_\text{S} = \frac{e^{-\beta H_\text{S}}}{\text{Tr} \{ e^{-\beta H_\text{S}} \}} \qquad (9)
$$

is a stationary state of Eq. (3).

II. CONSERVED QUANTITIES

Now assume that there exists a conserved quantity $N = N_S + N_B$, where N_S and N_B act only on system and bath, respectively. That is, we assume that $[H_\text{S}, N_S] = 0$, $[H_\text{B}, N_B] = 0$, and $[H_\text{SB}, N_S + N_B] = 0$, such that nontrivial evolution arises via $[H_\text{SB}, N_S] \neq 0$. Then, the invariance of H_SB with respect to global pseudo-rotations around the conserved axis $H_\text{SB} = e^{+\kappa(N_\text{S}+N_\text{B})} H_\text{SB} e^{-\kappa(N_\text{S}+N_\text{B})}$ leads to the identity

$$
\begin{aligned}
\sum_\alpha \big(e^{+\kappa N_\text{S}} A_\alpha e^{-\kappa N_\text{S}} \big) \otimes B_\alpha = {} \\
\sum_\alpha A_\alpha \otimes \big(e^{-\kappa N_\text{B}} B_\alpha e^{+\kappa N_\text{B}} \big),
\end{aligned} \qquad (10)
$$

which effectively transfers a pseudo-rotation of system operators into a pseudo-rotation of bath operators. We will show in the following, that this identity leads to additional properties of the dampening coefficients in Eq. (3), when the bath density matrix is assumed to be in the shifted equilibrium state with chemical potential μ

$$
\bar{\rho}_\text{B} = \frac{e^{-\beta(H_\text{B}-\mu N_\text{B})}}{\text{Tr}_\text{B} \left\{ e^{-\beta(H_\text{B}-\mu N_\text{B})} \right\}}. \qquad (11)
$$

Note that normalizability of $\bar{\rho}_\text{B}$ may impose constraints on the chemical potential, compare Sec. III B, Sec. III C, and Sec. III D. Evidently, as $[H_\text{S}, N_S] = 0$, we may also choose $\ket{a}$ to be the common eigenbasis of the two operators, such that $H_S \ket{a} = E_a \ket{a}$ and $N_S \ket{a} = N_a \ket{a}$.

When we multiply the Lamb-shift coefficients $\tilde{\sigma}_{ij}$ by a factor of the form $e^{+\beta\mu(N_i-N_j)}$, we may use Eq. (4) to replace the eigenvalues by operators, such that the system operators in Eq. (4) are rotated. Then, the identity (10) with Eq. (5) can be used to transfer the pseudo-rotation to the bath correlation functions. Finally, we may use the invariance of the trace over the bath degrees of freedom under cyclic permutations and $[N_\text{B}, \bar{\rho}_\text{B}] = 0$ to see that

$$
\tilde{\sigma}_{ij} e^{+\beta\mu(N_i-N_j)} = \tilde{\sigma}_{ij}, \qquad (12)
$$

i.e., the Lamb shift only acts on states with both degenerate energy and particle number. An analog calculation for the dissipative coefficients $\tilde{\gamma}_{ab,cd}$ reveals the identity

$$
\tilde{\gamma}_{aj,ai} e^{+\beta\mu(N_i-N_j)} = \tilde{\gamma}_{aj,ai}. \qquad (13)
$$

When we consider additional thermal Boltzmann factors, one needs to change the integration path in the Fourier transform (5) – using that the bath correlation functions are analytic – to show that the balance relation

$$
\tilde{\gamma}_{ia,ja} e^{-\beta(E_a-E_i)} e^{+\beta\mu(N_a-N_j)} = \tilde{\gamma}_{aj,ai} \qquad (14)
$$

holds. This fluctuation theorem [18] generalizes the KMS condition ($\mu = 0$) in Eq. (8) to systems with a conserved quantity.

