Bosonic quantum transport with power-law coupling: single-particle versus many-body treatment

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Abstract. Simulating boundary-driven quantum transport in open systems is quadratically more complex compared to an isolated quantum system, which already contains exponentially growing time-complexity as the number of sites grows. To efficiently solve the Lindblad master equation, one may restrict attention to the single-excitation problem, effectively mapping the problem to a tight-binding model or retain the many-body description by working with the covariance matrix via the Lyapunov equation. We show numerically for bosonic systems that these two approaches do not agree in general, except in a specific limit that is rarely stated explicitly: the dilute limit where the injection rate is much smaller than the extraction rate. We identify the regime for when each the single-particle sector is applicable.

1 Introduction

Open quantum systems driven out of equilibrium by boundary reservoirs represent a rich playground for exploring nonequilibrium transport phenomena [1,2]. When a quantum chain is coupled to particle baths of differing chemical potentials at its boundaries, a nonequilibrium steady state (NESS) emerges in which a constant particle current flows through the system. The study of such boundary-driven systems has attracted considerable attention across a wide range of platforms, from electron transport in mesoscopic devices [3] to energy transfer in photosynthetic complexes [4] and excitation transport in ultracold atomic gases [5].

A particularly interesting class of boundary-driven systems involves hopping interactions that decay as a power law of distance, $J_{nm} \sim \frac{1}{|n-m|^a}$. Such long-range interactions are naturally realized in several quantum simulation platforms: trapped ions exhibit effective spin-spin couplings with $0 \leq a \leq 3$ [6], polar molecules in optical lattices exhibit dipole-

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dipole interactions ($a = 3$) [7], and Rydberg atom arrays provide tunable power-law interactions [8]. In a recent work [9], we showed that the steady-state particle current in such a system can vary nonmonotonically as a function of the hopping exponent a, exhibiting a peak at a finite optimal value a^*. This enhancement depends sensitively on the exit site—the site coupled to the cold bath—and vanishes for certain special placements due to interference effects.

In that earlier study, the single-excitation (single-particle) sector of the Lindblad master equation was used to efficiently compute the NESS. This approach is common in the literature and is exact in the limit of low injection rate. However, the regime of validity of this approximation and its relation to the full many-body description via the covariance matrix Lyapunov equation have not been carefully examined. In this paper, we address this gap. We show that the two approaches—single-particle and many-body—do not in general agree, and that the discrepancy is not merely quantitative but can be qualitatively significant: the nonmonotonic current profile, including the existence and position of the peak, can differ between the two treatments.

This paper is organized as follows. In Section 2 we define the model. Section 3 derives both the single-particle and many-body calculations and identifies the conditions under which they agree. Section 4 presents our key numerical results. Section 5 is the conclusion.

2 Model

We consider a clean one-dimensional chain of L coupled bosonic modes with power-law hopping, described by the tight-binding Hamiltonian (setting $\hbar = 1$):

$$H = -\sum_{n<m} \frac{J}{|n-m|^a}\left(a_n^\dagger a_m + \text{H. c.}\right), \tag{1}$$

where $a_n^\dagger$ (a_n) is the bosonic creation (annihilation) operator at site n. The long-range hopping rate $J_{nm} = J/|n-m|^a$ decays as a power law with exponent $a \geq 0$, with J setting the energy scale. In the limit $a \to \infty$ the model reduces to the nearest-neighbour tight-binding chain, while $a = 0$ corresponds to all-to-all equal hopping in the complete graph.

