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Thermalization in Open Quantum Systems

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We study thermalization in open quantum systems using the Lindblad formalism. A method that both thermalizes and couples to Lindblad operators only at edges of the system is introduced. Our method leads to a Gibbs state of the system, satisfies fluctuation-dissipation relations, and applies both to integrable and non-integrable systems. Possible applications of the method include the study of systems coupled locally to multiple reservoirs. Our analysis highlights the limits of applicability of the Lindblad approach to study strongly driven systems.

I. INTRODUCTION

One of the basic problems in many-body physics is conduction between two baths, which act as heat and particle reservoirs. The problem has been addressed using a host of approaches, for both classical and quantum systems^{1–8}. More recently, much work has been done using quantum Markov processes based on the Lindblad approach^{9,10}. These give a host of novel effects, surprisingly even for non-interacting systems. These include bounds on ballistic transport in the XXZ chain¹¹, phase transitions in non-interacting chains held far from equilibrium¹², and a resonant structure in the thermopower generated between two edges with different temperatures¹³.

Broadly, one can identify two general approaches for using Lindblad operators to drive quantum systems. In the first, the reservoir are modeled by Lindblad operators acting globally on the whole system^{13–19}. The advantages of this approach are that it can be microscopically justified from the derivation of the Lindblad equation^{20,21}, in the limit of a weak coupling between the system and the reservoir; and that, when the system is coupled to a single reservoir, the system equilibrates. It is important to keep in mind that in this approach fluctuation-dissipation relations are violated if the coupling to the reservoir is pushed beyond the weak coupling limit²². In the second approach, the reservoirs are modeled by Lindblad operators acting locally on a few sites at the edges of the system^{11,12,16,23–27}. This approach has the advantage that the non-unitary effect of the reservoirs acts only at the edges, and not in the bulk of the system. However, it is not clear if the local approach can actually model an equilibrated reservoir, namely one that would equilibrate the system when no other reservoirs are present²⁸. This may be responsible for apparent violations of the second law of thermodynamics, as discussed in Ref. 29. It would be useful to have a method that bridges these two approaches.

In this paper we introduce such a method. Within our approach the reservoir is coupled to the system on one edge, thermalizes it and satisfies fluctuation-dissipation relations. To achieve this, we model the reservoir as a non-interacting lead together with a bath, which acts

on the lead through Lindblad operators. The lead is, in turn, coupled to the system at a single site. Under certain conditions that we specify, both non-interacting and interacting systems, including non-integrable, thermalize. The method provides a first step toward using the Lindblad approach to study non-equilibrium situations where the system is coupled to several reservoirs at different points. It also clarifies when the global approach can be applied. A similar approach was introduced in Refs. 30–33 to study thermalization in non-interacting systems.

Our results highlight the limit of applicability of the Lindblad formalism to study driven system. We show that it works only in a weak coupling limit. In particular, this approach does not allow the study of large currents which do not occur in this limit.

II. THE MODEL

We consider the setup depicted in Fig. 1. A one dimensional quantum system, described by a Hamiltonian H_S , is coupled to a reservoir through a single link on one of its edges. The reservoir is composed of a non-interacting one-dimensional lead, described by a Hamiltonian H_L , and a bath, which is modeled by a dissipative generator $\hat{\Gamma}$. The evolution of the total density matrix ρ of the system and lead is then given by

$$\partial_t \rho = -i [H_L + H_S + H_{\text{int}}, \rho] + \hat{\Gamma} \rho \quad (2.1)$$

where H_{int} is the coupling between the system and the lead. The dissipative generator is given by

$$\hat{\Gamma} \rho = \frac{1}{2} \sum_{\nu} \gamma_{\nu} (2\Gamma_{\nu} \rho \Gamma_{\nu}^{\dagger} - \rho \Gamma_{\nu}^{\dagger} \Gamma_{\nu} - \Gamma_{\nu}^{\dagger} \Gamma_{\nu} \rho), \quad (2.2)$$

where Γ_{ν} are quantum jump operators, which act only on the sites of the lead, and γ_{ν} are rates with dimensions of energy. These are chosen such that when $H_{\text{int}} = 0$, the lead reaches thermal equilibrium with a Boltzmann measure with inverse temperature β and chemical potential μ .

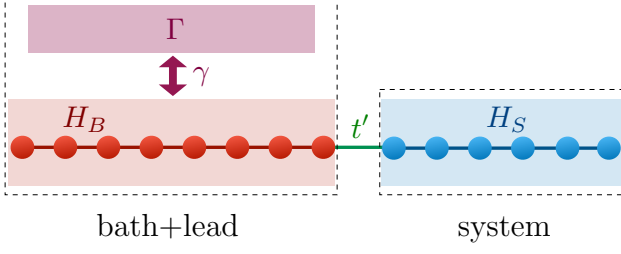


FIG. 1. Illustration of the model. The reservoir consists of a bath, modeled by Lindblad operators Γ , acting on a non-interacting lead. For simplicity, we use periodic boundary conditions in the lead.

We consider a lead Hamiltonian of the form,

$$H_L = -t_L \sum_{j=1}^M \left(b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right), \quad (2.3)$$

where b_j, b_j^\dagger are annihilation and creation operators for a spinless fermion on site j of the lead, which has M sites. For simplicity, we consider periodic boundary conditions in the lead, such that $b_{M+1} = b_1$. Then, H_L can be diagonalized in Fourier space, by introducing

$$b_m = \frac{1}{\sqrt{M}} \sum_j b_j e^{i2\pi m j} \quad (2.4)$$

which yields

$$H_L = \sum_m \epsilon_m^L b_m^\dagger b_m \quad (2.5)$$

where $\epsilon_m^L = -2t_L \cos(2\pi m)$.

To ensure that the lead thermalizes whenever $H_{\text{int}} = 0$, we impose detailed balance with respect to the lead eigenstates m . For each m , we introduce two jump operators: $\Gamma_{m-} = b_m$ removes a fermion with rate $\gamma_{m-} = \gamma_m(1 - f_m)$, while $\Gamma_{m+} = b_m^\dagger$ injects a fermion with rate $\gamma_{m+} = \gamma_m f_m$. Here, $f_m = f_{\text{FD}}(\epsilon_m^L)$ and

$$f_{\text{FD}}(\epsilon) \equiv \frac{1}{1 + e^{\beta(\epsilon - \mu)}} \quad (2.6)$$

is the Fermi-Dirac distribution. Then,

$$\frac{\gamma_{m+}}{\gamma_{m-}} = \frac{f_m}{1 - f_m} = e^{-\beta(\epsilon_m^L - \mu)}, \quad (2.7)$$

and Eq. (2.2) becomes

$$\begin{aligned} \hat{\Gamma}\rho = & \frac{1}{2} \sum_m \gamma_m [f_m (b_m^\dagger \rho b_m - b_m b_m^\dagger \rho - \rho b_m b_m^\dagger) \\ & + (1 - f_m) (b_m \rho b_m^\dagger - b_m^\dagger b_m \rho - \rho b_m^\dagger b_m)]. \end{aligned} \quad (2.8)$$

Throughout, unless otherwise stated, we will concentrate on the case $\mu = 0$.

