Non-Markovian master equation for quantum transport of fermionic carriers

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Abstract

We propose a simple, yet feasible, model for quantum transport of fermionic carriers across tight-binding chain connecting two reservoirs maintained at arbitrary temperatures and chemical potentials. The model allows for elementary derivation of the master equation for the reduced single particle density matrix (SPDM) in a closed form in both Markov and Born approximations. In the Markov approximation the master equation is solved analytically, whereas in the Born approximation the problem is reduced to an algebraic equation for the SPDM in the Redfield form. The non-Markovian equation is shown to lead to resonant transport similar to Landauer’s conductance. It is shown that in the deep non-Markovian regime the transport current can be matched with that obtained by the non-equilibrium Green’s function method.

Keywords: quantum transport, master equation, non-equilibrium Green’s functions

1. Introduction

Recently, we have witnessed a lot of interest to quantum transport [1–11] across systems connecting two atomic reservoirs (batteries) [12, 13]. Specifically, such system can nowadays be set experimentally with ultracold atomic gases [14–16]. One of the major tools for theoretical analysis of such systems is the master equation approach [17–21]. Despite the enormous progress, so far the approach has been fully established only in the framework of the Born-Markov approximation [5, 6, 18, 19, 22–25]. To handle the non-Markovian regimes for fermionic carriers the stochastic Schrödinger equation approaches with the correlated noise [26–29] have been put forward. As it is demonstrated in [29], these approaches result in a hierarchy of stochastic evolution equations of the diffusion type with Grassmannian noise making it difficult to simulate numerically due to anticommutative multiplication. In this paper we analyze a model for quantum transport of fermionic carriers recently proposed in [30]. We will show that the model allows for elementary derivation of a numerically tractable non-Markovian master equation in a closed form whereas in the Markov approximation the model is solvable analytically.

We consider the set-up consisting of a linear tight-binding chain of $L$ sites coupled at both ends with two tight-binding rings of $M$ sites each [30, 31] as shown in figure 1. Throughout the text the chain is termed system, whereas the rings are going to be referred to as reservoirs. Non-interacting spinless fermions can move between the sites of the system and the sites of the reservoirs with hopping rates $J_{s, r}$, correspondingly. The hopping between the system and the reservoirs is quantified by the coupling constant $\epsilon$. The dynamics is controlled by the master equation for the total density matrix

$$\frac{\partial \hat{\rho}}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho} \right] + \gamma \sum_{\ell=1}^L \sum_{\nu=1}^M \left( \hat{L}^{(s)}_{\ell, \nu} + \hat{L}^{(d)}_{\ell, \nu} \right).$$

(1)

The Hamiltonian in equation (1) is written as

$$\hat{H} = \hat{H}_s + \sum_{\ell=1}^L \left( \hat{H}_{s, \ell} + \hat{H}_{c, \ell} \right).$$

(2)
isolated reservoir relaxes to the thermodynamic equilibrium. 

\[ \tilde{H}_{\ell} = -J_{\ell} \sum_{\nu=1}^{M} \cos(k_{\nu}) \hat{a}_{\nu} \hat{a}_{\nu}^{\dagger} + h.c. \]  

(3)

is the system’s Hamiltonian with \( \hat{a}_{\nu}^{\dagger}, \hat{a}_{\nu} \) being fermionic creation and annihilation operators at the \( \ell_{th} \) site. The reservoirs’ \( \tilde{H}_{\ell,\ell} \) and the coupling \( \tilde{H}_{c,\ell} \) Hamiltonians are indexed with subscript \( \ell \) specifying the connection site. For further convenience we write each reservoir Hamiltonian in terms of fermionic operators acting in the Fock space of the Bloch eigenstates of the ring

\[ \tilde{H}_{\ell} = -\frac{\epsilon}{2\sqrt{M}} \sum_{\nu=1}^{M} \hat{a}_{\nu}^{\dagger} \hat{a}_{\nu} + h.c. \]  

(5)

To prescribe thermodynamic quantities to each reservoir we introduced the particle drain

\[ \tilde{E}_{\ell,\nu} = \frac{\tilde{E}_{\ell,\nu}}{2} \left( \hat{a}_{\nu}^{\dagger} \hat{a}_{\nu} - 2\hat{a}_{\nu} \hat{\mathcal{R}} \hat{a}_{\nu}^{\dagger} + \hat{\mathcal{R}} \hat{a}_{\nu}^{\dagger} \hat{a}_{\nu} \right), \]  

(6)

and the particle gain

\[ \tilde{E}_{\ell,\nu} = \frac{-\tilde{E}_{\ell,\nu}}{2} \left( \hat{a}_{\nu}^{\dagger} \hat{a}_{\nu} - 2\hat{a}_{\nu} \hat{\mathcal{R}} \hat{a}_{\nu}^{\dagger} + \hat{\mathcal{R}} \hat{a}_{\nu}^{\dagger} \hat{a}_{\nu} \right). \]  

(7)

Lindblad operators [20], where

\[ \tilde{h}_{\ell,\nu} = \frac{1}{e^{-\beta_{\ell}(\epsilon(k_{\nu})+\mu)} + 1} \]  

(8)

ensures that due to coupling with Lindblad bath [32–34] each reservoir is populated according to the Fermi–Dirac distribution \( n = (e^{\beta_{\ell}(\epsilon-k_{\nu}+\mu)} + 1)^{-1} \) with given chemical potential \( \mu_{\ell} \) and inverse temperature \( \beta_{\ell} \). The reservoirs are labeled by their connection site \( \ell = 1, L \). Finally, the constant \( \gamma \) in equation (1) is the reservoir relaxation rate which determines how fast the isolated reservoir relaxes to the thermodynamic equilibrium.