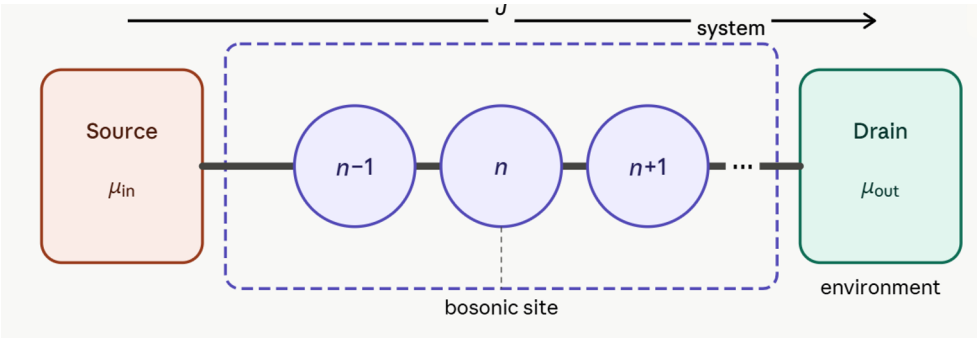

Fig. 1. Illustration of the open bosonic chain considered in the text. The transport is originates from a particle source and exited in the drain connected to l-th site (not necessarily the end site).

The system is coupled to two Markovian baths via the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation [10,11]:

$$\frac{d\rho}{dt} = \mathcal{L}\rho = -i[H,\rho] + \mu_{\text{in}}\mathcal{D}[a_1]\rho + \mu_{\text{out}}\mathcal{D}[a_l]\rho \tag{2}$$

where $\mathcal{D}[L]\rho = L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}$ is the Lindblad dissipator. The hot bath injects particles at site 1 with rate μ_{in}, while the cold bath extracts particles at exit site l with rate μ_{out}. We vary

μ_{in} and μ_{out} to study the single-particle and many-body effects. The steady-state particle current is:

$$J = -\text{Tr}(N\mathcal{D}_{\text{out}}\rho_{\text{NESS}}) = -\mu_{\text{out}}\text{Tr}(\mathcal{D}[a_l]\rho_{NESS}) = \mu_{\text{out}}C_{ll}, \tag{3}$$

where $N = \sum_n a_n^\dagger a_n$ is the total excitation number operator and $C_{nm} = \langle a_n^\dagger a_m \rangle$ the covariance matrix element of the NESS density matrix ρ_{NESS}, which is the solution of $\frac{d\rho}{dt} = 0$. The last equality is obtained by using only commutation relation for bosons $[a_n, a_m^\dagger] = \delta_{nm}$.

Note that for the closed system the particle number is conserved, since $[H, N] = 0$. Thus the change of particle number in the chain is only done by the Lindblad dissipators, which act as the particle source and drain.

3 Results and Discussions

3.1 Single-particle (tight-binding) model

When the injection ratio is sufficiently small, $\mu_{\text{in}}/\mu_{\text{out}} \ll 1$, the system is predominantly in the vacuum or single-excitation sector. The full density matrix takes the form:

$$\rho_{\text{NESS}} = p_0|0\rangle\langle 0| + \sum_{nm} \rho_{nm}^{(1)}|n\rangle\langle m| + O\left(\left(\frac{\mu_{\text{in}}}{\mu_{\text{out}}}\right)^2\right), \tag{4}$$

where $|0\rangle$ is the vacuum (0-excitation) state $|n\rangle$ denotes the single-excitation state at site n and $p_0 = 1 - \langle N \rangle$ is the vacuum population. Here the operating Hilbert space is $\mathcal{H}_0 \times \mathcal{H}_1$ where $\mathcal{H}_n$ is the n-excitation subspace, truncated from the total Fock space. This approach implies that the normalization is $p_0 + \sum_n \rho_{nn}^{(1)} = p_0 + \langle N \rangle = 1$. In this limit one can project the Lindblad equation onto the single-excitation manifold, obtaining an effective non-Hermitian Schrödinger equation. The covariance matrix element reduces to $C_{nm} \approx \rho_{nm}^{(1)}$, and the NESS is found by solving a linear system of size $(N+1) \times (N+1)$. Numerically this is implemented via mesolve in QuTiP [15] by considering a single-particle Hamiltonian working to the enlarged (vacuum $\oplus$ 1-particle) Hilbert space, that is by writing

$$a_n \to |0\rangle\langle n|, \qquad a_n^\dagger a_m \to |n\rangle\langle m|. \tag{5}$$

Consequently, the covariance matrix element reads as $C_{nm} = \langle n|\rho_{nm}^{(1)}|m\rangle$.