In what follows, we will consider separately both non-interacting and interacting system Hamiltonians H_S . We start with a non-interacting system, because its description in terms of one-particle eigenstates allows for a simpler analysis and a more intuitive reasoning. Then, we extend the study to an interacting system. We would like to clarify, however, that no fundamentally different behavior is exhibited between the two system types. In the non-interacting case,

$$H_S = -t_S \sum_{j=1}^{N-1} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right), \quad (2.9)$$

where c_j, c_j^\dagger are annihilation and creation operators for a spinless fermion on site j of the system, which has N sites. In this case one can express H_S in terms of the one-particle energy eigenstates,

$$H_S = \sum_n \epsilon_n^S c_n^\dagger c_n, \quad (2.10)$$

where ϵ_n^S is the energy of the n^{th} eigenstates. In the interacting case, we extend the tight-binding Hamiltonian to include Hubbard-like repulsion terms between neighboring sites,

$$\begin{aligned} H_S = & -t_S \sum_{j=1}^{N-1} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) \\ & + U \sum_{j=1}^{N-1} n_j n_{j+1} + V \sum_{j=1}^{N-2} n_j n_{j+2}. \end{aligned} \quad (2.11)$$

where $n_j = c_j^\dagger c_j$ is the number of fermions in site j . For finite, non-zero U and V , the system is non-integrable. Throughout, we set $t_S = 1$.

Finally, we take the coupling between the system and lead to be:

$$H_{\text{int}} = -t' \left(b_M^\dagger c_1 + c_1^\dagger b_M \right). \quad (2.12)$$

As we show later, the simple choice of coupling only at one site is not crucial for the discussion.

While the model defined above stands as a phenomenological model on its own, it can in principle be derived from an underlying microscopic description, using standard approaches^{24,34,35}. Consider three chains of sizes L, M , and N , with $L \gg M$ and $L \gg N$, and hopping rate t within each chain. Suppose the L chain is coupled to the M chain by a single link of strength t'' , and the M chain is coupled to the N chain by a link of strength t' , with $t' \ll t$ and $t'' \ll t$ both weak. The L chain is held at thermal equilibrium. In the limit $t' \ll t''$, we can at first think of the N chain as being decoupled, and consider the $L + M$ subsystem by itself. Then, following standard arguments³⁶, the L chain can be modeled as by a Lindblad equation, in which a reservoir acts globally on the M chain, thermalizing it with the rates given in Eq. (2.8). The coupling to the bath γ is of order $t'^2 \nu_0$, where $\nu_0 \sim 1/t$ is the density of states of the L chain. Then, we obtain our full model by reinstating the weakly coupled N chain.

III. NON-INTERACTING SYSTEM

We note that, in the non-interacting case, the entire Lindblad equation is quadratic in fermionic operators. This makes it amenable to analytic approaches, as described below.

A. One Site Lead ($M = 1$)

The first case that we investigate is a non-interacting system with a one site lead, with total Hamiltonian

$$H = -t' \left(c_1^\dagger b + b^\dagger c_1 \right) - t_S \sum_{i=1}^{N-1} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) \quad (3.1)$$

and dissipative generator,

$$\hat{\Gamma}\rho = \frac{1}{2}\gamma \left[f_0 (2b^\dagger \rho b - b b^\dagger \rho - b b^\dagger \rho) + (1 - f_0) (2b \rho b^\dagger - b^\dagger b \rho - b^\dagger b \rho) \right], \quad (3.2)$$

with $f_0 = \frac{1}{1+e^{-\beta\epsilon_0}}$. This corresponds to a lead Hamiltonian, $H_L = \epsilon_0 b^\dagger b$ (this differs from the convention above, since one cannot define a tight binding model on one site). As we show in Appendix A, independently of β , the steady state corresponds to an infinite temperature state. Namely, the reduced density matrix of the system (after tracing out the lead) becomes, in the energy basis,

$$\rho_S = \prod_n (f_0 c_n^\dagger c_n + (1 - f_0) c_n c_n^\dagger). \quad (3.3)$$

This result holds even for more general tight-binding models.

It is natural to ask whether this result is an artifact of the single-site lead, and whether thermal equilibrium is achieved by considering a more realistic lead composed of multiple sites. As we will show next, while the situation does improve when the lead is enlarged, thermalization is not achieved even in the infinite lead limit.

B. Multiple Site Lead

We proceed by extending the setup above to a lead with multiple sites. In the non-interacting case, the Lindblad equation is quadratic in fermionic operators, and hence can be solved using a third quantization method³⁷. This method involves the diagonalization of a $4(N + M)$ -dimensional matrix, allowing us to study fairly large leads and systems numerically. A detailed description of the third quantization method applied to this class of systems is given in Ref. 37.

In Fig. 2 we show the occupation g_n of one-particle system eigenstates as a function of energy, for a system with $N = 80$ sites. We take $t' = 1$, $t_L = 1.2$, $\beta = 10$, and

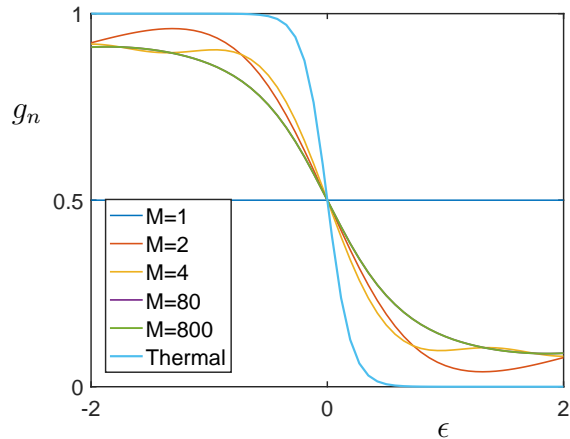


FIG. 2. Steady-state occupations of the single particle energy eigenstates, for different lead sizes, as a function of the single particle state energies. Here: $t' = 1$, $\beta = 10$, $\mu = 0$, $\gamma = 1$, $t_L = 1.2$ and $N = 80$. The thermalization error (Eq. (3.4)) saturates to a value of $\Delta = 0.14$ for $M > 50$.

constant rates $\gamma_m \equiv \gamma = 1$. The results are displayed for different values of the lead size M .

As expected from the previous section, for $M = 1$ the occupation of states is independent of their energy. This ceases to be true for $M > 1$. However, even for leads that are much larger than the system size, $M \gg N$, the one-particle occupations g_n are far from a thermal distribution with inverse temperature β . To quantify the error, we introduce the measure

$$\Delta \equiv \sqrt{\frac{1}{N} \sum_n (g_n - f_{\text{FD}}(\epsilon_n^S))^2} \quad (3.4)$$

where ϵ_n^S are the system one-particle energies, see Eq. (2.10). For the parameters considered above, the error already saturates to the large lead value for $M > 50$ at $\Delta = 0.14$. This implies that the average deviation from the thermal occupation is 14%, even for an infinite lead.