A. Stationary state

The matrix elements of the generalized Gibbs state read

$$\langle i | \bar{\rho}_{\mathrm{S}} | j \rangle = \frac{\langle i | e^{-\beta(H_{\mathrm{S}} - \mu N_{\mathrm{S}})} | j \rangle}{Z} = \frac{\delta_{ij} e^{-\beta(E_i - \mu N_i)}}{Z} , \quad (15)$$

where $Z = \mathrm{Tr}\left\{ e^{-\beta(H_{\mathrm{S}} - \mu N_{\mathrm{S}})} \right\}$ denotes the normalization. For such a diagonal density matrix, the time-evolution of off-diagonal matrix elements is still influenced by the diagonals, as Eq. (3) reduces to

$$\dot{\rho}_{ij}\big|_{\bar{\rho}_{\mathrm{S}}} = -i\tilde{\sigma}_{ij} (\rho_{jj} - \rho_{ii}) + \sum_a \tilde{\gamma}_{ia,ja} \rho_{aa}$$
$$- \frac{1}{2} \sum_a \tilde{\gamma}_{aj,ai} (\rho_{ii} + \rho_{jj}) . \quad (16)$$

To show stationarity of the Gibbs state (15), it is convenient to distinguish some different cases:

a. Trivially, when $i \neq j$ and also $E_i \neq E_j$ in Eq. (16), we have $\dot{\rho}_{ij}\big|_{\bar{\rho}_{\mathrm{S}}} = 0$, since all coefficients simply vanish, cf. Eq. (4).

b. When $i = j$ and evidently also $E_i = E_j$, Eq. (16) reduces to the rate equation system

$$\dot{\rho}_{ii}\big|_{\bar{\rho}_{\mathrm{S}}} = +\sum_a \tilde{\gamma}_{ia,ia} \rho_{aa} - \sum_a \tilde{\gamma}_{ai,ai} \rho_{ii} , \quad (17)$$

which vanishes due to the detailed balance relation (14), evaluated for $i = j$.

c. For degenerate energy levels we have the additional possibility that $i \neq j$ but $E_i = E_j$. Cancellation of the Lamb-shift terms in (16) results from Eq. (12). Showing that the remaining dissipative terms also vanish amounts to

$$0 = \sum_a \tilde{\gamma}_{ia,ja} e^{-\beta(E_a - E_i)} e^{+\beta\mu(N_a - N_j)}$$
$$- \frac{1}{2} \sum_a \gamma_{aj,ai} \left[e^{+\beta\mu(N_i - N_j)} + 1 \right] , \quad (18)$$

which is directly evident from relations (13) and (14).

To summarize, we have shown that the state (15) is a stationary state of the master equation (3), when the reservoir density matrix is of the form (11). Generally of course, the existence of further stationary states is possible, but for an ergodic [3] evolution the BMS approximation scheme leads to *equilibration of both temperature and chemical potential* between system and reservoir. This generalizes previous findings for the BMS approximation [19, 20] and for rate equations [21], but has also be observed for local equilibration [22].

B. Multiple Reservoirs

When the system of interest is is not only coupled to a single, but multiple (K) reservoirs

$$H_{\mathrm{SB}} = \sum_\alpha A_\alpha \otimes \sum_{k=1}^{K} B_\alpha^{(k)} , \quad H_{\mathrm{B}} = \sum_{k=1}^{K} H_{\mathrm{B}}^{(k)} , \quad (19)$$

where varying coupling strengths are absorbed in the $B_\alpha^{(k)}$ operators and the reservoirs are characterized by different inverse temperatures $\beta^{(k)}$ and different chemical potentials $\mu^{(k)}$

$$\bar{\rho}_{\mathrm{B}} = \bigotimes_{k=1}^{K} \frac{e^{-\beta^{(k)}\left(H_{\mathrm{B}}^{(k)} - \mu^{(k)} N_B^{(k)} \right)}}{\mathrm{Tr}_{\mathrm{B}}^{(k)} \left\{ e^{-\beta^{(k)}\left(H_{\mathrm{B}}^{(k)} - \mu^{(k)} N_B^{(k)} \right)} \right\}} , \quad (20)$$

much less is known about the resulting stationary state [23]. We assume that some interaction Hamiltonians may obey a conserved quantity $N^{(k)} \equiv N_S + N_B^{(k)}$, where $\left[N_B^{(k)}, H_B^{(k)} \right] = 0 = \left[N_S + N_B^{(k)}, \sum_\alpha A_\alpha \otimes B_\alpha^{(k)} \right]$ A decomposition of the interaction Hamiltonian in the form of Eq. (19) with identical system coupling operators for each bath is always possible, as we have chosen the A_α operators to form a complete basis set for hermitian operators in the system Hilbert space. Evidently, the form of Eq. (3) remains invariant with

$$\tilde{\gamma}_{ab,cd} = \sum_{k=1}^{K} \tilde{\gamma}_{ab,cd}^{(k)} , \qquad \tilde{\sigma}_{ab} = \sum_{k=1}^{K} \tilde{\sigma}_{ab}^{(k)} , \quad (21)$$

where $\tilde{\gamma}_{ab,cd}^{(k)}$ and $\tilde{\sigma}_{ab}^{(k)}$ describe the dissipation and Lamb-shift, respectively, due to the k-th bath only. Accordingly, each bath yields separate detailed balance conditions of the form of Eqns. (12), (13), and (14).