Intuitively, the condition for validity of this approximation is that the mean particle number satisfies $\langle N \rangle \leq 1$, which is achieved when the injection rate is very small compared to the extraction rate, that is $\mu_{\text{in}}/\mu_{\text{out}} \ll 1$. Nevertheless, is there a more general condition that is not restricting the injection rate that still satisfies $\langle N \rangle \leq 1$? We will come to this issue later on. For comparison, in a nearest-neighbor chain, the 1-excitation sector is still justifiable for $\mu_{\text{in}} = \mu_{out}$ if the following conditions apply [9,14],

$$\langle N \rangle = \frac{K}{K+1}, \qquad K = N + \frac{N+1}{4}\frac{\mu_{\text{out}}^2}{J}. \tag{6}$$

Note that in our previous paper, Ref. [9], we made an oversight by taking this condition to be applicable as well for a long-range system. Instead, the appropriate condition for the long-range chain should be considered separately. In later part we will see that the necessary is not $\langle N \rangle \leq 1$ but instead the stronger $\langle N \rangle \ll 1$.

3.2 Many-body approach and relation to single-particle sector

From the master equation (2), we can derive the equation for the covariance matrix C, its elements satisfy

$$\dot{C}_{nm} = -i[H,C]_{nm} + \mu_{\text{in}}\left(\delta_{n1}\delta_{m1} - \frac{1}{2}\delta_{n1}C_{1m} - \frac{1}{2}\delta_{m1}C_{n1}\right) - \frac{\mu_{\text{out}}}{2}(\delta_{nl} + \delta_{ml})C_{nm} \quad (7)$$

where

$$-i[H,C]_{nm} = -i\sum_{k}(h_{nk}C_{km} - C_{nk}h_{km})\,. \quad (8)$$

In matrix form, the steady state equation $\dot{C}_{nm} = 0$ becomes

$$AC + CA^{\dagger} = P \quad (9)$$

where

$$A = -ih - \frac{\mu_{\text{in}}}{2}|1\rangle\langle 1| - \frac{\mu_{\text{out}}}{2}|l\rangle\langle l|, \qquad P = -\mu_{\text{in}}|1\rangle\langle 1|, \quad (10)$$

where $h = (h)_{mn}$ is an $N \times N$ matrix of the power-law hopping. This is referred to as the Lyapunov equation [12], similar to the one in control theory.

Equation (9) works for any quadratic Hamiltonian, allowing for more efficient and systematic computing task, both analitically and numerically, compared to solving the full Lindbladian. The difference between many-body and single-particle approaches is that, despite obeying the same Lyapunov equation, the Hamiltonian differs (as mentioned above),

$$H = \sum_{n,m} h_{nm}|n\rangle\langle m| = \sum_{n<m}\frac{-J}{|n-m|^{a}}(|n\rangle\langle m| + |m\rangle\langle n|)\,. \quad (11)$$

Since $[H,N] = 0$ and $[N,L_{\alpha}] \propto L_{\alpha}$ for $\alpha = \{1,l\}$, the Liouvillian superoperator $\mathcal{L}$ satisfies $U(1)$ symmetry. Another way to show that this symmetry exist in the open system is to check whether $[\mathcal{L},\mathcal{N}] = 0$ where $\mathcal{N}\rho = [N,\rho]$. This way we can show the $U(1)$ symmetry, $[\mathcal{L},\mathcal{U}_{\phi}] = 0$ where $\mathcal{U}_{\phi}\rho = U(\phi)\rho U^{\dagger}(\phi)$ for $\phi \in \mathbb{R}$. Hence, the full density matrix consists of k-particle sector blocks,

$$\rho_{\text{NESS}} = \bigoplus_{k=0}^{\infty}\rho^{(k)}, \qquad \text{Tr}\,\rho_{\text{NESS}} = 1, \quad (12)$$

the many-body covariance matrix element becomes

$$C_{nm} = \text{Tr}\left(a_n^{\dagger}a_m\rho\right) = \sum_{k}\text{Tr}\left(a_n^{\dagger}a_m\rho^{(k)}\right). \quad (13)$$