We now turn to investigate the effect of varying the values of the dissipation rate γ and the system-lead coupling t' . Figure 3 shows the error Δ as a function of t' , for different values of γ , and a large lead. One can see that Δ increases monotonically with t' , as one may expect from general statistical physics arguments: large values of t' increase the subextensive corrections to the system's energy. Note, however, that the error saturates at small t' to a γ -dependent value, which is monotonically increasing with γ . This implies that, even for leads that are much larger than the system size, the only hope of achieving thermalization is by taking both t' and γ to be small.

At first glance, the requirement of small γ is counter-intuitive, as one may have expected a strong dissipative coupling to lead to better equilibration. However, as we show in the next section, a large γ introduces an uncertainty in the system's energy, which reduces its ability to

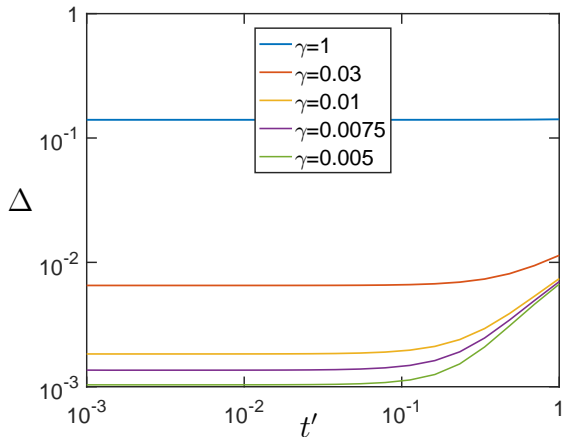


FIG. 3. Thermalization error as a function of t' , for different values of γ . Here: $\beta = 10$, $t_L = 1.2$, $N = 80$ and $M = 400$.

equilibrate at the desired temperature.

As discussed at the end of Sec. II, in microscopic derivations of the dissipative term, it is natural to consider the limit $t' \ll \gamma$. Therefore, in what follows we will take the limit $t' \rightarrow 0$ first. In this limit, we derive closed form expressions for the steady state density matrix and study the dependence of Δ on γ and other parameters.

IV. WEAK LEAD COUPLING ($t' \rightarrow 0$)

A. Degenerate Perturbation Theory – Non-interacting System

In this section, we will show that in the limit of infinitesimal coupling between system and lead, $t' \rightarrow 0$, the steady-state density matrix is given by

$$\rho \equiv \prod_m (f_m b_m^\dagger b_m + (1 - f_m) b_m b_m^\dagger) \times \prod_n (g_n c_n^\dagger c_n + (1 - g_n) c_n c_n^\dagger) \quad (4.1)$$

where $0 \leq g_n \leq 1$ are the occupations of the system eigenstates, given by

$$g_n = \frac{\sum_m |t'_{mn}|^2 Q_{nm} f_m}{\sum_m |t'_{mn}|^2 Q_{nm}} \quad (4.2)$$

where $Q_{nm} = \Upsilon(\epsilon_m^L - \epsilon_n^S)$ and

$$\Upsilon(\Delta\epsilon) = \frac{\gamma}{(\Delta\epsilon)^2 + \gamma^2/4}. \quad (4.3)$$

Here we assume, for simplicity, that $\gamma_m = \gamma$. The hopping amplitudes t'_{mn} are defined through

$$H_{\text{int}} = - \sum_{mn} t'_{mn} b_m^\dagger c_n + \text{h.c.}, \quad (4.4)$$

that is, t'_{mn} is the coupling between lead and system in the energy basis of both. Note that the density matrix in Eq. (4.1) is diagonal in the energy basis, as must be the case in order for ρ to commute with the system Hamiltonian in the steady state.

Equation (4.2) can be interpreted as a balance equation between particles hopping in and out of the system state n , via particle exchange with the lead:

$$0 = (1 - g_n) R_n^{\text{in}} - g_n R_n^{\text{out}} \quad (4.5)$$

where the rates R_n^{in} , R_n^{out} include all possible hopping processes:

$$R_n^{\text{in}} = \sum_m |t'_{nm}|^2 Q_{nm} f_m$$

$$R_n^{\text{out}} = \sum_m |t'_{nm}|^2 Q_{nm} (1 - f_m) \quad (4.6)$$

The factors $1 - g_n$ (in Eq. (4.5)) and $1 - f_m$ (in Eq. (4.6)) appear due to Pauli exclusion. In the limit $\gamma \rightarrow 0$, $Q_{nm} \rightarrow 2\pi\delta(\epsilon_n^S - \epsilon_m^L)$, and these rates reduce to the standard result expected from Fermi's Golden Rule. More generally, for non-zero γ_m , the dissipative term broadens the energy-conserving δ -function into a Lorentzian Q_{nm} .

This imposes constraints on when the equilibrium density matrix,

$$\rho_S = \prod_n (f_{\text{FD}}(\epsilon_n^S) c_n^\dagger c_n + (1 - f_{\text{FD}}(\epsilon_n^S)) c_n c_n^\dagger), \quad (4.7)$$

(corresponding to taking $g_n = f_{\text{FD}}(\epsilon_n^S)$ in Eq. (4.1)) can be obtained. Specifically, in the limit $\gamma \rightarrow 0$, we require that the lead is infinite and its bandwidth is larger than or equal to that of the system. To understand these conditions, note that when $\gamma \rightarrow 0$, the Lorentzian Q_{mn} selects the energy $\epsilon_n^S = \epsilon_m^L$. When the lead is infinite and its bandwidth is large, one is guaranteed to find a state in the lead that matches each level in the system.

Equation (4.2) is much simpler to use than the third quantization method, as it only requires a diagonalization of the system Hamiltonian. It applies to the class of non-interacting systems described above, and to more general tight-binding models. It only relies on the weak coupling between system and lead and not on specifics, such as the exact number of links. It can be generalized to systems with anomalous fermion hopping $c_j^\dagger c_{j'}$, which are relevant for superconducting systems and to quantum Ising chains.

The full derivation of the above results is given in Appendix B. Here, we outline its main steps. This derivation is similar to previous studies of the perturbative approach to the Lindblad equation (see Refs. 31, 38–42), with appropriate modifications relevant to our physical setup. First, we write the Lindblad equation for the steady state in the form:

$$0 = \hat{H}_0 \rho + \hat{\Gamma} \rho + \hat{V} \rho \quad (4.8)$$

with the superoperators \hat{H}_0 and \hat{V} defined by,

$$\begin{aligned}\hat{H}_0\rho &= -i[H_S + H_L, \rho], \\ \hat{V}\rho &= -i[H_{\text{int}}, \rho],\end{aligned}\quad (4.9)$$

and $\hat{\Gamma}$ given in Eq. (2.8). We are interested in the steady state ρ in the limit of weak system-lead coupling $\hat{V} \rightarrow 0$.

Let's consider first the case $\hat{V} = 0$. Then, the density matrix ρ factorizes into system and lead components. The lead component is thermal by construction. The system component is a steady state, provided it commutes with H_S . This implies that ρ is of the form in Eq. (4.1), where the parameters g_n are at this point arbitrary. For simplicity, we assume H_S has a non-degenerate spectrum.

In order to obtain the density matrix to leading order in t' , the coefficients g_n have to be determined using degenerate perturbation theory, within the Hilbert space of states of the form in Eq. (4.1). The details are given in Appendix B.