### 2. Single particle density matrix (SPDM)

Equation (1) only contains pairwise combinations of the creation and annihilation operators. This allows us to rewrite it in terms of the total SPDM \( \tilde{\rho} \). The entries of the SPDM are defined as follows

\[ \rho_{\nu',\nu} = \text{tr} \left( \hat{a}_{\nu'}^{\dagger} \hat{a}_{\nu} \tilde{R} \right), \]  

(9)

where \( \nu \) spans all Bloch degrees of freedom \( \nu \) in the reservoirs as well as the Wannier degrees of freedom \( \ell \) in the system. Let us assume for a moment that only one reservoir is attached to the system at \( \ell = 1 \), then the SPDM takes the following block form

\[ \tilde{\rho} = \begin{pmatrix} \tilde{\rho}_{1} & \tilde{\rho}_{1,1} \\ \tilde{\rho}_{1,1}^{\dagger} & \tilde{\rho}_{1,1} \end{pmatrix}, \]  

(10)

where \( \tilde{\rho}_{1} \) is the SPDM of the reservoir, \( \tilde{\rho}_{1,1} \) is the SPDM of the system, and \( \tilde{\rho}_{1,1}^{\dagger} \) accounts for reservoir-system correlations. The following three equations can be obtained by applying equation (10) to equation (1)

\[ \frac{\partial \tilde{\rho}_{1}}{\partial t} = -i \left[ \tilde{H}_{1}, \tilde{\rho}_{1} \right] - ic \left( \tilde{V}_{1}^{\dagger} \tilde{\rho}_{1} - \tilde{\rho}_{1} \tilde{V}_{1} \right), \]  

(11)

\[ \frac{\partial \tilde{\rho}_{1,1}}{\partial t} = -i \tilde{H}_{1} \tilde{\rho}_{1} + i \tilde{\rho}_{1} \tilde{H}_{1} - \frac{\gamma}{2} \tilde{\rho}_{1} - ic \left( \tilde{V}_{1} \tilde{\rho}_{1}^{\dagger} - \tilde{\rho}_{1}^{\dagger} \tilde{V}_{1} \right), \]  

(12)

\[ \frac{\partial \tilde{\rho}_{1,1}^{\dagger}}{\partial t} = -i \left[ \tilde{H}_{1}, \tilde{\rho}_{1,1}^{\dagger} \right] - ic \left( \tilde{V}_{1} \tilde{\rho}_{1,1}^{\dagger} - \tilde{\rho}_{1,1}^{\dagger} \tilde{V}_{1} \right) + \gamma \left( \tilde{\rho}_{1}^{(0)} - \tilde{\rho}_{1} \right), \]  

(13)

where \( \tilde{\rho}_{1}^{(0)} \) is the Fermi–Dirac SPDM of the reservoir

\[ \tilde{\rho}_{1}^{(0)} = \sum_{\nu=1}^{M} \frac{|\nu\rangle \langle \nu|}{e^{-\beta_{1}(\epsilon(k_{\nu})+\mu_{1})} + 1}, \]  

(14)

while the Hamiltonian

\[ \tilde{H} = \left( \tilde{H}_{1} \right)_{\epsilon \tilde{V}_{1} \tilde{H}_{1}} \]  

(15)

is composed of the single particle Hamiltonian of the system

\[ \tilde{H}_{1} = -\frac{J_{1}}{2} \sum_{\ell=1}^{L-1} (|1+\ell\rangle \langle \ell| + h.c.), \]  

(16)

the single particle Hamiltonian of the reservoir

\[ \tilde{H}_{1} = -J_{1} \sum_{\nu=1}^{M} \cos \left( \frac{2\pi \nu}{M} \right) |\nu\rangle \langle \nu|, \]  

(17)

and the coupling operator

\[ \tilde{V}_{1} = -\frac{1}{2\sqrt{M}} \sum_{\nu=1}^{M} |\nu\rangle \langle \nu|. \]  

(18)
From equation (12) we find the solution with the initial condition \( \hat{\rho}_s(0) = 0 \)

\[
\hat{\rho}_s = i e \int_0^t d\tau e^{i(\tau - \tau')} \hat{U}_t(t - \tau) \left[ \hat{\rho}_s(\tau) \hat{V}_1 - \hat{V}_1 \hat{\rho}_s(\tau) \right] \hat{U}_t^\dagger(t - \tau),
\]

(19)

where \( \hat{U}_t(t) = e^{-i\hat{H}_s t} \) are the evolution operators and the initial condition \( \hat{\rho}_s(0) = 0 \) corresponds to the absence of initial reservoir-system correlations.

The above procedure can be applied to a reservoir attached to an arbitrary site of the chain. To address the transport problem the second reservoir is reattached to the \( L_{th} \) site. From now on we apply the notations \( \hat{\rho}_s \) for the SPDM of the reservoir at the \( \ell_{th} \) site. By substituting equation (19) into equation (11) and changing variables \( \tau - t \rightarrow \tau \) one finds

\[
\frac{\partial \hat{\rho}_s}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s \right] + \sum_{\ell=1,L} \left( \hat{L}_\ell + \hat{L}_\ell^\dagger \right),
\]

(20)

where

\[
\hat{L}_\ell = e^\tau \int_0^\tau d\tau' e^{-i\tau'} \hat{V}_\ell^\dagger(\tau') \left[ \hat{\rho}_s(\tau + \tau') \hat{V}_\ell - \hat{V}_\ell \hat{\rho}_s(\tau + \tau') \right] \hat{U}_\ell(\tau).
\]

(21)

3. Markov approximation

The Markov approximation consists of assuming no memory in integral equation (19). The Markov approximation makes it possible to derive the master equation for \( \hat{\rho}_s \) as a set of ordinary differential equations. The elementary derivation is presented in appendix. The final result is

\[
\frac{\partial \hat{\rho}_s}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s \right] - \frac{\epsilon^2}{\gamma^2} \sum_{\ell=1,L} \{ |\ell\rangle \langle \ell|, \hat{\rho}_s \} + \frac{\epsilon^2}{\gamma} \sum_{\ell=1,L} \left( \frac{\gamma^2 \hat{n}_\ell}{\gamma^2 + \epsilon^2} + \frac{\epsilon^2}{\gamma^2 + \epsilon^2} \langle |\ell\rangle \langle \ell| \hat{\rho}_s |\ell\rangle \langle \ell| \right),
\]