For the single-particle, k =1,

$$\text{Tr}\left(a_n^{\dagger}a_m\rho^{(1)}\right) = \rho_{mn}^{(1)}. \quad (14)$$

For the $k = 2$ sector,

$$\text{Tr}\left(a_n^{\dagger}a_m\rho^{(2)}\right) = \sum_{p\le q}\rho_{pq,pq}^{(2)}\langle p,q|a_n^{\dagger}a_m|p,q\rangle = 2\sum_{p}\rho_{np,mp}^{(2)} \quad (15)$$

by only using the bosonic commutation relations. Here, $|p,q\rangle$ means there is an excitation in site p and the other one is in site q. The factor 2 appears since

$$a_m|p,q\rangle = \frac{1}{\sqrt{1+\delta_{pq}}}\left(\delta_{mp}|q\rangle + \delta_{mq}|p\rangle\right) \quad (16)$$

works to each of the 2 particles. Similarly for 3 particles, there will be three terms. Thus, we can write

$$C_{nm} = \sum_{k=1}^{L} k \sum_{\{p\}} \rho^{(k)}_{m\{p\},n\{p\}} = \rho^{(1)}_{mn} + 2\sum_{p} \rho^{(2)}_{mp,np} + 3\sum_{p,q} \rho^{(3)}_{mpq,npq} + \cdots \tag{17}$$

where $\{p\}$ indicates all the site indices for the other $k-1$ excitations. In trace notation, this is more concise,

$$C = \sum_{k=1}^{L} k \,\mathrm{Tr}_{k-1}\rho^{(k)}. \tag{18}$$

For the single-particle approach, we truncate all the multiple particle sector and the corresponding normalization becomes $p_0 + \mathrm{Tr}\big(\rho^{(1)}\big) = p_0 + \mathrm{Tr}\big(C^{(1)}\big) = 1$, where $C^{(1)}$ denotes the single-particle covariance matrix. Note that in equation (16) the contribution from the vacuum ($k = 0$) is zero so that the sum starts from $k = 1$.

Additionally, in the case of hard-core bosons the site occupation is limited to be one boson for each site. That is, $n_i \in \{0,1\}$ for all the sites. Thus the many body part covariance matrix element is simply zero if at least two indices coincide. Hence, for hard-core bosons,

$$C = \sum_{k=1}^{L} \mathrm{Tr}_{k-1}\rho^{(k)}. \tag{19}$$

3.3 Single-particle sector vs. single-particle *model*

It should be noted that the NESS from single-particle sector $\rho^{(1)}$ is different to single-particle model. The former is just a subspace of the full many-body covariance matrix C, while the latter is strictly the NESS obtained by solving the single-particle (tight-binding) model. From hereafter, we denote the latter as ρ_{sp} to differentiate it from $\rho^{(1)}$.

The single-particle model lives in the Hilbert space $\mathcal{H} = \mathrm{span}\{|0\rangle, |1\rangle, \ldots, |L\rangle\}$ where $|0\rangle$ denotes the vacuum. The steady-state $\rho_{\mathrm{sp}} = p_0|0\rangle\langle 0| + \rho^{(1)}$ has a normalization constraint $p_0 + \mathrm{Tr}\,\rho^{(1)} = 1$, or more explicitly,

$$\rho_{\mathrm{sp}} = \begin{pmatrix} \tilde{C} & 0 \\ 0 & 1 - \mathrm{Tr}\,\tilde{C} \end{pmatrix}, \qquad H = \begin{pmatrix} h & 0 \\ 0 & 0 \end{pmatrix}, \tag{20}$$

where $\tilde{C} = \rho^{(1)}$ with the above normalization constraint. Notice that we have added the vacuum block in the last row and column. Hence, the Lyapunov equation becomes

$$A\tilde{C} + \tilde{C}A = -\mu_{\mathrm{in}}\big(1 - \mathrm{Tr}\,\tilde{C}\big)|1\rangle\langle 1|. \tag{21}$$

Thus the equation becomes nonlinear and in practice it is more straightforward to use steady-state solver in QuTiP. Important note is that, if the NESS is nonunique then we cannot trust the numerical result from QuTiP since it only gives one possibility of zero eigenvalues of the Liouvillian. Rather, the true steady state must be the linear combination of all the degenerate steady states. The nonuniqueness is indeed the case in our model if the exit site corresponds to the dark states, such as exactly in the middle of an odd L chain (node of the closed system eigenstates, see Ref [9]).