B. Fluctuation-Dissipation Relation

It has been shown that the Lindblad equation does not in general satisfy fluctuation-dissipation relations^{22,43,44}. This is true even in cases where the Lindblad operator acts globally on the whole system and when the steady state is Gibbs. Fluctuation-dissipation relations hold only in the weak coupling limit and are violated otherwise. This can be understood by recalling that unitary dynamics together with Gibbs initial condition for the density matrix ensure the fluctuation-dissipation relations. The dynamics of the system are unitary over time scales shorter than $1/\gamma$, and therefore the fluctuation-dissipation relations become exact in the weak coupling limit $\gamma \rightarrow 0$.

In our settings we saw that a small γ (and t') limit is required for obtaining a Gibbs density matrix. With the above in mind this automatically ensures the existence of fluctuation-dissipation relations.

C. Error Analysis

We have shown that in order to obtain thermalization, we must take the limit of small t' and γ , while holding a large lead $M \gg N$. It is interesting to quantify the error. As argued above, it is natural to consider the limit $t' \ll \gamma$. Therefore, we estimate the error as a function of γ , to leading order in $t' \rightarrow 0$, using the results of Sec. IV A. Throughout, we work with an infinite lead of infinite bandwidth.

Using Eq. (4.2), we obtain

$$g(\epsilon_n^S) = \frac{\int d\epsilon \Upsilon(\epsilon - \epsilon_n^S) f_{\text{FD}}(\epsilon)}{\int d\epsilon \Upsilon(\epsilon - \epsilon_n^S)}. \quad (4.10)$$

Here, as above, we assume that the system couples to the lead on a single site, and that the lead has periodic

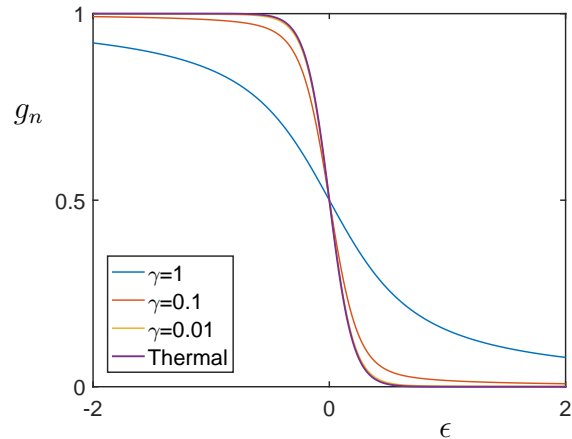


FIG. 4. Steady-state occupations of the single particle energy eigenstates for $\beta = 10$, in the limit $t' \rightarrow 0$ and an infinite size lead.

boundary conditions. Then, $|t'_{mn}|^2$ is independent of m , and it drops out of the sum in Eq. (4.2). For simplicity, we have also assumed that the density of states varies slowly relative to both γ and β^{-1} , which are also taken to be small relative to the system bandwidth. Then, the density of states also drops out, and the integrals above can be taken to extend from $-\infty$ to ∞ . In this case, the denominator becomes $\int d\epsilon \Upsilon(\epsilon - \epsilon_n^S) = 2\pi$.

Equation (4.10) shows that the occupation is smeared by the Lorentzian resulting from the dissipative terms. This implies a condition for thermalization, $\gamma \ll \beta^{-1}$. Figure 4 shows the occupation function for different values of γ , at a fixed value $\beta = 10$. As can be clearly seen, only for $\gamma\beta \ll 1$ does the occupation approximate well the thermal distribution.

In the opposite limit, when $\beta\gamma \gg 1$, Eq. (4.10) evaluates to

$$g(\epsilon_n^S) = \frac{1}{2} - \frac{1}{\pi} \tan^{-1}\left(\frac{2\epsilon_n^S}{\gamma}\right). \quad (4.11)$$

Note that this result is independent of β , as one may expect in this regime. The occupation is controlled by the Lorentzian, which has broad tails, as shown in Fig. 5. This leads to a slow decay of the occupation, which behaves as $\sim \frac{\gamma}{2\pi\epsilon_n^S}$ well above the chemical potential of the lead, and therefore cannot be described by a Fermi distribution with an effective temperature. The thermalization error in this regime is dictated by the system size. As clearly seen in Fig. 6, in the limit $\gamma N \ll 1$ it behaves as $\Delta^2 \propto \gamma^2$, whereas in the opposite limit $\gamma N \gg 1$ it behaves as $\Delta^2 \propto \gamma$. To explain this, we note that for finite systems, the energy level spacing scales as $\frac{1}{N}$. Therefore, the main contributions to the error near the Fermi surface ($\epsilon_n^S = 0$) are simply

$$g(\epsilon_n^S)_{\gamma N \ll 1} \sim \begin{cases} 1 - \gamma N & \epsilon_n^S < 0 \\ \gamma N & \epsilon_n^S > 0 \end{cases} \quad (4.12)$$

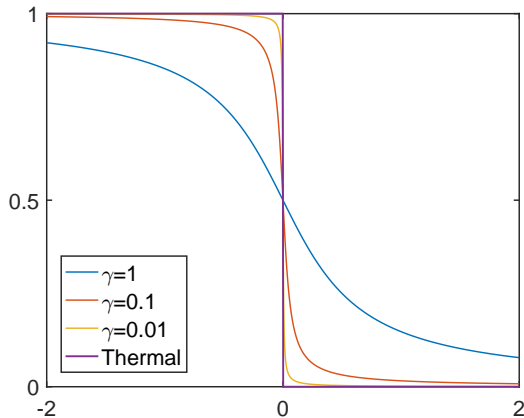


FIG. 5. Steady-state occupations of the single particle energy eigenstates at zero temperature, in the limit $t' \rightarrow 0$ and for an infinite lead size.

and clearly $\Delta^2 \propto \gamma^2 N$ (see Fig. 6 inset). On the other hand, for infinite systems the summation can be replaced by an integral,

$$\Delta^2 = 2 \cdot \int_0^W d\epsilon D(\epsilon) \left(\frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{2\epsilon}{\gamma} \right) \right)^2 \quad (4.13)$$

with $D(\epsilon)$ being the density of states and W is a characteristic bandwidth, of order 1. Assuming that the density of states does not change abruptly, namely $D'(\epsilon) \ll \frac{1}{\gamma}$, it can be approximated to a constant. Then, doing a simple change of variables and noting that $\frac{W}{\gamma} \gg 1$ leads to $\Delta^2 \propto \gamma$.

In Fig. 7, we plot the error for finite temperatures, but still low enough such that $\beta \gg 1$. The error saturates for large values of β , as well as for large values of γ .

V. GENERALIZATION TO INTERACTING SYSTEMS

In the interacting case, in order to study many-body systems, we write the system Hamiltonian (such as (Eq. 2.11)) in terms of the many-body eigenstates:

$$H_S = \sum_{\nu=1}^{2^N} E_\nu^S |\psi_\nu\rangle \langle \psi_\nu| \quad (5.1)$$

with $|\psi_\nu\rangle$ a many-body eigenstate and E_ν^S its corresponding energy. For simplicity, we keep studying particle number conserving Hamiltonians, such as Eq. (2.11). In this case, each eigenstate has a well defined particle number, such that

$$\hat{\mathcal{N}} |\psi_\nu\rangle = \mathcal{N}_\nu |\psi_\nu\rangle \quad (5.2)$$

with $\hat{\mathcal{N}} = \sum_{i=1}^N c_i^\dagger c_i$ and \mathcal{N}_ν an integer between 0 and N .