The question which we seek to answer is whether these K local balance conditions can be compatible with a single global balance condition, eventually leading to thermalization in a Gibbs state with average temperature $\bar{\beta}$ and average chemical potential $\bar{\mu}$.

An affirmative answer can be given for a class of systems that fulfill

a. $H_{\mathrm{S}} = \Delta\epsilon N_S$, i.e., non-interacting models with an equidistant spectrum,

b. the system coupling operators act identically on energetically degenerate states $\langle j | A_\alpha | a \rangle = \langle i | A_\alpha | a \rangle$ for $E_i = E_j$,

c. the structure of the dampening coefficients allows only the single transition frequency $\pm\Delta\epsilon$ (and hence particle number difference ± 1).

Due to the first condition, relations (12) and (13) are automatically fulfilled, as for the nonvanishing coefficients $\tilde{\sigma}_{ij}^{(k)}$ and $\tilde{\gamma}_{aj,ai}^{(k)}$ we have $E_i = E_j$ and consequently also

$N_i = N_j$. The second condition implies that $\tilde{\gamma}_{ia,ja}^{(k)} = \tilde{\gamma}_{ia,ia}^{(k)} \equiv \tilde{\gamma}_{ia}^{(k)}$ and analogously $\tilde{\gamma}_{aj,ai}^{(k)} = \tilde{\gamma}_{ai,ai}^{(k)} \equiv \tilde{\gamma}_{ai}^{(k)}$. Finally, the third condition implies that relations (14) only have to be fulfilled at a single transition frequency $E_a - E_i = \pm\Delta\epsilon$ and $N_a - N_i = \pm 1$. Performing a summation over k with Eq. (14) we then obtain

$$
\begin{aligned}
\sum_k \tilde{\gamma}_{ai}^{(k)} &= \sum_k \tilde{\gamma}_{ia}^{(k)} e^{-\beta^{(k)}(E_a - E_i)} e^{+\beta^{(k)}\mu^{(k)}(N_a - N_i)} \\
&\stackrel{!}{=} e^{\mp\bar{\beta}(\Delta\epsilon - \bar{\mu})} \sum_k \tilde{\gamma}_{ia}^{(k)} \quad : \quad E_a = E_i \pm \Delta\epsilon \quad (22)
\end{aligned}
$$

In order to make this a valid definition for a generalized Boltzmann factor, it is necessary that

$$
e^{-\bar{\beta}(\Delta\epsilon - \bar{\mu})} \stackrel{(E_a = E_i + \Delta\epsilon)}{=} \frac{\sum_k \tilde{\gamma}_{ia}^{(k)} e^{-\beta^{(k)}(\Delta\epsilon - \mu^{(k)})}}{\sum_k \tilde{\gamma}_{ia}^{(k)}} > 0 \,. \quad (23)
$$

In addition, common sense suggests that the average Boltzmann factor should be a *convex* combination of the K bath Boltzmann factors. Both conditions are fulfilled due to

$$
\gamma_{ia}^{(k)} = \sum_{\alpha\beta} \langle i| A_\alpha |a\rangle^* \gamma_{\alpha\beta}^{(k)}(E_a - E_i) \langle i| A_\beta |a\rangle \geq 0 \,, \quad (24)
$$

since $\gamma_{\alpha\beta}^{(k)}(\omega)$ is a positive semidefinite matrix, which follows from Bochners theorem [3, 24]. In consequence, we obtain thermalization at an average temperature and average chemical potential for this class of systems, where average temperature and chemical potential are defined by Eq. (23).

III. EXAMPLES

For a single reservoir the equilibration of both temperature and chemical potential has been observed even for interacting systems [19]. Therefore, we only give examples to illustrate the results in Sec. II B. Naturally, in case of only a single coupling bath, the non-interacting case of Sec. II A is also reproduced here.

A. Non-Interacting Electronic Nanostructure

Consider a nanostructure with N sites for non-interacting electrons $H_S = \Delta\epsilon \sum_{i=1}^{N} d_i^\dagger d_i$, at first coupled to a single lead $H_B = \sum_k \epsilon_k c_k^\dagger c_k$ at temperature β and chemical potential μ via the tunneling Hamiltonian [27] $H_{SB} = D \otimes \sum_k g_k c_k^\dagger + D^\dagger \otimes \sum_k g_k^* c_k$, where $D \equiv \sum_{i=1}^{N} d_i$, g_k represents a frequency-dependent coupling constant, and c_k are fermionic annihilation operators acting on the lead Hilbert space. The conserved quantity is composed from $N_S = \sum_{i=1}^{N} d_i^\dagger d_i$ and $N_B = \sum_k c_k^\dagger c_k$. We may write the interaction Hamiltonian also as $H_{SB} = A_1 \otimes B_1 +$

$A_2 \otimes B_2$, with the hermitian and trace-orthogonal (not-normalized) system coupling operators $A_1 = \left(D^\dagger + D\right)$ and $A_2 = i\left(D^\dagger - D\right)$, and the associated bath coupling operators $B_1 = \sum_k \left(g_k c_k^\dagger + g_k^* c_k\right)/2$ and $B_2 = i\sum_k \left(g_k c_k^\dagger - g_k^* c_k\right)/2$. For a single bath in thermal equilibrium β and with chemical potential μ, such that $\bar{\rho}_B = e^{-\beta(H_B - \mu N_B)}/Z$, we obtain for Fourier transforms (5) of the bath correlation functions $\gamma_{11}(\omega) = \gamma_{22}(\omega) = \Gamma(+\omega)\left[1 - f(+\omega)\right]/4 + \Gamma(-\omega)f(-\omega)/4$ and $\gamma_{12}(\omega) = \gamma_{21}^*(\omega) = i\Gamma(+\omega)\left[1 - f(+\omega)\right]/4 - i\Gamma(-\omega)f(-\omega)/4$, where $\Gamma(\omega) \equiv 2\pi \sum_k |g_k|^2 \delta(\omega - \epsilon_k)$ is the tunneling rate and the Fermi function $f(\omega) \equiv 1/(e^{\beta(\omega-\mu)} + 1)$ encodes the bath properties β and μ. Obviously, the Fourier-transform matrix of bath correlation functions has non-negative eigenvalues. In addition, for $N = 1$ we recover the single resonant level [25].

For $N > 1$, the spectrum of the Hamiltonian is degenerate, but the permutational symmetry suggests to use the symmetrized basis $|N, m+1\rangle \equiv \frac{1}{\sqrt{(N-m)(m+1)}} D^\dagger |N, m\rangle$ with $0 \leq m \leq N$, where $|N, 0\rangle = |0, \ldots, 0\rangle$ represents the N particle Fock space vacuum. Clearly, it is an eigenbasis of H_S and N_S. We obtain for the nonvanishing coefficients

$$
\begin{aligned}
\tilde{\gamma}_{m,m+1} &= (N-m)(m+1)\Gamma(+\Delta\epsilon)\left[1 - f(+\Delta\epsilon)\right] \,, \\
\tilde{\gamma}_{m+1,m} &= (N-m)(m+1)\Gamma(+\Delta\epsilon)f(+\Delta\epsilon) \,. \quad (25)
\end{aligned}
$$

The generalized KMS condition (14) therefore simply reduces to $f(+\Delta\epsilon) = e^{-\beta(\Delta\epsilon - \mu)}\left[1 - f(+\Delta\epsilon)\right]$, which is a general property of the Fermi functions. The corresponding rate equation reads with $\rho_m \equiv \langle N, m| \rho_S |N, m\rangle$

$$
\begin{aligned}
\dot{\rho}_m &= \tilde{\gamma}_{m,m-1}\rho_{m-1} + \tilde{\gamma}_{m,m+1}\rho_{m+1} \\
&\quad - \left[\tilde{\gamma}_{m-1,m} + \tilde{\gamma}_{m+1,m}\right]\rho_m \,, \quad (26)
\end{aligned}
$$

where it becomes visible that in the chosen basis, the Lamb-shift terms are irrelevant.

Now we consider tunnel couplings to multiple baths with factorizing density matrices as in Eq. (20). The form of Eq. (26) remains invariant, and we simply have $\tilde{\gamma}_{m,m\pm 1} = \sum_k \tilde{\gamma}_{m,m\pm 1}^{(k)}$, with different temperatures $\beta^{(k)}$ and chemical potentials $\mu^{(k)}$ entering the rates as in Eq. (25). In this case, one may check explicitly that the stationary state of Eq. (26) is a thermal one with average Boltzmann factor

$$
e^{-\bar{\beta}(\Delta\epsilon - \bar{\mu})} = \frac{\sum_k \Gamma^{(k)}(\Delta\epsilon) f^{(k)}(\Delta\epsilon)}{\sum_k \Gamma^{(k)}(\Delta\epsilon)\left[1 - f^{(k)}(\Delta\epsilon)\right]} \quad (27)
$$

which is consistent with Eq. (23). The same factor would be obtained when the system was coupled to a hypothetical single bath with average Fermi function $\bar{f}(\Delta\epsilon) = \left[\sum_k \Gamma^{(k)}(\Delta\epsilon) f^{(k)}(\Delta\epsilon)\right] / \left[\sum_k \Gamma^{(k)}(\Delta\epsilon)\right]$.

B. Coupled oscillators

We consider a harmonic oscillator $H_S = \Omega b^\dagger b$ coupled to many others $H_B = \sum_k \omega_k b_k^\dagger b_k$ with positive eigenfrequencies $\omega_k > 0$ via quasi-particle tunneling $H_{SB} = b \otimes \sum_k h_k b_k^\dagger + b^\dagger \otimes \sum_k h_k^* b_k$. The conserved quantity is composed from $N_S = b^\dagger b$ and $N_B = \sum_k b_k^\dagger b_k$. Rewriting the interaction Hamiltonian in terms of hermitian operators, we obtain $A_1 = (b^\dagger + b)$, $A_2 = i(b^\dagger - b)$, $B_1 = \sum_k (h_k b_k^\dagger + h_k^* b_k)/2$, and $B_2 = i \sum_k (h_k b_k^\dagger - h_k^* b_k)/2$. The matrix elements of the Fourier transforms (5) of the bath correlation functions equate to $\gamma_{11}(\omega) = \gamma_{22}(\omega) = 1/4 [+\Theta(+\omega)[1 + n(+\omega)]\Gamma(+\omega) + \Theta(-\omega)n(-\omega)\Gamma(-\omega)]$ and $\gamma_{21}^*(\omega) = \gamma_{12}(\omega) = i/4 [+\Theta(+\omega)[1 + n(+\omega)]\Gamma(+\omega) - \Theta(-\omega)n(-\omega)\Gamma(-\omega)]$, where $\Theta(\omega)$ denotes the Heavyside step function, $\Gamma(\omega) = 2\pi \sum_k |h_k|^2 \delta(\omega - \omega_k)$ the quasi-particle tunneling rate, and $n(\omega) \equiv 1/(e^{\beta(\omega-\mu)} - 1)$ denotes the bosonic occupation number. The condition that $\mu < \min_k(\omega_k)$ grants positivity of all bath occupations. In addition, it implies that $\Gamma(\Omega)|_{\Omega<\mu} = 0$, such that we assume also $\Omega > \mu$ throughout. Accordingly, the Fourier transform matrix of the bath correlation functions is positive semidefinite at all frequencies. In the Fock space basis (where $b^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$), we obtain a rate equation of the form (26), where $0 \le n < \infty$. However, since the eigenstates are non-degenerate, the dampening coefficients equate (with $\Omega > 0$) to

$$\begin{aligned}
\tilde{\gamma}_{n,n+1} &= (n+1)[1 + n(\Omega)]\Gamma(\Omega), \\
\tilde{\gamma}_{n+1,n} &= (n+1)n(\Omega)\Gamma(\Omega).
\end{aligned} \tag{28}$$

The resulting system is infinitely large, one may however, introduce a cutoff size N_{cut} and solve for the stationary state of the rate equations for finite N_{cut}. The ratio ρ_{n+1}/ρ_n of two successive populations yields the desired Boltzmann factor, which even happens to be independent of N_{cut}.

For multiple baths, we obtain equilibration in an average thermal state with the average Boltzmann factor

$$e^{-\bar{\beta}(\Omega-\bar{\mu})} = \frac{\sum_k \Gamma^{(k)}(\Omega)n^{(k)}(\Omega)}{\sum_k \Gamma^{(k)}(\Omega)[1 + n^{(k)}(\Omega)]}, \tag{29}$$

consistent with Eq. (23). This Boltzmann factor is the same that one would obtain for contact with a hypothetical single bath at an average occupation $\bar{n}(\Omega) = [\sum_k \Gamma^{(k)}(\Omega)n^{(k)}(\Omega)]/[\sum_k \Gamma^{(k)}(\Omega)]$, which in the classical (high-temperature and $\mu^{(k)} \to 0$) limit reduces to the average temperature $\bar{T} \approx [\sum_k \Gamma^{(k)}(\Omega)T^{(k)}]/[\sum_k \Gamma^{(k)}(\Omega)]$, which coincides well with classical expectations and previous results [10].

C. Spin-Boson Model

A variant of the spin-boson model coupled to a single bath has already been provided in Ref. [26], such

that we here only generalize to $K \ge 2$ baths and non-vanishing chemical potentials. We consider a large spin system $H_S = \Omega/2 J^z$ with $\Omega > 0$, coupled to a bath of harmonic oscillators $H_B = \sum_k \omega_k b_k^\dagger b_k$ with $\omega_k > 0$ via $H_{SB} = J^x \otimes \sum_k \left[h_k b_k^\dagger + h_k b_k \right]$, where $J^\alpha \equiv \sum_{i=1}^N \sigma_i^\alpha$, and where the coupling operators are hermitian already. At first sight, the total Hamiltonian does not obey a conserved quantity of the discussed type. However, within the BMS approximation, the model is identical to one with the modified interaction Hamiltonian $H_{SB}^* = J^+ \otimes \sum_k h_k b_k^\dagger + J^- \otimes \sum_k h_k b_k$ with the conserved quantity $N_S + N_B = -J^z/2 + \sum_k b_k^\dagger b_k$ and where $J^\pm \equiv (J^x \pm iJ^y)/2$. We impose the same conditions on the chemical potential(s) as before: $\mu < \min_k(\omega_k)$ and $\mu < \Omega$. From the previous section, the Fourier transform (5) of the bath correlation function is evidently $\gamma(\omega) = +\Theta(+\omega)[1 + n(+\omega)]\Gamma(+\omega) + \Theta(-\omega)n(-\omega)\Gamma(-\omega)$. In order to calculate the dampening coefficients, permutational symmetry suggests to use the angular momentum basis $|N/2, m\rangle$ with $-N/2 \le m \le +N/2$. Using that $J^x = J^+ + J^-$ with $J^\pm |j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)} |j, m\rangle$, we obtain a rate equation of the form (26) with the coefficients $\tilde{\gamma}_{m,m+1} = \Gamma(\Omega)[1 + n(\Omega)][N/2(N/2+1) - m(m+1)]$ and $\tilde{\gamma}_{m+1,m} = \Gamma(\Omega)n(\Omega)[N/2(N/2+1) - m(m+1)]$.

Solving this rate equation with multiple baths for its steady state yields a thermal bath with the same average Boltzmann factor as Eq. (29), as predicted by Eq. (23).

D. Mixed Spin Model

We consider a spin-1/2 system $H_S = \Omega/2\sigma^z$ that is firstly coupled to a bosonic bath $H_B^{(1)} = \sum_k \omega_k b_k^\dagger b_k$ via the dissipative coupling $H_{SB}^{(1)} = \sigma^x \otimes \sum_k \left[h_k b_k^\dagger + h_k^* b_k \right]$, and secondly to a fermionic bath $H_B^{(2)} = \sum_k \epsilon_k c_k^\dagger c_k$ via the coupling $H_{SB}^{(2)} = \sigma^+ \otimes \sum_k g_k c_k^\dagger + \sigma^- \otimes \sum_k g_k^* c_k$. The second interaction Hamiltonian explicitly obeys the conserved quantity constructed from $N_S = -\sigma^z/2$ and $N_B^{(2)} = \sum_k c_k^\dagger c_k$, and under the BMS approximation the first interaction Hamiltonian is equivalent to $H_{SB}^{*(1)} = \sigma^+ \otimes \sum_k h_k b_k^\dagger + \sigma^- \otimes \sum_k h_k^* b_k$. Note that $H_{SB}^{(2)}$ does not conserve the number of fermions, but such a model may represent scattering processes with a further fermionic bath. As before, we require that $\mu^{(1)} < \Omega$ and $\mu^{(1)} < \min_k(\omega_k)$. Choosing the system coupling operators as $A_1 = \sigma^x$ and $A_2 = \sigma^y$, we obtain $B_1^{(1)} = \sum_k \left(h_k b_k^\dagger + h_k^* b_k \right)$, $B_2^{(1)} = 0$, and $B_1^{(2)} = 1/2 \sum_k \left(g_k c_k^\dagger + g_k^* c_k \right)$ with $B_2^{(2)} = i/2 \sum_k \left(g_k c_k^\dagger - g_k^* c_k \right)$. The Fourier transform of the bath correlation function for the first bath corresponds to Sec. III C, whereas the Fourier transform matrix for the second bath is identical to that of Sec. III A. Accordingly, we obtain in the σ^z-eigenbasis $\sigma^z |a\rangle = (-1)^a |a\rangle$

with $a \in \{0, 1\}$ and $\rho_a \equiv \langle a | \rho_S | a \rangle$ the master equation

$$\rho_0 = -\left[\tilde{\gamma}_{1,0}^{(1)} + \gamma_{1,0}^{(2)}\right]\rho_0 + \left[\tilde{\gamma}_{0,1}^{(1)} + \gamma_{0,1}^{(2)}\right]\rho_1 ,$$
$$\rho_1 = +\left[\tilde{\gamma}_{1,0}^{(1)} + \gamma_{1,0}^{(2)}\right]\rho_0 - \left[\tilde{\gamma}_{0,1}^{(1)} + \gamma_{0,1}^{(2)}\right]\rho_1 \quad (30)$$

with the dampening coefficients $\tilde{\gamma}_{0,1}^{(1)} = \Gamma_1(\Omega)\left[1 + \mathrm{n}(\Omega)\right]$, $\tilde{\gamma}_{1,0}^{(1)} = \Gamma_1(\Omega)\mathrm{n}(\Omega)$, $\tilde{\gamma}_{0,1}^{(2)} = \Gamma_2(\Omega)\left[1 - \mathrm{f}(\Omega)\right]$, and $\tilde{\gamma}_{1,0}^{(2)} = \Gamma_2(\Omega)\mathrm{f}(\Omega)$, where $\mathrm{f}(\omega)$ and $\mathrm{n}(\omega)$ have been defined in Sec. III A and Sec. III B, respectively, and $\Gamma_1(\omega) = 2\pi \sum_k |h_k|^2 \delta(\omega - \omega_k)$ with $\Gamma_2(\omega) = 2\pi \sum_k |g_k|^2 \delta(\omega - \epsilon_k)$ represent the coupling strengths to the two baths, respectively. The stationary state of Eq. (30) is a thermal one with average Boltzmann factor

$$e^{-\bar{\beta}(\Omega - \bar{\mu})} = \frac{\Gamma_1(\Omega)\mathrm{n}(\Omega) + \Gamma_2(\Omega)\mathrm{f}(\Omega)}{\Gamma_1(\Omega)\left[1 + \mathrm{n}(\Omega)\right] + \Gamma_2(\Omega)\left[1 - \mathrm{f}(\Omega)\right]} , \quad (31)$$

which is consistent with Eq. (23).

IV. CONCLUSIONS

Under the Born, Markov, and secular approximations, quantum systems coupled to a single bath described by inverse temperature β and chemical potential μ do not only equilibrate their temperature, but – when the total Hamiltonian conserves a (quasi-)particle number – also their chemical potential with that of the bath. As long as only a single bath is involved, this holds for interacting and non-interacting systems.

When the system is coupled to multiple baths, equilibration in an average thermal state may still occur when there exists only a single transition frequency, as e.g. in two-level systems. However, also for higher-dimensional systems, an average equilibration may occur when rigid symmetry assumptions are imposed. When the coupling baths have the same character (e.g., fermionic), the resulting stationary state is the same as the one reached by interaction with a hypothetical average bath.

There are several interesting consequences: Firstly, by using equilibration under side constraints one should be able to prepare not only the ground state of a system Hamiltonian by dissipative means but also an energy eigenstate with a desired particle number when bath temperature and chemical potential are tuned accordingly. Secondly, in order to generate interesting non-equilibrium stationary states via coupling to multiple baths, it is necessary (though not sufficient) to consider systems with more than a single allowed transition frequency. Finally, when the focus is on particle or thermal transport, analytic knowledge of the flow equilibrium state in the non-interacting limit as presented here may aid the corresponding calculations.

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