(22)

where

\[
\hat{n}_\ell = \frac{1}{M} \sum_{\nu=1}^M e^{-\beta[\hat{J}_\ell(\nu) + \mu]} + 1
\]

(23)

is the mean population of each site of the reservoir at the \( \ell_{th} \) site in the absence of coupling \( \epsilon = 0 \) and \{ \ldots \} designates the anticommutator. Equation (22) can be solved with a three diagonal time-stationary Ansatz

\[
\hat{\rho}_s = \sum_{\ell=1,L} A_\ell |\ell\rangle \langle \ell| + B \sum_{\ell=1}^{L-1} \langle i |\ell + 1 \rangle |\ell\rangle + \text{c.c.} + C \sum_{\ell=2}^{L-1} \langle \ell | |\ell - 1\rangle + \text{c.c.}
\]

(24)

which, upon substitution into equation (22), yields

\[
A_1 = C + \frac{\epsilon^2}{\gamma J_1}, A_L = C - \frac{\epsilon^2}{\gamma J_1},
\]

\[
B = \frac{1}{2} \frac{(n_1 - n_L) J_1 \gamma^2}{\gamma^2 + \epsilon^2}, C = \frac{n_1 + n_L}{2}.
\]

(25)

The stationary probability current along any bond in the system can be found as \( \langle j \rangle = J B \). Thus, we have

\[
\langle j \rangle = \frac{1}{2} \frac{(n_1 - n_L) J^2 \gamma^2}{\gamma^2 + \epsilon^2}.
\]

(26)

where we introduced

\[
\gamma = \frac{\epsilon^2}{\gamma}.
\]

(27)

If \( \gamma \gg \epsilon \), equation (22) simplifies to

\[
\frac{\partial \hat{\rho}_s}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s \right] - \gamma \sum_{\ell=1,L} \text{tr} \left( \frac{1}{2} \langle |\ell\rangle \langle \ell|, \hat{\rho}_s \rangle - \hat{n}_\ell |\ell\rangle \langle \ell| \right).
\]

(28)

The condition \( \gamma \gg \epsilon \) implies that the thermalization time of the reservoirs is much shorter than the time-scale of the dynamics induced by the system-reservoir coupling, i.e. the system interacts with a quasi-thermalized reservoir. It is not difficult to see that equation (28) can be derived from the following many particle master equation for the reduced density matrix \( \hat{\rho}_s = \text{tr}_r(\hat{\rho}) \)

\[
\frac{\partial \hat{\rho}_s}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s \right] + \sum_{\ell=1,L} \left( \hat{L}_\ell + \hat{L}_\ell^\dagger \right) + \tilde{\gamma}_\ell \hat{L}_\ell^\dagger + \tilde{\gamma}_\ell \hat{L}_\ell,
\]

(29)

with \( \tilde{\gamma} \) playing the role of the effective reservoir relaxation rate, and \( \tilde{\gamma}_\ell \) the standard gain and drain Lindblad operators of the form equations (6) and (7), but now acting directly on the Wannier state of the connection sites. Equation (29) is usually obtained with application of both Markov and Born approximations [35]. Physically, the Born approximation implies weak coupling between the system and the reservoir \( J_{sL} \gg \epsilon \). Often [35] the Born approximation is introduced as \( \hat{\rho} = \hat{\rho}_s \odot \hat{\rho}_s \). It can be easily seen that in the SPDM language the above becomes \( \hat{\rho} = \hat{\rho}_s \odot \hat{\rho}_s \). In our case the latter formula does not hold true [36] as it can be easily seen from equation (19). In fact, the zeroth order Born approximation emerges as

\[
\hat{\rho}_s = \hat{\rho}_s^{(0)}
\]

(30)

meaning that the reservoir’s SPDM is not perturbed by the state of the system.
4. Born approximation

Let us apply the Born approximation to equation (21) not involving the Markov approximation at the initial step. Substituting equation (30) into equation (21) and taking the limit $M \to \infty$ one finds

$$
\widetilde{L}_t = \frac{\ell}{4} |\ell\rangle \langle \ell| \int_{-\tau}^{0} d\tau e^{F_t} \left[ J_{\ell}(J_\tau) \tilde{\rho}_0 - J_{\ell}(J_\tau) \tilde{\rho}_0(\tau + t) \right] \tilde{U}_s(\tau),
$$

where $J_\ell$ is the zeroth order Bessel function of the first kind, $\tilde{\rho}_0$ the identity operator in the Wannier basis of the system, and

$$
J_{\ell}(J_\tau) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\tau \frac{e^{-i\ell \cos(\tau)} - e^{-2i\ell \cos(\tau) + \mu(\tau)}}{1 + e^{-2i\ell \cos(\tau) + \mu(\tau)}}.
$$

Equation (31) together with equation (20) constitute the non-Markovian master equation in the Born approximation. Notice the key role of $\gamma$ in equation (31); since the Bessel function at large $t$ decays as $1/\sqrt{t}$ the integral in equation (31) is only convergent with non-zero $\gamma$.

If the difference between the chemical potentials $\Delta \mu = \mu_R - \mu_L$ is small in comparison to the $H_s$ level spacing, the system’s SPDM can be written as

$$
\tilde{\rho}_s = \hat{\rho}_s^{(0)} + \Delta \mu \hat{\rho}_s^{(1)}.
$$

Note that $\hat{\rho}_s^{(0)}$ corresponds to equilibrium, and, thus, does not support a probability current. From equation (20) we have

$$
\frac{\partial \hat{\rho}_s^{(1)}}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s^{(1)} \right] + \sum_{\ell = 0,L} \left( \hat{\Delta}_\ell + \hat{\Delta}^\dagger_\ell \right).
$$