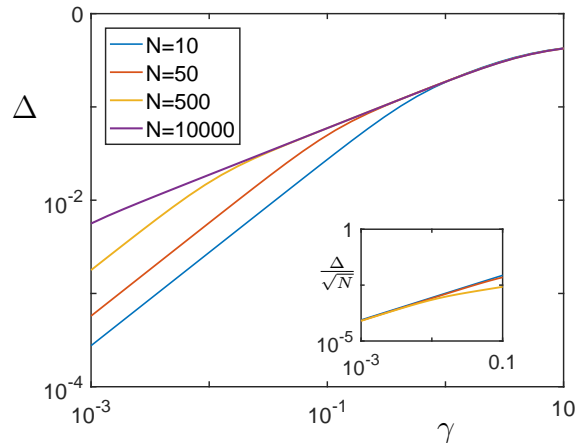


FIG. 6. Thermalization error at $\beta = \infty$ as a function of γ for different values of N , in the limit $t' \rightarrow 0$ and for an infinite lead size. Inset: the same data, scaled with $\frac{1}{\sqrt{N}}$. Note that the plot for $N = 10000$ has been omitted from the inset, since it is practically an infinite system for the values of γ considered here.

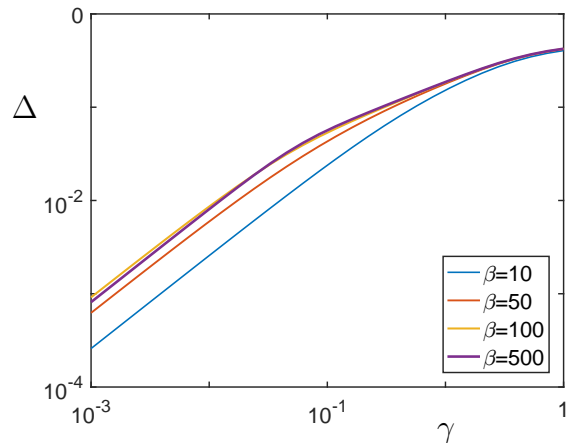


FIG. 7. Thermalization error as a function of γ for different values of β , in the limit $t' \rightarrow 0$ and an infinite size lead. System size is finite and chosen as $N = 100$.

The coupling Hamiltonian, Eq. (2.12), exchanges one particle between the system and the lead, and therefore can be written in terms of energy eigenstates as follows:

$$H_{\text{int}} = \sum_{m,\nu,\nu'} T_{m\nu\nu'} b_m^\dagger |\psi_{\nu'}\rangle \langle \psi_\nu| + \text{h.c.} \quad (5.3)$$

with

$$T_{m\nu\nu'} = -\frac{e^{-2\pi i m M}}{\sqrt{M}} t' \langle \psi_{\nu'} | c_1 | \psi_\nu \rangle. \quad (5.4)$$

This matrix element connects eigenstates which differ by one particle, namely $\mathcal{N}_\nu = 1 + \mathcal{N}_{\nu'}$.

As before, we start by studying the case of $H_{\text{int}} = 0$. Then, the steady state density matrix factorizes into a

system component and a thermal density matrix for the lead. Assuming that there are no degeneracies, it can therefore be written as follows:

$$\rho = \prod_{m=1}^M (f_m b_m^\dagger b_m + (1 - f_m) b_m b_m^\dagger) \otimes \sum_{\nu=1}^{2^N} G_\nu |\psi_\nu\rangle \langle \psi_\nu| \quad (5.5)$$

with $0 \leq G_\nu \leq 1$ arbitrary and subject to the normalization condition $\sum_\nu G_\nu = 1$. As a side remark, we point out that degeneracies can arise due to the particle-hole symmetry in our system at $\mu = 0$. These can be simply taken into account by a simultaneous diagonalization of H_S and \hat{N}^{45} .

To proceed we carry out a degenerate perturbation theory in t' . This fixes the values of G_ν . The analysis is very similar to the non-interacting case, as presented in Appendix B, and results in the following equation for each state $|\psi_\nu\rangle$:

$$0 = \sum_{m,\nu'} |T_{m\nu\nu'}|^2 Q_{m\nu\nu'} (f_m G_{\nu'} - (1 - f_m) G_\nu) + \sum_{m,\nu''} |T_{m\nu''\nu}|^2 Q_{m\nu''\nu} ((1 - f_m) G_{\nu''} - f_m G_\nu) \quad (5.6)$$

where the summation runs over eigenstates such that

$$\begin{aligned} \mathcal{N}_{\nu'} &= \mathcal{N}_\nu - 1 \\ \mathcal{N}_{\nu''} &= \mathcal{N}_\nu + 1 \end{aligned} \quad (5.7)$$

In addition,

$$Q_{m\nu\nu'} = \Upsilon (\epsilon_m^L - (E_\nu^S - E_{\nu'}^S)) \quad (5.8)$$

with $\Upsilon(\Delta\epsilon)$ defined in Eq. (4.3). The steady state values of G_ν are then obtained by solving the 2^N coupled linear equations of Eq. (5.6).

Equation (5.6) generalizes Eq. (4.5) to a many-body context. It can be rephrased as a global balance equation for the flow in and out of the state $|\psi_\nu\rangle$:

$$0 = \sum_{\nu'} (G_{\nu'} R_{\nu'\rightarrow\nu} - G_\nu R_{\nu\rightarrow\nu'}) + \sum_{\nu''} (G_{\nu''} R_{\nu''\rightarrow\nu} - G_\nu R_{\nu\rightarrow\nu''}) \quad (5.9)$$

with G_ν again being the probability for the eigenstate ν , and where the rates R sum over all possible particle exchanges with the lead:

$$\begin{aligned} R_{\nu'\rightarrow\nu} &= \sum_m |T_{m\nu\nu'}|^2 Q_{m\nu\nu'} f_m \\ R_{\nu\rightarrow\nu'} &= \sum_m |T_{m\nu\nu'}|^2 Q_{m\nu\nu'} (1 - f_m) \\ R_{\nu''\rightarrow\nu} &= \sum_m |T_{m\nu''\nu}|^2 Q_{m\nu''\nu} (1 - f_m) \\ R_{\nu\rightarrow\nu''} &= \sum_m |T_{m\nu''\nu}|^2 Q_{m\nu''\nu} f_m. \end{aligned} \quad (5.10)$$

Note that the expression for the rates depends on whether a particle is being added or removed into the lead. Since Eq. (5.9) is a balance equation for a probability conserving process, there is always a solution for the probabilities G_ν . If the process is ergodic, then the solution is unique.

As in the non-interacting case, the system thermalizes for $\gamma \rightarrow 0$. In this limit, $Q_{m\nu\nu'} \rightarrow 2\pi\delta(\epsilon_m^L - (E_\nu^S - E_{\nu'}^S))$ and we obtain the many-body equivalent of Fermi's Golden Rule. Then, for an infinite lead where the bandwidth is infinite, the rates in Eq. (5.10) satisfy detailed balance:

$$\frac{R_{\nu'\rightarrow\nu}}{R_{\nu\rightarrow\nu'}} = e^{-\beta(E_\nu^S - E_{\nu'}^S - \mu)} \quad (5.11)$$

and similarly for the ratio $\frac{R_{\nu\rightarrow\nu''}}{R_{\nu''\rightarrow\nu}}$. Hence, the steady state probabilities are

$$G_\nu = G_\nu^{\text{thermal}} \equiv \frac{1}{\mathcal{Q}} e^{-(\beta E_\nu^S - \mu \mathcal{N}_\nu)} \quad (5.12)$$

where \mathcal{Q} is the grand-canonical partition function:

$$\mathcal{Q} \equiv \sum_\nu e^{-(\beta E_\nu^S - \mu \mathcal{N}_\nu)} \quad (5.13)$$

Figure 8 shows the steady state value of G_ν , as a function of energy, for two different values of γ . To ensure non-integrability, we set $U = 0.5$ and $V = 0.25$. As expected, when γ is small, the system is close to a thermal distribution. Significant deviations from thermalization are only noticeable on a logarithmic scale, for excited states whose probability is $G_\nu \leq 10^{-5}$. On the other hand, when γ is not small, there are significant deviations even for the ground state.

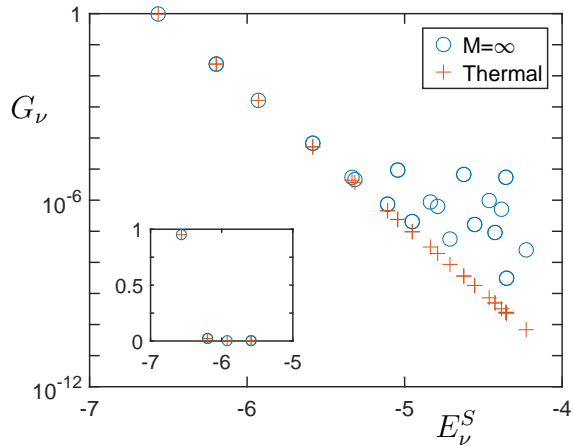
In order to quantify the many-body thermalization error, we define:

$$\Delta = \sqrt{\frac{1}{N} \sum_{\nu=1}^{2^N} (G_\nu - G_\nu^{\text{thermal}})^2}. \quad (5.14)$$

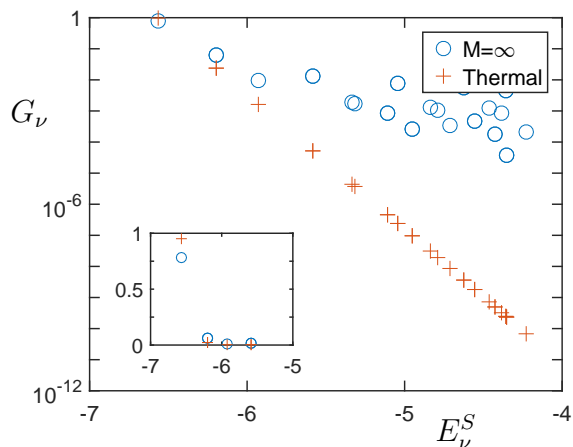
In Fig (9) we present the thermalization error as a function of γ . As seen in the figure, strict thermalization is only achieved for $\gamma \rightarrow 0$, and for small γ the thermalization error Δ is linear in γ . The results are shown for several system sizes and are consistent with an error scaling as $N^{1/2}$ (see inset). This is the same behavior argued for in the non-interacting case, see Sec. IV C.

VI. DISCUSSION

The paper addresses thermalization of quantum system using a Lindblad approach. A new method was devised which allows the Lindblad operators to thermalize the system without coupling to the whole system. The method relies on acting on a lead with Lindblad jump operators and coupling the lead to the system, which is



(a)



(b)

FIG. 8. Steady state occupations of the first 30 many-particle energy eigenstates in the limit $t' \rightarrow 0$ and for an infinite size lead. Here: $\beta = 10$, $N = 10$, $U = 0.5$, $V = 0.25$. Inset: the same graph, on a linear scale, for the first 4 eigenstates. In (a), $\gamma = 10^{-4}$, while in (b), $\gamma = 0.1$.

subjected to Hamiltonian dynamics only. For the method to be properly applied, the coupling of the system to the lead and of the Lindblad operators to the lead have to be weak. In these limits, the method ensures that there is both thermalization into a Gibbs state and that fluctuation-dissipation relations are satisfied. The corresponding errors as a function of the coupling were estimated. The study also shows the limitations of applying the Lindblad approach to strongly driven systems.

This approach can serve as the starting point to study transport in situations where the system is coupled to multiple leads. The resulting behavior of the system is expected to be similar to that obtained by a Landauer approach for non-interacting systems and weakly interacting systems^{1,7,46}. However, the method can also be applied to systems of arbitrarily strong interactions, and gives access to the full density matrix of the system.

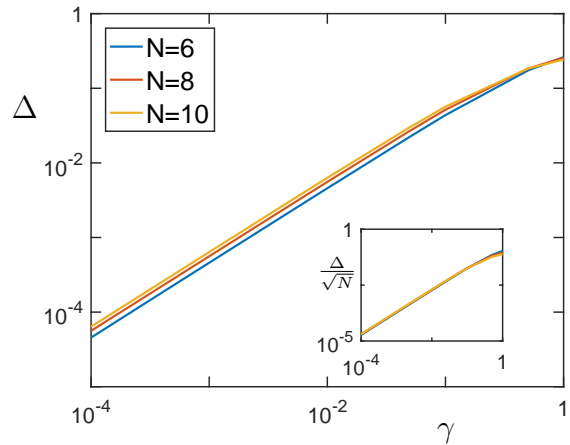


FIG. 9. Many-body thermalization error (Eq. (5.14)) as a function of γ for different system sizes and an infinite size lead (Here: $\beta = 10$, $U = 0.5$, $V = 0.25$). Inset: the same data, scaled by $\frac{1}{\sqrt{N}}$.

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Appendix A: Single-Site Coupling

We note that the Lindblad equation, with the unitary part of the evolution given in Eq. (3.1) and the dissipative generator in Eq. (3.2), represents a Markov process which is ergodic. Therefore, its steady state is unique. This steady state can be found by considering the following Ansatz,

$$\tilde{\rho} = (g_L b^\dagger b + (1 - g_L) b b^\dagger) \times \prod_{i=1}^N (g_i c_i^\dagger c_i + (1 - g_i) c_i c_i^\dagger), \quad (\text{A1})$$

corresponding to a product density matrix in the site basis, with the parameters g_L and g_i to be determined. Substituting Eq. (A1) into the dissipative generator we find,

$$\hat{\Gamma} \tilde{\rho} = \gamma [f_0 (1 - g_L) (b^\dagger b - b b^\dagger) + (1 - f_0) g_L (b b^\dagger - b^\dagger b)] \times \prod_{i=1}^N (g_i c_i^\dagger c_i + (1 - g_i) c_i c_i^\dagger), \quad (\text{A2})$$

which vanishes for $g_L = f_0$. Similarly, substituting into the unitary part of the evolution,

$$\begin{aligned}
[H, \hat{\rho}] &= t' (g_L - g_1) \left(c_1^\dagger b - b^\dagger c_1 \right) \\
&\times \prod_{j=2}^{N-1} \left(g_j c_j^\dagger c_j + (1 - g_j) c_j c_j^\dagger \right) \\
&+ \sum_{i=1}^N (g_i - g_{i+1}) \left(c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1} \right) \\
&\times \prod_{j \neq i, i+1}^{N-1} \left(g_j c_j^\dagger c_j + (1 - g_j) c_j c_j^\dagger \right) \\
&\times (g_L b^\dagger b + (1 - g_L) b b^\dagger). \tag{A3}
\end{aligned}$$

We thus see that for

$$g_L = g_j = f_0 \quad \forall j \tag{A4}$$

the unitary evolution $-i[H, \hat{\rho}] = 0$ also vanishes.

The analysis above shows that within this coupling protocol, different sites are uncorrelated in the steady state. In fact, since the occupations are site-independent, it follows that the density matrix factorizes and is state independent for any one-particle basis. In particular, the reduced density matrix of the system (after tracing out the lead) becomes, in the energy basis,

$$\rho_S = \prod_n (f_0 c_n^\dagger c_n + (1 - f_0) c_n c_n^\dagger). \tag{A5}$$

Hence, a state's occupation is seen to be independent of its energy, corresponding to an infinite temperature steady state, regardless of the value of β . From the derivation above, it is clear that this result holds for more general tight-binding models.

Appendix B: Perturbation Theory

In this Appendix, we consider general tight binding models. The setup is similar to Fig. 1:

$$H = H_L + H_S + H_{\text{int}} \tag{B1}$$

Here, it is more convenient to work with the one-particle eigenstates of the lead and system Hamiltonians. Therefore,

$$\begin{aligned}
H_L &= \sum_m \epsilon_m^L b_m^\dagger b_m \\
H_S &= \sum_n \epsilon_n^S c_n^\dagger c_n \\
H_{\text{int}} &= \sum_{m,n} t'_{mn} b_m^\dagger c_n + \text{h.c.} \tag{B2}
\end{aligned}$$

where m, n are the eigenstates of the lead, system Hamiltonians, respectively, b_m, c_n are their corresponding annihilation operators and $\epsilon_m^L, \epsilon_n^S$ the corresponding energies.

Right now, we don't assume specific details about the Hamiltonians, except that H_{int} is governed by an overall scale t' and vanishes as $t' \rightarrow 0$.

Our goal is to obtain the solution to Eq. (4.8) order by order in t' . In particular, we show that in the limit $t' \rightarrow 0$, the results in Sec. IV A hold.

We begin by denoting:

$$\rho = \sum_{k=0}^{\infty} \rho_k \tag{B3}$$

With $\rho_k \sim (t')^k$. Plugging Eq. (B3) into Eq. (4.8) and comparing terms of the same order, we can solve for the density matrix iteratively:

$$(\hat{H}_0 + \hat{\Gamma}) \rho_0 = 0 \tag{B4}$$

$$k \geq 1: \quad \rho_k = \left(\hat{H}_0 + \hat{\Gamma} \right)^{-1} \left(-\hat{V} \right) \rho_{k-1} \tag{B5}$$

Here, we focus on computations up to second order in t' . Higher order terms can be obtained iteratively, but are outside the scope of this paper.

Eq. (B4) can be satisfied by choosing a factorizable density matrix as follows:

$$\begin{aligned}
\rho_0 &= \prod_m (f_m b_m^\dagger b_m + (1 - f_m) b_m b_m^\dagger) \\
&\times \prod_n (g_n c_n^\dagger c_n + (1 - g_n) c_n c_n^\dagger) \tag{B6}
\end{aligned}$$

with $0 \leq g_n \leq 1$, at this point arbitrary. Without loss of generality (see remark at the end of the Appendix), we assume that H_S is non-degenerate. In this case, the above form of density matrix is the only possible choice to satisfy Eq. (B4). However, the subspace of solutions to this equation is largely degenerate. Therefore, to determine ρ_0 , a degenerate perturbation theory has to be employed.

Note that here, in contrast to a usual perturbation theory, the Schrodinger equation is replaced by the Lindblad equation, and the Fock space by the space of the linear operators which act on Fock states. Also, since we are interested in the steady state, the eigenvalue of $\hat{H}_0 + \hat{\Gamma} + \hat{V}$ is 0 to all orders in t' .

For convenience, we introduce some notation. Since the unperturbed operator $\hat{H}_0 + \hat{\Gamma}$ is a sum of one-particle operators, its eigenstates can be factorized:

$$\rho_{\{i_m, i_n\}} = \prod_m \Omega_{i_m, m}^L \otimes \prod_n \Omega_{i_n, n}^S, \tag{B7}$$

where i_m, i_n are indices taking the values of 0 – 3, and $\Omega_{i_m, m}^L$ ($\Omega_{i_n, n}^S$) are one-particle lead (system) eigenstates, respectively, specified in Table I. The corresponding eigenvalue of $\rho_{\{i_m, i_n\}}$ is

$$\begin{aligned}
\left(\hat{H}_0 + \hat{\Gamma} \right) \rho_{\{i_m, i_n\}} &= \rho_{\{i_m, i_n\}} \times \\
&\left(\sum_m \omega_{i_m, m}^L + \sum_n \omega_{i_n, n}^S \right) \tag{B8}
\end{aligned}$$

with $\omega_{i_m, m}^L, \omega_{i_n, n}^S$ the one-particle eigenvalues (also specified in Table I). Note that $\Omega_{0, n}^S, \Omega_{3, n}^S$ are degenerate, and we emphasize again that the g_n 's are arbitrary. This apparently cumbersome choice of $\Omega_{0, n}^S, \Omega_{3, n}^S$ will prove to be useful later.

To formulate the perturbation theory in the space of linear operators, we define the inner product between two states ρ_a and ρ_b :

$$\langle \rho_a, \rho_b \rangle \equiv \text{Tr}(\tilde{\rho}_a \rho_b), \quad (\text{B9})$$

with $\tilde{\rho}_a$ being the dual state of ρ_a . This dual state is the analog of the "bra" state with respect to some "ket" state. However, it is not necessarily its Hermitian conjugate, since we study eigenstates of a non-Hermitian operator. The dual state is computed as follows: The dual eigenstates $\tilde{\rho}_{\{i_m, i_n\}}$ are obtained by factorizing dual one-particle eigenstates, which are given in Table II. These, in turn, were obtained by requiring

$$\begin{aligned} \langle \Omega_{i_m, m}^L, \Omega_{j_m, m}^L \rangle &= \delta_{i_m, j_m} \\ \langle \Omega_{i_n, n}^S, \Omega_{j_n, n}^S \rangle &= \delta_{i_n, j_n} \end{aligned} \quad (\text{B10})$$

Employing the above notations, ρ_0 can be written simply as

$$\rho_0 = \prod_m \Omega_{0, m}^L \prod_n \Omega_{0, n}^S \quad (\text{B11})$$

We now proceed to find other solutions to Eq. (B4). These solutions form a subspace, which we name the

TABLE I. Eigenstates of $\hat{H}_0 + \hat{\Gamma}$

Name	Expression	Eigenvalue
$\Omega_{0, m}^L$	$f_m b_m^\dagger b_m + (1 - f_m) b_m b_m^\dagger$	0
$\Omega_{1, m}^L$	b_m^\dagger	$-i\epsilon_m^L - \frac{\gamma}{2}$
$\Omega_{2, m}^L$	b_m	$i\epsilon_m^L - \frac{\gamma}{2}$
$\Omega_{3, m}^L$	$b_m^\dagger b_m - b_m b_m^\dagger$	$-\gamma_m$
$\Omega_{0, n}^S$	$g_n c_n^\dagger c_n + (1 - g_n) c_n c_n^\dagger$	0
$\Omega_{1, n}^S$	c_n^\dagger	$-i\epsilon_n^S$
$\Omega_{2, n}^S$	c_n	$i\epsilon_n^S$
$\Omega_{3, n}^S$	$c_n^\dagger c_n - c_n c_n^\dagger$	0

TABLE II. Dual Eigenstates of $\hat{H}_0 + \hat{\Gamma}$

Name	Expression	Eigenvalue
$\tilde{\Omega}_{0, m}^L$	$b_m^\dagger b_m + b_m b_m^\dagger = \mathbb{I}_m$	0
$\tilde{\Omega}_{1, m}^L$	b_m	$-i\epsilon_m^L - \frac{\gamma}{2}$
$\tilde{\Omega}_{2, m}^L$	b_m^\dagger	$i\epsilon_m^L - \frac{\gamma}{2}$
$\tilde{\Omega}_{3, m}^L$	$(1 - f_m) b_m^\dagger b_m - f_m b_m b_m^\dagger$	$-\gamma_m$
$\tilde{\Omega}_{0, n}^S$	$c_n^\dagger c_n + c_n c_n^\dagger = \mathbb{I}_n$	0
$\tilde{\Omega}_{1, n}^S$	c_n	$-i\epsilon_n^S$
$\tilde{\Omega}_{2, n}^S$	c_n^\dagger	$i\epsilon_n^S$
$\tilde{\Omega}_{3, n}^S$	$(1 - g_n) c_n^\dagger c_n - g_n c_n c_n^\dagger$	0

"ground state manifold", that is spanned by the following basis vectors:

$$\rho_{\{i_{0, n}\}} = \prod_m \Omega_{0, m}^L \prod_n \Omega_{i_{0, n}, n}^S \quad i_{0, n} = 0 \text{ or } 3 \quad (\text{B12})$$

The degenerate perturbation theory requires that ρ_1 (Eq. (B5)) has zero overlap with any $\rho_{\{i_{0, n}\}}$. By applying \hat{V} one obtains the following:

$$\begin{aligned} (-\hat{V}) \rho_0 &= i \sum_{m, n} t'_{mn} b_m^\dagger c_n \times \\ &\prod_{\mu \neq m} \Omega_{0, \mu}^L \prod_{\nu \neq n} \Omega_{0, \nu}^S (g_n - f_m) + \text{h.c.} \end{aligned} \quad (\text{B13})$$

and, trivially, ρ_1 has no overlap with the ground state manifold. Therefore, we proceed to second order in t' :

$$\begin{aligned} \hat{V} \left(\hat{H}_0 + \hat{\Gamma} \right)^{-1} \hat{V} \rho_0 &= \prod_{\mu} \Omega_{0, \mu}^L \times \\ &\sum_{m, n} \frac{|t'_{mn}|^2 \gamma_m (g_n - f_m)}{\left(\frac{\gamma_m}{2} \right)^2 + (\epsilon_m^L - \epsilon_n^S)^2} \times \\ &\left(\prod_{\nu \neq n} \Omega_{0, \nu}^S \right) \Omega_{3, n}^S \\ &+ \rho_2^\perp \end{aligned} \quad (\text{B14})$$

with ρ_2^\perp being terms outside the ground-state manifold. The requirement that $\langle \rho_2, \rho_{\{i_{0, n}\}} \rangle = 0$ for any $\rho_{\{i_{0, n}\}}$ is mostly trivial, except for the set of N independent equations:

$$\sum_m \frac{|t'_{mn}|^2 \gamma_m (g_n - f_m)}{\left(\frac{\gamma_m}{2} \right)^2 + (\epsilon_m^L - \epsilon_n^S)^2} = 0 \quad \forall \quad n \quad (\text{B15})$$

which results in Eq (4.2), as expected. In addition to the occupations g_n , we can obtain different correlation functions from ρ_2^\perp (Eq. (B14)), up to second order:

$$\begin{aligned} \langle b_m^\dagger b_{m'} \rangle_{m \neq m'}^{(2)} &= \frac{1}{-i(\epsilon_m^L - \epsilon_{m'}^L) - \frac{\gamma_m + \gamma_{m'}}{2}} \times \\ &\sum_n \frac{(t'_{mn})^* t'_{m'n} (g_n - f_m)}{i(\epsilon_m^L - \epsilon_n^S) - \frac{\gamma_m}{2}} \\ &+ \text{c.c.}, m \leftrightarrow m' \end{aligned} \quad (\text{B16})$$

$$\begin{aligned} \langle b_m^\dagger b_m - b_m b_m^\dagger \rangle^{(2)} &= \frac{1}{-\gamma_m} \sum_n \frac{|t'_{mn}|^2 (g_n - f_m)}{-i(\epsilon_m^L - \epsilon_n^S) - \frac{\gamma_m}{2}} \\ &+ \text{c.c.} \end{aligned} \quad (\text{B17})$$

$$\begin{aligned} \langle c_n^\dagger c_{n'} \rangle_{n \neq n'}^{(2)} &= \frac{1}{-i(\epsilon_n^S - \epsilon_{n'}^S)} \times \\ &\sum_{m, n''} \frac{t'_{mn} (t'_{m'n''})^* (g_n - f_m)}{-i(\epsilon_m^L - \epsilon_n^S) - \frac{\gamma_m}{2}} \\ &+ \text{c.c.}, n \leftrightarrow n' \end{aligned} \quad (\text{B18})$$

The lead-system correlations can be obtained as well, and are needed for computing the current in out of equilibrium setups:

$$\langle b_m^\dagger c_n \rangle^{(1)} = \frac{i (t'_{mn})^* (g_n - f_m)}{i (\epsilon_m^L - \epsilon_n^s) - \frac{\gamma_m}{2}} \quad (\text{B19})$$

Note that these processes reflect the virtual creation and annihilation of the particles in the lead and system via

the weak coupling.

As a final remark, we would like to clarify that this treatment can be generalized to a degenerate H_S . For example, in the simplest case, if the degeneracy results from known symmetries, H_S can be diagonalized simultaneously with the additional conserved quantities, and then these eigenstates are chosen as the constituents of Eq. (B6).

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