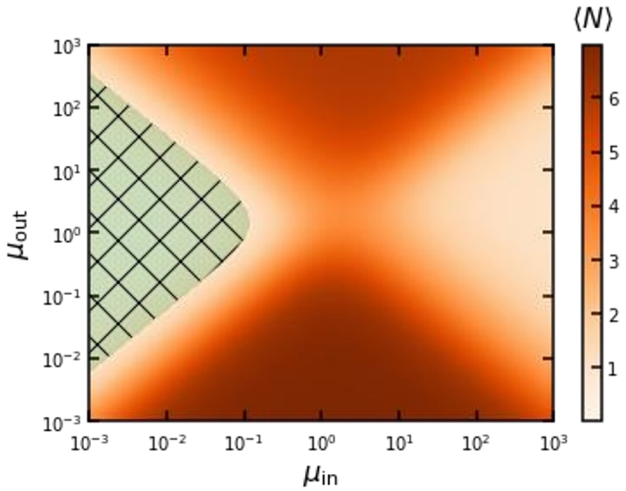

Fig. 2. Steady-state excitation number $\langle N\rangle$ for $L = 7$ and long-range hopping exponent $a = 1$, as a function of the injection and extraction rates. The hatched region corresponds to $\langle N\rangle \leq 1$.

3.4 Numerical Results

We now turn to the steady-state total excitation number $\langle N\rangle$. For a bosonic chain with number-conserving Hamiltonian $[N, H] = 0$, subject to incoherent injection at site 1 and extraction at site $l = L$ (end-to-end transport). Despite the absence of any intrinsic occupation constraint in the bosonic Hilbert space, we find that N remains finite over a broad region of parameter space, and can even be restricted to the effective single-particle sector $N \lesssim 1$.

Figure 2 shows the steady-state excitation number for $L = 7$ and long-range hopping exponent $a = 1$, as a function of the injection and extraction rates. The hatched region corresponds to $N \leq 1$. Remarkably, this region occupies a finite area in parameter space, demonstrating that the dynamics alone can suppress multi-particle occupation, even in a bosonic system. This behavior can be understood from the continuity equation for the total particle number. Since the Hamiltonian conserves N, the steady state is determined entirely by the balance between boundary driving processes,

$$\frac{d}{dt}\langle N\rangle = \mu_{\text{in}} - \mu_{\text{out}}\langle n_l\rangle, \tag{20}$$

so that $\langle n_l\rangle = \mu_{\text{in}}/\mu_{\text{out}}$ at steady state. Thus, the occupation at the drain site is fixed by the ratio of injection and extraction rates. However, the total excitation number depends crucially on the ability of the system to transport particles from the source to the drain. In particular, the steady-state current is controlled by both coherent hopping and dissipative broadening, leading to an effective transport rate that competes with the boundary driving.

The resulting steady state is therefore governed by a competition between three processes: injection, extraction, and bulk transport. When injection is weak compared to extraction, particles are removed faster than they are supplied, and the system remains close to the vacuum. Conversely, when extraction is inefficient, particles accumulate and the total excitation number grows. Between these limits lies a transport-limited regime, where the current through the system is bounded by the bulk dynamics. In this regime, the excitation number remains finite and can be of order unity, giving rise to the observed “single-particle” region. The structure of the phase diagram reflects this competition. The approximately X-

shaped crossover separating low- and high-density regions corresponds to the condition where injection, extraction, and transport rates become comparable. Notably, the position of this crossover depends on the long-range exponent a, indicating that the bulk transport properties—rather than purely boundary rates—control the steady-state occupation. In particular, long-range hopping enhances transport and shifts the crossover region, consistent with an increased effective conductance of the system.

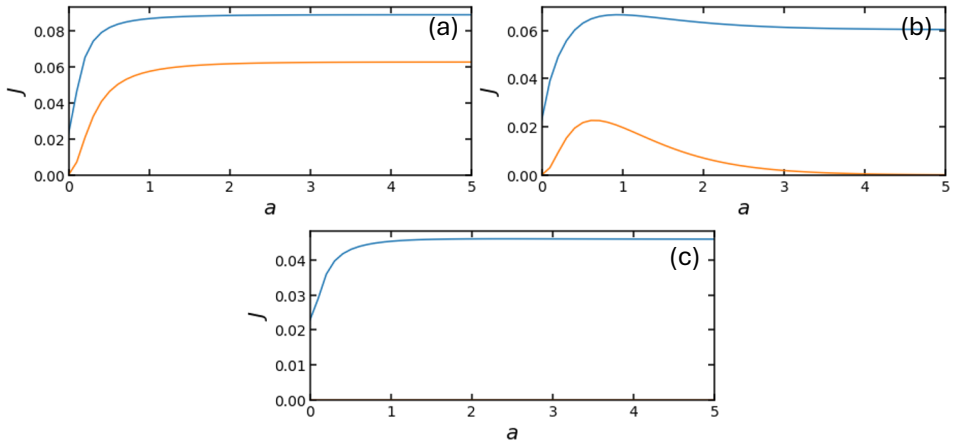

Fig. 3. Steady-state particle current J. (Blue) many-body results and (orange) single-particle model. $N = 5, \mu_{\text{in}} = 0.1J, \mu_{\text{in}} = J$. (a) Exit site $l = 5$, (b) $l = 4$, (c) $l = 3$.

Figure 3 shows the comparison between full many-body calculation of particle current J as a function of the power-law exponent a. It is shown that the single-particle model always underestimate the current value for all a. We can understand this by looking at equation 17, where (unnormalized) C includes the single particle sector $\rho^{(1)}$ plus higher sector terms. In the single-particle model the vacuum plus single-particle population is normalized. The results from many-body (bosonic) and single-particle models result in converge when $\frac{\mu_{\text{in}}}{\mu_{\text{out}}} \ll 1$ (sufficient condition), while the necessary condition is $\langle N \rangle \ll 1$. The condition $\langle N \rangle \leq 1$ is not enough because we can have, for example, total single-particle particle population 0.5 and 2-particle population 0.5. The total $\langle N \rangle$ is 1 but obviously it is not strictly a single-particle problem since the higher sector has nonzero weight. To ensure the entire dynamics live in $N = 0{,}1$ sectors we need $\langle N \rangle \ll 1$. Another important note is in figure 3(c), where the exit site is located at the center of the chain. In this case the single-particle model NESS is nonunique (in fact there are 4 zero eigenvalues of the Liouvillian $\mathcal{L}$. Moreover, for $l = 3$ in infinitesimal $a \to 1$ regime, $\langle N \rangle$ is close to 1, while for finite a, $\langle N \rangle > 2$. This clearly shows the breakdown of the single-particle approximation.

These results show that the use of full many-body calculation is crucial for boundary-transport systems, particularly in long-range systems. On the other hand, bounded excitation in driven bosonic systems does not rely on statistical constraints (i.e. that infinitely many bosons per site), but instead emerges dynamically from the interplay of coherent transport and boundary dissipation. In this sense, the steady state can be viewed as a transport-limited nonequilibrium state, whose properties are controlled by an effective conductance determined by the underlying Hamiltonian. Further studies may include the effects of mobility edges [13] and periodic driving [14].

4 Conclusion

We have examined the relationship between the single-particle (tight-binding) and many-body (Lyapunov equation) descriptions of boundary-driven bosonic transport with power-law hopping. The two approaches agree only when $\langle N \rangle \ll 1$ and $\frac{\mu_{\text{in}}}{\mu_{\text{out}}} \ll 1$. Whether the qualitative behavior of the current (e.g. existence of peak) is a subject to a further study.

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Numerical computations were performed using the QuTiP [15] and SciPy package in Python 3.x.

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