At low temperatures, $\beta \gg J_\ell$ the Fermi–Dirac distribution is

$$
\lim_{\beta \to \infty} \eta(E, \mu + \Delta \mu) = \theta(\mu - E) - \Delta \mu \delta(E - \mu),
$$

where $\theta$ is the Heaviside theta. Thus, for the operators $\hat{\Delta}_\ell$ one finds

$$
\hat{\Delta}_\ell = \frac{\ell^2}{4} |\ell\rangle \langle \ell| \int_{-\tau}^{0} d\tau e^{F_t} \left[ \frac{d(\mu)}{M} \frac{\delta_1 \ell}{\pi \sqrt{F_\ell - \mu^2}} e^{i\mu \gamma_s} \hat{U}_s(\tau) \right],
$$

where $d(\mu)$ is the $M$-site reservoir density of states

$$
d(\mu) = \begin{cases} 
\frac{M \eta}{\pi \sqrt{\mu^2 - \gamma_s^2}}, & \text{if } |J_\ell| > |\mu|, \\
0, & \text{if } |J_\ell| < |\mu|.
\end{cases}
$$

Finally, let us find the stationary equation for the matrix $\hat{\rho}_s^{(1)}$. Using the eigenenergies $E_m$ and eigenstates $|m\rangle$ of $H_s$

$$
E_m = -J \cos \left( \frac{\pi m}{L+1} \right), \quad m = 1, 2, \ldots, L,
$$

$$
|m\rangle = \sqrt{\frac{2}{L+1}} \sum_{\ell = 1}^{L} \sin \left( \frac{\pi m \ell}{L+1} \right) |\ell\rangle,
$$

we write both $\hat{\rho}_s^{(1)}$ and $\hat{\Gamma}_s$ as a series expansion

$$
\hat{\rho}_s^{(1)} = \sum_{m,m' = 1}^{L} \rho_{m,m'} |m\rangle \langle m'|,
$$

$$
\hat{\Gamma}_s = \sum_{m = 1}^{L} \rho_{m,m} |m\rangle \langle m|.
$$

By substituting equation (39) into equation (34) we obtain

$$
i \sum_{m,m' = 1}^{L} \rho_{m,m'} (E_m - E_{m'}) |m\rangle \langle m'| = \sum_{\ell = 1,L} \left[ \hat{\Delta}_\ell (t_\infty) + \hat{\Delta}_\ell^\dagger (t_\infty) \right],
$$

where we used

$$
\int_{-\infty}^{0} d\tau e^{F_t} \frac{\delta_1 \ell}{\pi \sqrt{F_\ell - \mu^2}} \sum_{m = 1}^{L} i |m\rangle \langle m| E_m - \mu + i \frac{\gamma_s}{2} = \frac{1}{\sqrt{F_\ell - (E_m + i \frac{\gamma_s}{2})^2}},
$$

Multiplying equation (40) by $|m\rangle$ from the left and by $|m'|$ from the right we find

$$
i (E_m - E_{m'}) \rho_{m,m'} = \frac{\ell^2}{4} \left( Q_{m,m'} - \sum_{\ell = 1,L} \sum_{m,m' = 1} \mathbb{B}_{m,m',m,m'}^{(\ell)} \rho_{m,m'} \right),
$$

where the source term $Q_{m,m'}$, and the Redfield relaxation tensor $\mathbb{B}_{m,m',m,m'}^{(\ell)}$, are given by

$$
Q_{m,m'} = \frac{J_\ell |m\rangle \langle m'|}{\pi \sqrt{F_\ell - \mu^2}} \left( \frac{i}{E_{m'} - \mu + i \frac{\gamma_s}{2}} - \frac{i}{E_m - \mu - i \frac{\gamma_s}{2}} \right),
$$

$$
\mathbb{B}_{m,m',m,m'}^{(\ell)} = \frac{(m |\ell\rangle \langle \ell| \delta_{m,m'})}{\sqrt{F_\ell - (E_{m'} + i \frac{\gamma_s}{2})^2}} + \frac{(m |\ell\rangle \langle \ell| \delta_{m,m'})}{\sqrt{F_\ell - (E_m - i \frac{\gamma_s}{2})^2}}.
$$
are interested in the stationary current across the chain as the energies in a window centered around 0.2, μ = 0.1. By applying the analytic solution equation (45) to remove the singularity we regularized the source term by integrating over 0.1, while the right at 0.1; solid lines show theoretical result obtained with the Markov approximation, equation (26), dashed and dotted lines—exact numerical solutions.

5. Numerical validation

Let us assume that the left reservoir is maintained at chemical potential μ + Δμ, while the right at μ. The other parameters of the reservoirs are the same if not stated otherwise. We are interested in the stationary current across the chain as the function of the chemical potential μ and the relaxation constant γ. We can calculate the current by using the following approaches:

(i) by straightforward numerical simulation of the system’s dynamics according to equations (11)–(13), which does not involve any approximation but is very time consuming;

(ii) by simulating the system dynamics on the basis of non-Markovian master equations (20) and (31), which implies validity of the Born approximation, and

(iii) by using the stationary Redfield equation equations (43) and (44), which also assumes low temperatures and the limit Δμ → 0;

(iv) by applying the analytic solution equation (26) which, however, implies validity of the Markov approximation.

In figures 2(a) and (b) we compare the probability currents obtained by using (i) and (ii). In figures 2(a) and (b) one can see a good coincidence between the two approaches for μ spanning the whole propagation band of Hr in a broad range of γ. Importantly, at small γ we observed four resonant peaks coinciding with the positions of the eigenvalues of Hr, which can be explained by the onset of resonant transport.

Figure 2. Quantum transport of fermionic carriers, L = 4, M = 80, J = 1. (a) The probability current versus γ and μ computed from numerical solution of equations (11)–(13), Δμ = 0.1, 1/β = 0.02, ε = 0.2. The vertical dashed lines show the eigenvalues of Hr. (b) Same as (a) but computed by numerically solving the non-Markovian master equation, equation (20) and (31). (c) The probability current against chemical potential with 1/β = 0.02, ε = 0.2, γ = 0.2, Δμ = 0.025; dash-dot black shows the data obtained from numerical solution of equations (11)–(13), solid red line—from the non-Markovian master equations (20) and (31), and dash blue line from the stationary Redfield equations (43) and (44). (d) Trace normalized eigenvalues of ˆρ11 for the same parameters as in (c), (e), (f) The probability current against γ for Δμ = 0.1; solid lines show theoretical result obtained with the Markov approximation, equation (26), dashed and dotted lines—exact numerical solutions.
due to the coupling suppressed with small $\varepsilon$. This resonant picture resembles Landauer’s conductance in which the transport solution is the pure scattering state with the energy equal to the chemical potential $\mathcal{E}$ [37]. The key to onset of the resonant transport is $\Delta \mu$ smaller than the spacing between the eigenstates of $\hat{H}_r$. On the other hand a small $\Delta \mu$ is difficult to handle with equations (11)–(13) since $\Delta \mu$ must be much larger than the level spacing in the reservoirs which otherwise would exhibit discrete eigenenergies rather than the continuous density of states equation (37). In figure 2(c) we, however, managed to achieve a reasonable coincidence between (i), (ii), and (iii), where the latter explicitly assumes infinite size reservoirs. In figure 2(d) we plotted the trace-normalized eigenvalues of the transport state $\rho_s^{(1)}(\mu)$. One can see that despite the superficial resemblance to Landauer’s conductance $\rho_s^{(1)}(\mu)$ only approaches a pure state near the resonant eigenvalues. Finally, in figures 2(e) and (f) we compared the numerical data with the Markovian analytic solution (iv). As expected equation (26) is only valid at large $\gamma$. One can see from figures 2(e) and (f) that the Markovian solution is incapable of describing the resonant transport at small $\gamma$. Notice that equation (26) is only plotted for $\mu = 0$ since for $\mu = 0.309$ the plots are almost identical. As it is seen from figure 2(f), it is possible to approach the maximum of equation (26) by increasing $\epsilon$ and $1/\beta$, but the Markov approximation unavoidably breaks down at $\gamma \approx J_{r,s}$.

Let us now examine the effect of temperature on quantum transport in more detail. In figure 3(a) we show the dependence of the current on the chemical potentials for three different temperatures for a fixed $\Delta \mu$. One can see in figure 3(a) that the temperature increase eliminates the resonant transport. This effect could be easily understood by smoothing of the Fermi distribution at larger temperature so that a significant difference between the Fermi functions of the reservoirs occurs at a broader range of energies. In figure 3(b) we present the data for the case of temperature increase only in the left reservoir. Notice that even with a larger chemical potential of the left reservoir $\Delta \mu = 0.01$ one can observe a flow of particles from the right to the left $\langle j \rangle < 0$ at $\mu = 0.42$. To understand this effect in figure 3(c) we plotted the Fermi–Dirac distributions in both reservoirs superposed with the eigenvalues of $\hat{H}_r$. One can see that all but the third eigenvalue occur at the points where the populations are almost equal. The third eigenvalue, though, occurs in the point where the population in the right reservoir is larger leading to enhancement of the resonant transport from the right to the left.

6. Transport in the chain between the rings with non-equilibrium Green’s functions

In this section we provide the theoretical description of the resonant transport in the system using the standard non-equilibrium Green’s function (NEGF) technique which will be used as the benchmark method. Let us assume that the chain is coupled with the rings with $M \rightarrow \infty$ playing a role of macroscopic contacts [37]. In other words, particles that populate them are thermalized under a given temperature and chemical potential and are reinjected back into the system. The Hamiltonian of the $j$th macroscopic contact ($j = 1, 2$) is

$$
\hat{H}_j = \sum_\nu \zeta_{\mu j} \hat{a}_{\mu j}^\dagger \hat{a}_{\mu j},
$$

where $\zeta_{\mu j} = -J_r \cos(k_{\nu j}) - \mu_j$; $\hat{a}_{\mu j}$ — an annihilator operator of electron with a wave vector $k_{\nu j}$, characterized by the dispersion relation $-J_r \cos(k_{\nu j})$ in the $j$th contact; $\mu_j = \mu + \eta_j V/2$ — an electrochemical potential of the $j$th contact (hereinafter $e = 1$); $V$ — a bias voltage; $\eta_1, \eta_2 = \pm 1$.

The tunneling between the macroscopic reservoirs and the system can be described by the operators which are analogous to (5). For the convenience of further derivation of the current, we rewrite these tunneling Hamiltonians using a field operator $\hat{\Psi}$ with $L$ components, $\Psi = [\hat{a}_1 \ldots \hat{a}_L]^T$, and projection operators $\hat{P}_1 = [1 \ldots 0]^T$, $\hat{P}_L = [0 \ldots 0 \; 1]^T$, such that

$$
\hat{T}_1 = -\sum_{\nu} \hat{a}_{1 \nu}^\dagger \hat{T}_1^\dagger \hat{\Psi} + h.c., \quad \hat{T}_2 = -\sum_{\nu} \hat{a}_{2 \nu}^\dagger \hat{T}_2^\dagger \hat{\Psi} + h.c.,
$$

where $\hat{T}_{1(2)} = \frac{\gamma}{\sqrt{\Psi}} \hat{P}_{1(2)}$. 

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Figure 3. Temperature effect on transport, $L = 4$, $M = 80$, $J_s = 1$, $J_r = 1.1$, $\gamma = 0.2$, $\varepsilon = 0.2$. (a) The effect of increasing temperature in both reservoirs, $\Delta \mu = 0.025$. (b) The effect of different temperatures; temperature in the left reservoir $1/\beta = 0.06$, temperature in the right reservoir $1/\beta = 0.02$. (c) Fermi–Dirac distributions in the reservoirs for subplot (b) with $\mu = 0.42$ and $\Delta \mu = 0.01$. Vertical black lines show the eigenvalues of $\hat{H}_r$. 

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The stationary current of fermions in the 1st contact is \( I_1 = \frac{\partial}{\partial \tau} \sum_{\nu} \langle \hat{N}_{1\nu}(t) \rangle \), where \( \hat{N}_{1\nu} = \hat{a}_{1\nu}^\dagger \hat{a}_{1\nu} \) is the number operator in the left contact. Using the Heisenberg equation one can easily obtain

\[
I_1 = -\sum_{\nu} \left( \epsilon \langle \hat{a}_{1\nu}^\dagger \hat{a}_{1\nu} \rangle - \epsilon^* \langle \hat{a}_{1\nu}^\dagger \hat{a}_{1\nu} \rangle \right).
\]

In the above expression we introduced NEGFs as follows [38]

\[
G^a_{1\nu}(\tau_a, \tau_b) = -i \left\{ \hat{T}_C \hat{P}_1^a \hat{\Psi}(\tau_a) \hat{a}_{1\nu}(\tau_b) \right\} \equiv \left\langle \hat{a}_{1\nu}(\tau_b) \right\rangle_{\text{con}},
\]

where \( \hat{T}_C \) orders the second-quantization operators on the Keldysh time contour \( C \) and \( a, b = +, - \) are the indices of its branches. Importantly, in the first line of (49) the averaging of the operators in the Heisenberg representation is over the ground state of the system with interaction (47). In the second line, the operators in the interaction representation are averaged over the known ground state without the perturbation, as indicated by the subscript 0. Such a simplification is achieved by introducing an evolution operator \( \hat{S} \) on the Keldysh contour,

\[
\hat{S}(\infty, -\infty) = \hat{T}_C \exp \left\{ -i \int_C (\hat{T}_1^+ + \hat{T}_2) \right\} \text{d} \tau,
\]

defining the perturbation expansion of the NEGFs where only connected diagrams have to be considered, as indicated by superscript \( \text{con} \) in equation (49).

Analyzing the diagrammatic series generated by the \( S \) operator (50) one can express the NEGFs included in (48) as

\[
G^+_{1\nu}(t, \tau_a) = -\int_C \text{d} \tau \hat{P}_1^a \hat{T}_1 \hat{a}_{1\nu}(\tau_a) \text{d} \tau - \int_C \text{d} \tau \hat{a}_{1\nu}(\tau_a) \hat{T}_1 \hat{G}^+ - \int_C \text{d} \tau \hat{G}^+ \text{d} \tau_e \hat{P}_1^a,
\]

where \( g^{ab}_{1\nu}(\tau_a - \tau_b) \) is the bare NEGFs of the 1st contact. The full NEGFs of the structure satisfy the Dyson equation of the general form

\[
\hat{G}(\tau - \tau') = \hat{g}(\tau - \tau') + \int_C \text{d} \tau_1 \text{d} \tau_2 \hat{g}(\tau - \tau_1) \hat{S}(\tau_1 - \tau_2) \hat{G}(\tau_2 - \tau'),
\]

Here the self-energy reflects the effect of the macroscopic contacts, i.e.

\[
\hat{S}(\tau_1 - \tau_2) = \sum_{\nu} \left[ \hat{T}_1 g_{1\nu}(\tau_1 - \tau_2) \hat{T}_1^+ + \hat{T}_1 g_{2\nu}(\tau_1 - \tau_2) \hat{T}_1^+ \right] \equiv \hat{S}_1 + \hat{S}_2.
\]

Further, it is convenient to replace the linearly dependent functions \( G^{ab} \) and \( \Sigma^{ab} \) with the independent ones, so-called NEGF triangular representation, including retarded, advanced, and Keldysh NEGFs and the corresponding self-energies. In case of the \( j_{ab} \), isolated macroscopic contact these quantities as functions of frequency are given by

\[
g^{r,a}_{j\nu}(\omega) = \frac{1}{\omega - \xi_{j\nu} \pm i\delta},
\]

where \( n_{aj} \) is the Fermi–Dirac distribution function defined in (8). If the bandwidths of the macroscopic contacts are wide in comparison with the bias electric field energy, one can approximate that \( \Sigma^{r,a}_{j\nu} \approx i \pi \Gamma/2 \) \( \delta (\omega - \xi_{j\nu}) \), where \( \Gamma(\omega) = 2 \pi \left( \frac{\tau}{\sqrt{2\pi}} \right) \text{d}(\omega), \text{d}(\omega) \) the density of states of the contacts defined by the expression (37) valid for \( M \to \infty; n_j \equiv n(\omega + \eta_j V/2) \) is the Fermi–Dirac distribution functions. The matrix self-energies of the contacts are \( \hat{S}_{1,2} = \hat{P}_{1,2} \hat{S}^{\pm}_{1,2} \hat{P}_{1,2}^\dagger \), and \( i = r, a, K \).

Substituting equation (51) into equation (48) and performing the Fourier transformation, the particle current becomes

\[
I_1 = i \int_{-\infty}^{+\infty} \text{d} \omega \frac{2\pi}{\omega} \left\langle \text{Im} \left\{ \hat{S}_{1\nu}(\omega) \right\} G^a_{1\nu}(\omega) \right\rangle - \text{Im} \left\{ \hat{S}_{1\nu}(\omega) \right\} G^a_{1\nu}(\omega),
\]

To obtain (55) the relations between the NEGFs are used, namely, \( G^K = G^{++} + G^{++} \), \( G^L = G^{++} - G^{+-} \) and \( G^L = G^{++} - G^{--} \), \( G^L(\omega) = \langle G^L(\omega) \rangle \).

Green’s functions in equation (55) can be found using the Keldysh equation

\[
G_{11}^K = \hat{P}_1^a \hat{G}^+ \hat{S}^K \hat{G}^a \hat{P}_1,
\]

\[
2 \text{Im} \left\{ \hat{G}_{11}^a \right\} = \hat{P}_1^a \hat{G}^+ \left[ \hat{S}^K - 2\hat{S}^+ \right] \hat{G}^a \hat{P}_1.
\]

Taking these relations into account, we finally obtain

\[
I_1 = \int_{-\infty}^{+\infty} \text{d} \omega \frac{2\pi}{\omega} \left\langle \hat{G}_1 \hat{G}_2 \hat{G}_3 \right\rangle (n_2 - n_1),
\]

where \( \hat{G}_{1,2} = \hat{G}_1 \hat{G}_2 \hat{G}_3 \). A similar approach for the current in the right contact yields

\[
I_2 = \int_{-\infty}^{+\infty} \text{d} \omega \frac{2\pi}{\omega} \left\langle \hat{G}_1 \hat{G}_2 \hat{G}_3 \right\rangle (n_1 - n_2).
\]

Note that the factors before the difference of the distribution functions in (57) and (58) can be treated as transmission coefficients. As a result, the obtained formulae for the current are equivalent to those of the Landauer-Büttiker formalism dealing with the scattering problem [39–41].
Using the Dyson equation in the $\omega$-representation one can show that the device spectral function is [37]

\[
\hat{A} = i \left( \hat{G}^r - \hat{G}^\lambda \right) = \hat{G}^r \left( \hat{\Gamma}_1 + \hat{\Gamma}_2 \right) \hat{G}^\lambda = \hat{G}^\lambda \left( \hat{\Gamma}_1 + \hat{\Gamma}_2 \right) \hat{G}^r.
\] (59)

The last equality leads to $\text{tr} \left[ \hat{\Gamma}_2 \hat{G}^r \hat{\Gamma}_1 \hat{G}^\lambda \right] = \text{tr} \left[ \hat{\Gamma}_1 \hat{G}^\lambda \hat{\Gamma}_2 \hat{G}^r \right]$ and $I_2 = -I_1 \equiv \langle j \rangle$ that is a well-known result. In figure 4 we compare the results found using the non-Markovian master equation and the NEGF method. One can observe a qualitative agreement for different values of $\gamma$. Quantitatively, there are two tendencies as the relaxation rate changes. The resonant peaks widen when the relaxation rate approaches $\epsilon$. In the opposite case, if $\gamma \ll \epsilon$, the four resonances become sharper and the two pictures match with good accuracy.

7. Summary

In summary, we analyzed a fermionic model that allows for elementary derivation of transport master equation which can be solved analytically in the Markov approximation. In the Born approximation we have derived a non-Markovian master equation for quantum transport of fermionic carriers in the Redfield form. The equation obtained is shown to predict the effect of resonant transport which cannot be accounted for by the exact Markovian solution. A similar phenomenon of resonant excitation transfer has been recently predicted in [42] in the set-up consisting of a block of sender sites, each hosting one excitation, weakly coupled to a quantum tight-binding wire at one edge with the block of receiver sites weakly coupled at the opposite edge. Here we have demonstrated the effect of resonant transport with thermalized sender and receiver. The results obtained in the deep non-Markovian regime show a qualitative agreement with those obtained with the non-equilibrium Green’s function method. Two ingredients are essential for the correct derivation of the non-Markovian master equation. First, the explicit account of the relaxation rate in the microscopic model of the reservoir. The reservoir relaxation rate is found to be of key importance to ensure convergence of the memory integral and onset of the resonant transport. The second ingredient is the account of correlations between the state of the reservoir and the state of the system. Such correlations do not allow to write the total density matrix as the tensor product of the density matrices of the reservoir and the system, but, nonetheless, do not invalidate the Born approximation at weak couplings. We speculate that the above conclusion can be applied to quite arbitrary set-ups of reservoir-coupled conductors. The benefit of the set-up considered, though, is the simplicity of derivation that paves a way to generalizing the results for interparticle interactions in the system.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Appendix. Markovian master equation for system’s SPDM

In equations (21) and (22) of the main text we arrived at the following equation for the system’s SPDM

\[
\frac{\partial \hat{\rho}_s}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s \right] + \sum_{\ell=1,k} \left( \hat{L}_{\ell} + \hat{L}_{\ell}^\dagger \right),
\]
\[ \hat{L}_t = c^2 \int_{-t}^{0} d\tau e^{2\gamma \tau} \hat{V}_t^\dagger(t) \left[ \hat{\rho}_t(\tau + t) \hat{V}_t - \hat{V}_t \hat{\rho}_t(\tau + t) \right] \hat{U}_t(t). \]  
(A.1)

In the similar fashion equations (18) and (19) of the main text can be resolved to

\[ \frac{\partial \hat{\rho}_t}{\partial t} = -i \left[ \hat{H}_t, \hat{\rho}_t \right] + \hat{K}_t + \hat{K}_t^\dagger + \gamma \left( \hat{\rho}_t^{(0)} - \hat{\rho}_t \right), \]
\[ \hat{K}_t = \frac{c^2}{2} \int_{-t}^{0} d\tau e^{2\gamma \tau} \hat{V}_t^\dagger(t) \left[ \hat{V}_t \hat{\rho}_t(\tau + t) - \hat{\rho}_t(\tau + t) \hat{V}_t \right] \hat{U}_t(t), \]
\[ \hat{\rho}_t^{(0)} = \sum_{\nu = 1}^{M} \frac{|\nu\rangle \langle \nu|}{e^{-\beta \bar{e}[\cos(k_s) + \mu]} + 1}, \]  
(A.2)

where subscript \( \ell \) specifies the reservoir’s connection site. Together equations (A.1) and (A.2) constitute a set of tree integro-differential equations for \( \hat{\rho}_s \) and \( \hat{\rho}_t \) with \( \ell = 1, L \).

The Markov approximation consists of assuming no memory in integrals in equations (A.1) and (A.2). It can be applied under two assumptions:

- \( \gamma \gg J_s, J_t \); i.e. the reservoirs’ relaxation rate is much greater than the characteristic dynamic time-scales due to the evolution operators \( \hat{U}_{s,t}(t) \) of both reservoirs and system.
- The reservoirs and the system are near stationary. Thus, \( \hat{\rho}_s \) and \( \hat{\rho}_t \) are slow varying on the scale \( 1/\gamma \).

The memory effect can be removed by applying

\[ \int_{-t}^{0} d\tau e^{2\gamma \tau} \hat{A}(\tau + t) = \frac{2}{\gamma} \hat{A}(t) \]  
(A.3)

where \( \hat{A}(t) \) is any operator quantity slow varying on the scale \( 1/\gamma \). Under the Markov approximation one finds

\[ \hat{L}_t = \gamma \gamma \hat{V}_t \hat{\rho}_t \hat{V}_t - \hat{V}_t \hat{\rho}_t \hat{V}_t, \]
\[ \hat{K}_t = \gamma \gamma \left( \hat{V}_t \hat{V}_t^\dagger \hat{\rho}_t - \hat{\rho}_t \hat{V}_t \hat{V}_t^\dagger \right) \hat{V}_t. \]  
(A.4)

Substituting the above into the first line equation (A.1) one finds

\[ \frac{\partial \hat{\rho}_t}{\partial t} = -i \left[ \hat{H}_t, \hat{\rho}_t \right] + \gamma \left( \hat{\rho}_t^{(0)} - \hat{\rho}_t \right) \]
\[ - \frac{c^2}{\gamma} \left( \hat{V}_t \hat{\rho}_t \hat{V}_t^\dagger - 2 \hat{V}_t \hat{\rho}_t \hat{V}_t \right), \]  
(A.5)

where \{ \ldots \} designates the anticommutator. With the initial condition \( \hat{\rho}_t(0) = 0 \) and \( J_t \ll \gamma \) the solution of equation (A.5) reads

\[ \hat{\rho}_t = \int_{-t}^{0} d\tau \hat{F}(\tau) \left[ \gamma \hat{\rho}_t^{(0)}(\tau + t) + 4 \gamma \hat{V}_t \hat{\rho}_t(\tau + t) \hat{V}_t^\dagger \right] \hat{F}(\tau), \]  
(A.6)

where

\[ \hat{F}(t) = e^{2\gamma t} \hat{V}_t \hat{V}_t^\dagger. \]  
(A.7)

Notice that the initial condition \( \hat{\rho}_t(0) = 0 \) is far from the thermodynamic equilibrium which seemingly contradicts our initial assumptions. Yet, for large times \( t \gg 1/\gamma \), when the equilibrium in the isolated reservoirs is settled, the initial condition for the operator \( \hat{K}_t \) in equation (A.2) becomes irrelevant with all deviations from the equilibrium due to the coupling with the system that is accounted for exactly in both equations (A.5) and (A.6). By using the definition of the coupling operator

\[ \hat{V}_t = -\frac{1}{2\sqrt{M}} \sum_{\nu = 1}^{M} |\nu\rangle \langle \ell|. \]  
(A.8)

one finds

\[ \hat{F}(t) = \hat{V}_t^\dagger + \frac{e^{2\gamma t} - 1}{M} \sum_{\nu, \nu' = 1}^{M} |\nu\rangle \langle \nu'|. \]  
(A.9)

Now the quantity \( \hat{V}_t^\dagger \hat{\rho}_t \hat{V}_t \) that has emerged in equation (A.4) can be written as

\[ \hat{V}_t^\dagger \hat{\rho}_t \hat{V}_t = \int_{-t}^{0} d\tau e^{\gamma t + e^{-\gamma t}} \gamma \gamma \hat{V}_t \hat{\rho}_t \hat{V}_t \]
\[ \times \left[ \gamma \hat{\rho}_t + \frac{e^{2\gamma t} - 1}{4} \left( \hat{\rho}_t(\tau + t) |\ell\rangle \langle \ell| \right) |\ell\rangle \langle \ell| \right], \]  
(A.10)

where \( \bar{n}_t \) is the mean population of each site of the reservoir at the site in the absence of coupling \( \epsilon = 0 \)

\[ \bar{n}_t = \frac{1}{M} \sum_{\nu = 1}^{M} e^{-\beta \bar{e}[\cos(k_s) + \mu]} + 1. \]  
(A.11)

Assuming no memory again one rewrites equation (A.10) as

\[ \hat{V}_t^\dagger \hat{\rho}_t \hat{V}_t = \frac{1}{4} \left( \gamma \gamma \bar{n}_t + e^{2\gamma t} \gamma \gamma \hat{\rho}_t(\tau + t) \right) |\ell\rangle \langle \ell| \right] |\ell\rangle \langle \ell| \right], \]  
(A.12)

Finally, by combining equations (A.1), (A.4) and (A.12) we arrive at the Markovian master equation for the system’s SPDM

\[ \frac{\partial \hat{\rho}_s}{\partial t} = -i \left[ \hat{H}_s, \hat{\rho}_s \right] - \frac{e^2}{2\gamma} \sum_{\ell = 1}^{L} |\ell\rangle \langle \ell| \right] |\ell\rangle \langle \ell| \right], \]  
(A.13)

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References

[1] Dubi Y and Ventra M D 2009 Phys. Rev. E 79 042101
[2] Znidaric M 2010 J. Stat. Mech. L05002
[3] Bruderer M and Belzig W 2012 Phys. Rev. A 85 013623
[4] Ivanov A, Kordas G, Komnik A and Wimberger S 2013 Eur. Phys. J. B 86 345
[5] Nietner C, Schaller G and Brandes T 2014 Phys. Rev. A 89 052141
[6] Pershin Y V, Rossi M and Giuliano D 2021 Phys. Rev. B 103 115139
[7] Nava A, Rossi M and Giuliano D 2021 Phys. Rev. B 103 115139
[8] Xu X, Thingna J and Wang J-S 2017 Phys. Rev. B 85 035428
[9] De Raedt H, Jin F, Katsnelson M I and Michielsen K 2017 Phys. Rev. B 96 053306
[10] Kolovsky A R, Denis Z and Wimberger S 2018 Phys. Rev. A 98 043623
[11] Potts P P, Kalaeec A A S and Wacker A 2021 New J. Phys. 23 123013
[12] Zhao X, Shi W, Wu L A and Yu T 2012 Phys. Rev. A 86 032116
[13] Chen M and You J Q 2013 Phys. Rev. A 87 052108
[14] Nazir A and Schaller G 2018 The reaction coordinate mapping in quantum thermodynamics Thermodynamics in the Quantum Regime (Springer) pp 551–77
[15] 1997 Electronic Transport in Mesoscopic Systems (Cambridge University Press)
[16] