Resolving Discrepancy between Liouvillian Gap and Relaxation Time in Boundary-Dissipated Quantum Many-Body Systems

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The gap of the Liouvillian spectrum gives the asymptotic decay rate of a quantum dissipative system, and therefore its inverse has been identified as the slowest relaxation time. In contrary to this common belief, we show that the relaxation time due to diffusive transports in a boundary dissipated many-body quantum system is determined not by the gap or low-lying eigenvalues of the Liouvillian but by superexponentially large expansion coefficients for Liouvillian eigenvectors with non-small eigenvalues at an initial state. This finding resolves an apparent discrepancy reported in the literature between the inverse of the Liouvillian gap and the relaxation time in dissipative many-body quantum systems.

Introduction.— Understanding the nonequilibrium steady state (NESS) and the relaxation dynamics towards it in a macroscopic open quantum system driven at boundaries is a central problem of nonequilibrium statistical physics and condensed matter physics [1–4]. This problem is of practical importance in the context of quantum technologies since recent advancement in experiments using ultra-cold atoms allow us to implement highly controllable dissipative dynamics [5–7].

Since the relaxation to the NESS takes place via the transport of conserved quantities, its timescale is determined by the transport property of the bulk Hamiltonian. If the slowest process is the diffusive transport, the relaxation time is proportional to \( L^2 \), where \( L \) is the diameter of the system, while if all the transports are ballistic, it is proportional to \( L \).

The dynamics of an open quantum system is generated by the Liouvillian superoperator, and thus the inverse of the gap of the Liouvillian spectrum has been identified as the relaxation time. It is then natural to expect that, in the thermodynamic limit, the Liouvillian gap closes as \( L^{-2} \) in a boundary-dissipated quantum chaotic system in which transports are diffusive. However, numerical results for finite systems by Žnidarič [4] show that the Liouvillian gap closes slower than \( L^{-2} \) in various boundary-dissipated systems with diffusive transports. Is such a large gap of the Liouvillian just a finite-size effect and should the Liouvillian gap always close as \( L^{-2} \) for sufficiently large system sizes?

In this Letter, we address the above question. It turns out that the relaxation time due to diffusive transports is originated not from low-lying eigenvalues of the Liouvillian but from extraordinarily large (\( \sim e^{O(L^2)} \)) expansion coefficients at an initial state, which is due to non-Hermiticity of the Liouvillian. Slowly vanishing gap \( g^{-1} = o(L^2) \) for large \( L \) does not contradict the relaxation time of \( O(L^2) \) due to diffusive transports. Our result is contrary to a common belief that the Liouvillian gap determines the relaxation time, and hence we should take special care for discussing the relaxation time in dissipative quantum systems.

Liouvillian eigenvalues and eigenvectors.— The dissipative dynamics of the density matrix \( \rho(t) \) of an open quantum system is described by the Lindblad equation \[ \begin{aligned} \frac{d}{dt}\rho(t) &= \mathcal{L}\rho(t), \\ \mathcal{L}\rho &= -i[\hat{H}, \rho] + \sum_a \left( \hat{L}_a \rho \hat{L}_a^\dagger - \frac{1}{2} \{ \hat{L}_a^\dagger \hat{L}_a, \rho \} \right), \end{aligned} \] (1) where \( \hat{H} \) is the bulk Hamiltonian and \( \{ \hat{L}_a \} \) are called the Lindblad operators that characterize the dissipation. The commutator and the anti-commutator are denoted by \( \{ \cdot, \cdot \} \) and \( \{ \cdot, \cdot \} \), respectively. We consider a one-dimensional lattice system and assume that dissipation acts only at two ends of the system, i.e., Lindblad operators are local operators acting nontrivially to either the left or right boundary.

The superoperator \( \mathcal{L} \) is called the Liouvillian. Complex eigenvalues of the Liouvillian are denoted by \( \{ \lambda_n \}_{n=0,1,2,\ldots} \), which are sorted as \( 0 = \lambda_0 \geq \text{Re} \lambda_1 \geq \text{Re} \lambda_2 \geq \ldots \) (we assume that the zero eigenvalue is not degenerate). The corresponding right and left eigenvectors are denoted by \( \{ \rho_n \} \) and \( \{ \pi_n \} \), respectively. We normalize the eigenvectors using the trace norm, i.e.,
\[
\|\rho_n\|_\text{tr} = |\pi_n|_\text{tr} = 1, \tag{2}
\]
where \( \|\hat{A}\|_\text{tr} := \text{Tr} \sqrt{\hat{A}^\dagger \hat{A}} \) \[10\]. Let us define the inner product of two operators \( \hat{A} \) and \( \hat{B} \) as \( \langle \hat{A}, \hat{B} \rangle = \text{Tr} \hat{A}^\dagger \hat{B} \). The orthogonality of eigenvectors is then expressed as
\[
\langle \pi_n, \rho_m \rangle = 0 \quad \text{for all } n \neq m. \tag{3}
\]
The right eigenvector \( \rho_0 \) with zero eigenvalue corresponds to the density matrix of the NESS, so we write \( \rho_0 = \rho_{\text{ss}} \). If the initial state \( \rho(0) \) is expanded as
\[
\rho(0) = \rho_{\text{ss}} + \sum_{n \neq 0} c_n \rho_n, \tag{4}
\]
the state at time \( t \) is given by
\[
\rho(t) = \rho_{\text{ss}} + \sum_{n \neq 0} c_n e^{\lambda_n t} \rho_n. \tag{5}
\]
The Liouvillian gap $g$ is defined as
\[ g = -\text{Re} \lambda_1. \] (6)

The Liouvillian gap determines the asymptotic decay rate [11] and also carries information on some properties of the NESS [11–14]. Let us consider an initial state with a single excited mode $\rho(0) = \rho_{ss} + c_n \rho_n$, where we assume that $\lambda_n$ is real for simplicity (in this case $\rho_n = \rho_n^\dagger$ and $\pi_n = \pi_n^\dagger$ hold). The trace distance between $\rho(t)$ at $t \geq 0$ and $\rho_{ss}$ is given by
\[ \|\rho(t) - \rho_{ss}\|_\text{tr} = |c_n e^{\text{Re}(\lambda_n) t}|. \] (7)

It should be noted that $\|\rho(t) - \rho_{ss}\|_\text{tr}$ is bounded by 2, and hence $|c_n|$ is restricted by
\[ |c_n| \leq 2. \] (8)

For any $\epsilon \in (0, 1)$, $\|\rho(t) - \rho_{ss}\|_\text{tr} \leq 2\epsilon$ for any $t \geq |\ln(\epsilon)/\text{Re} \lambda_n|$, and hence the relaxation time $\tau$ for this initial state is given by $\tau \sim |\ln \lambda_n|^{-1}$. It takes maximum at $n = 1$, and hence the relaxation time for any initial state with a single excited mode is bounded by the inverse of the Liouvillian gap
\[ \tau \leq g^{-1}. \] (9)

**Evaluation of relaxation time.**—Žnidarič [4] reported that numerical calculations of the Liouvillian gap of some boundary-dissipated spin systems show $g \propto L^{-\frac{2}{z}}$ with $1 \leq z < 2$ although the bulk Hamiltonian is chaotic and there exist diffusive transports, which implies $\tau \propto L^2$. This result violates the relation (9).

Here we argue that the behavior of $g \propto L^{-\frac{2}{z}}$ with $z < 2$ does not contradict the existence of diffusive transports. Now let us consider a general initial state $\rho(0) = \rho_{ss} + \sum_{n \neq 0} c_n \rho_n$. The trace distance satisfies the inequality
\[ \|\rho(t) - \rho_{ss}\|_\text{tr} \leq \sum_{n \neq 0} |c_n| e^{\text{Re}(\lambda_n) t}. \] (10)

From this expression, the relaxation time is estimated by the condition $|c_n| e^{\text{Re}(\lambda_n) t} \ll 1$ for all $n \neq 0$.

For an initial state with a single excited right eigenvector, eq. (8) must be satisfied. However, for generic initial states, eq. (8) does not need to hold and $|c_n|$ may take a much larger value. To understand it, let us consider an initial state with a single left eigenvector excited:
\[ \rho(0) = \rho_{ss} + a_n \pi_n, \] (11)

where we again assume that $\lambda_n$ is real, for simplicity. Similarly to eq. (8), $a_n$ satisfies
\[ |a_n| \leq 2. \] (12)

Now let us expand this state in terms of the right eigenvectors, $\rho(0) = \rho_{ss} + \sum_{m \neq 0} c_m \rho_m$ with
\[ c_m = \frac{\langle \pi_m, \rho(0) \rangle}{\langle \pi_m, \rho_m \rangle} = \frac{\langle \pi_m, \pi_n \rangle}{\langle \pi_m, \rho_m \rangle} a_n. \] (13)

For $m = n$, we have $c_n = a_n \langle \pi_n, \pi_n \rangle / \langle \pi_n, \rho_n \rangle$, and thus by using eq. (12), we obtain
\[ |c_n| \leq 2 \left| \frac{\langle \pi_n, \pi_n \rangle}{\langle \pi_n, \rho_n \rangle} \right| = 2 \Phi_n. \] (14)

When $\lambda_n$ is not real, we have to consider $\rho(0) = \rho_{ss} + a_n \pi_n + a_n^\dagger \pi_n^\dagger$ to ensure the Hermiticity of the density matrix. In this case, by defining $\Phi_n$ as
\[ \Phi_n = \frac{1}{\langle \pi_n, \rho_n \rangle} \max_{\theta \in [0, \pi]} \left| \frac{\langle \pi_n, \rho_n e^{i\theta} + \pi_n^\dagger e^{-i\theta} \rangle}{\langle \pi_n e^{i\theta} + \pi_n^\dagger e^{-i\theta} \rangle} \right|, \] (15)

it is shown that $|c_n| \leq 2 \Phi_n$.

Since the relaxation time $\tau$ should satisfy the condition $|c_n| e^{\text{Re}(\lambda_n) t} \leq 2\epsilon$ for some fixed small constant $\epsilon \in (0, 1)$, we obtain
\[ \tau \sim \frac{\ln \epsilon}{\text{Re} \lambda_n} + \frac{\ln \Phi_n}{|\text{Re}(\lambda_n)|}. \] (16)

The first term of eq. (16) gives a contribution to the relaxation time that is roughly bounded from above by $g^{-1}$. When $z < 2$, this contribution is $O(L^2)$, which does not explain the relaxation time during diffusive transports. We therefore focus on the second term of eq. (16),
\[ \tau_n := \frac{\ln \Phi_n}{|\text{Re}(\lambda_n)|}, \] (17)

which roughly gives the maximum relaxation time for a class of initial states expressed by $\rho(0) = \rho_{ss} + a_n \pi_n$.

If the Liouvillian were (anti-)Hermitian, $\rho_n = \pi_n$ and therefore $\Phi_n = 1$. In this case, eq. (14) is reduced to eq. (8). However, the Liouvillian is actually not (anti-)Hermitian, and hence $\rho_n$ is not identical to $\pi_n$. In this case, there is no obvious upper bound of $\Phi_n$. The divergence of $\ln \Phi_n$ in the thermodynamic limit, which alters the system-size dependence of the relaxation time, is not ruled out. If such a thing happens, the relaxation time is not solely determined by the Liouvillian gap, and the apparent contradiction between $g \sim L^{-\frac{2}{z}}$ with $z < 2$ and $\tau \sim L^2$ may disappear.

Below, we numerically show that in a many-body chaotic quantum system with boundary dissipation, $\tau_{\text{max}} \propto L^2$ due to the existence of expansion coefficients superexponential in $L$, i.e., $\Phi_n = e^{O(L)}$ for $\text{Re} \lambda_n = O(L^0)$ [see eq. (18)]. This result implies that the timescale of diffusive transports is determined not by the gap or low-lying eigenvalues of the Liouvillian but by such extraordinarily large expansion coefficients for eigenvectors with non-small eigenvalues $\text{Re} \lambda_n = O(L^0)$. This is contrary to a common belief that the Liouvillian gap characterizes the relaxation time.

Since $|\langle \pi_n, \pi_n \rangle| \leq \|\pi_n\|^2 = 1$, the superexponential dependence $e^{O(L^2)}$ purely stems from an anomalously small overlap...
\[ \langle \pi_n, \rho_n \rangle \text{ of left and right eigenvectors. In a recent work [15], it is shown that an exponentially small overlap } \langle \pi_n, \rho_n \rangle = e^{-O(L)} \text{ arises due to the localization of left and right eigenmodes at the opposite boundaries of the system in a single-particle model under bulk dissipation. As far as we have calculated, however, the superexponentially small overlap } |\langle \pi_n, \rho_n \rangle| = e^{-O(L^2)} \text{ in a boundary-dissipated many-body system is not simply explained by such a localization.}

Model.— We consider one-dimensional hard-core Bose-Hubbard model, which is equivalent to a spin-1/2 chain, with boundary dissipation. The bulk Hamiltonian is given by

\[ \hat{H} = -\hbar \sum_{i=1}^{L-1} \left( \hat{b}_{i+1}^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{b}_{i+1} \right) - \hbar' \sum_{i=1}^{L-2} \left( \hat{b}_{i+2}^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{b}_{i+2} \right) + U \sum_{i=1}^{L-1} \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_{i+1} - \frac{1}{2} \right) + U' \sum_{i=1}^{L-2} \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_{i+2} - \frac{1}{2} \right), \tag{19} \]

where \( \hat{b}_i, \hat{b}_i^\dagger \) are annihilation and creation operators of a hard-core boson at site \( i \), respectively, which satisfy \( \{ \hat{b}_i, \hat{b}_j \} = [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0 \) for any \( i \) and \( j \), \( [\hat{b}_i, \hat{b}_j^\dagger] = 0 \) for any \( i \neq j \), and \( \{ \hat{b}_i, \hat{b}_j^\dagger \} = 1 \). The number operator is denoted by \( \hat{n}_i = \hat{b}_i^\dagger \hat{b}_i \). We fix the parameters as \( \hbar = U = 1 \) and \( \hbar' = U' = 0.24 \). This model is known to be chaotic [16].

We consider two types of boundary dissipation for the Lindblad equation (1). The first one is the dephasing dissipation on the first and the last site, which corresponds to the Lindblad operators \( \{ \hat{L}_a \}_{a=1,2} \) with

\[ \hat{L}_1 = \hat{b}_1^\dagger \hat{b}_1, \quad \hat{L}_2 = \hat{b}_L^\dagger \hat{b}_L. \tag{20} \]

This model conserves the total particle number \( N = \sum_{i=1}^L \hat{n}_i \), and hence we restrict ourselves to the sector of \( N = L/2 \) for \( L \) even and \( N = (L-1)/2 \) for \( L \) odd. The NESS is just the infinite-temperature ensemble with a fixed particle number \( N \), and so the NESS is trivial but the relaxation dynamics is complicated.

The second one is the particle-driving dissipation, which is expressed by the Lindblad operators \( \{ \hat{L}_a \}_{a=1,2} \) with

\[ \hat{L}_1 = \sqrt{\gamma} \hat{b}_1^\dagger, \quad \hat{L}_2 = \sqrt{\gamma} \hat{b}_L. \tag{21} \]

where we fix \( \gamma = 0.2 \) in this Letter. In this case, \( \hat{L}_1 \) adds a boson at site 1 and \( \hat{L}_2 \) removes a boson at site \( L \). As a result, particles flow from left to right, and a nontrivial NESS is formed.

The Liouvillian gap and the time evolution of the trace distance \( \| \rho(t) - \rho_{SS} \|_1 \) are presented in [17]. The Liouvillian gap \( g \) scales as \( L^{-\gamma} \) with \( \gamma \approx 1.6 \) for the dephasing dissipation and \( \gamma \approx 1.0 \) for the particle-driving dissipation. The dynamics of the trace distance shows that the relaxation time is proportional to \( L^2 \) in both cases, which is consistent with the presence of diffusive transports but not explained by \( g^{-1} \).

**Numerical Calculations of \( \Phi_n \) and \( \tau_{\max} \).**—Figure 1 shows numerically calculated values of \( \Phi_n \) as a function of \( |\text{Re } \lambda_n| \) up to \( L = 9 \) in the model with the dephasing dissipation. We see that the values of \( \{ \Phi_n \} \) rapidly grow with \( L \). In the same figure, the rescaled quantity \( \ln(\Phi_n)/L^2 \) is also shown. The system-size dependence disappears after rescaling, which means that \( \Phi_n \) typically behaves as \( \Phi_n \propto e^{O(L^2)} \).

Figure 2 shows \( \tau_n \) for varying \( L \) (Top) and the system-size dependence of \( \tau_{\max} = \max_n \tau_n =: \tau_n \) and \( \tau_1 \) (Bottom) in the model with the dephasing dissipation. The number written at each plot point in Fig. 2 (Bottom) represents \( |\text{Re } \lambda_n| \). We see that \( \tau_{\max} \propto L^2 \), which is consistent with the relaxation time due to diffusive transports. The value of \( |\text{Re } \lambda_n| \) does not seem to decrease with \( L \), which indicates that eigenmodes with non-small eigenvalues, \( \lambda_n = O(L^0) \), play a dominant role in determining the overall relaxation time. This conclusion is strengthened by the fact that \( \tau_1 \) increases with \( L \) but slower than \( O(L^2) \), which means that the first excited eigenmode giving the Liouvillian gap does not produce diffusive relaxation. The gap is not relevant in determining the overall relaxation time, although it determines the asymptotic decay rate in the long-time limit (see also [17]).

Similar results are also obtained for the particle-driving dissipation. Figure 3 shows \( \ln(\Phi_n)/L^2 \) (Top) and \( \ln(\Phi_n)/L^2 \) (Bottom), respectively, up to \( L = 7 \) except for \( \tau_1 \). We see that typical values of \( \ln(\Phi_n)/L^2 \) do not change with \( L \), which implies \( \Phi_n \propto e^{O(L^2)} \) and \( \tau_{\max} \propto L^2 \). In this model, in contrary to the dephasing dissipation, we also find \( \tau_1 \propto L^2 \), which...
FIG. 2. (Top) $\tau_n$ for varying system sizes $L$. (Bottom) Log-log plot of $\tau_{\text{max}}$ and $\tau_1$ against $L$. We find $\tau_{\text{max}} \propto L^2$, which agrees with diffusive transports, while $\tau_1$ looks increasing more slowly with $L$. The number indicated for each plot point of $\tau_{\text{max}}$ corresponds to $|\text{Re} \lambda_n|$.

indicates that the first excited eigenmode, as well as higher ones, can give a timescale of diffusion [18].

*Expansion coefficients for a specific initial state.*—We have considered a special class of initial states in the form $\rho(0) = \rho_{ss} + a_n \pi_n$. We have seen that for such an initial state one of the expansion coefficients can grow with $L$ as $c_n = e^{\mathcal{O}(L^2)}$.

Such a superexponentially large $c_n$ is not specific for this particular choice of the initial state. Let us consider the model with the dephasing dissipation and the initial state in which all the left-half sites are occupied and all the right-half sites are empty, i.e., $n_1 = n_2 = \cdots = n_{[L/2]} = 1$ and $n_{[L/2]+1} = \cdots = n_L = 0$. Starting from this initial state, bosons diffusively spread over the entire region, and hence the relaxation time is proportional to $L^2$. We calculate $\{|c_n|\}$ for varying $L$ and plot them in Fig. 4 (Top). We see explosive growth of some $|c_n|$ as $L$ increases. The relaxation time is estimated as $\tau \sim \max_n [\ln(|c_n|)/|\text{Re} \lambda_n|]$, which is plotted in Fig. 4 (Bottom). We see that it looks consistent with $\tau \propto L^2$, although data for larger system sizes are needed to definitely conclude $\tau \propto L^2$ (or $|c_n| = e^{\mathcal{O}(L^2)}$).

*Conclusion.*—We have discussed the problem of the discrepancy between the inverse of the Liouvillian gap and the relaxation time due to diffusive transports, which was already reported in Ref. [4]. This discrepancy is resolved by taking into account the system-size dependence of expansion coeffi-

FIG. 3. Numerically calculated values of $\ln(|\Phi_n|)/L^2$ (Top) and $(\tau_{\text{max}}, \tau_1)$ (Bottom). The results are similar to Fig. 1 and 2.

FIG. 4. (Top) Expansion coefficients $\{|c_n|\}$ for the initial state in which all the left-half sites are occupied. (Bottom) Log-log plot of the estimated relaxation time $\tau = \max_n [\ln(|c_n|)/|\text{Re} \lambda_n|]$ against $L$. 

We find that, rather surprisingly, $|\Phi_n|$ grows with $L$ superexponentially in $L$, $|\Phi_n| \sim e^{\Omega L^2}$. We also show that the relaxation time due to diffusive transports is determined not by low-lying eigenmodes but by eigenmodes with non-small eigenvalues. This is against a common belief that eigenmodes with small eigenvalues are dominantly important in a slow relaxation process like diffusive transports.

Theoretical framework leading to eq. (18) is generic as long as the dynamics is generated by a linear non-Hermitian operator. In particular, eq. (18) also holds in a classical stochastic process. In fact, it is known that nonequilibrium classical stochastic processes such as the boundary-driven symmetric (or asymmetric) simple exclusion process [19, 20] also exhibit the mismatch between the inverse of the spectral gap of the transition matrix and the relaxation time [21]. A superexponential dependence of $\{|\Phi_n|\}$ is also expected in such models. The result reported in this Letter is thus relevant beyond the context of quantum dissipative systems.

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A. LIOUVILLIAN GAP AND DYNAMICS

Let us consider the hard-core Bose-Hubbard chain with the boundary dephasing dissipation and that with the boundary particle-driving dissipation, both of which are introduced in the main text. For these models we have calculated the Liouvillian gap \( g = - \text{Re} \lambda_1 \). The system-size dependence of \( g \) is shown in Fig. S1 for (a) the dephasing dissipation and (b) the driving dissipation. We find \( g \sim L^{-1.6} \) in the model with the dephasing dissipation and \( g \sim L^{-1.0} \) in the model with the particle-driving dissipation.

Next, we calculate the dynamics of the trace distance between the current state \( \rho(t) \) and the NESS \( \rho_{ss} \), i.e.,

\[
d_T := \| \rho(t) - \rho_{ss} \|_\text{tr},
\]

in the model with the dephasing dissipation. We employ the initial state in which all the half-left sites are occupied and all the right-half sites are empty: \( n_1 = n_2 = \cdots = n_{L/2} = 1 \) and \( n_{L/2+1} = \cdots = n_L = 0 \) (\( L \) is even).

Dynamics of \( d_T \) is shown in Fig. S2 (a). Although the decay rate becomes asymptotically identical to \( g \) as indicated by dashed lines in Fig. S2 (a), the overall relaxation time is not fully determined by \( g \) because of the presence of a plateau for small \( t \).

![Figure S1](image1.png)

**FIG. S1.** System-size dependence of the Liouvillian gap for (a) the model with the dephasing dissipation and (b) the model with the particle-driving dissipation.

![Figure S2](image2.png)

**FIG. S2.** (a) Dynamics of the trace distance \( d_T \) for various system sizes. The dashed lines have the slope \(-g\) for each \( L \). (b) Time \( \tau \) at which \( d_T \) becomes 1.5. Clearly \( \tau \propto L^2 \), which is consistent with the timescale of diffusive transports.
Timescale of the persistence of the plateau increases with $L$, so we measure this system-size dependence. To do so, we calculate the time $\tau$ at which $d_T$ becomes 1.5 (the initial value of $d_T$ is almost the maximum value 2). As a result, we find $\tau \propto L^2$ as shown in Fig. S2 (b), which implies that observed plateaus result from diffusive transports. Since the inverse of the Liouvillian gap is much smaller than $L^2$, the lifetime of this initial plateau dominantly determines the overall relaxation time. This is the reason why the relaxation time is not given by the inverse of the Liouvillian gap.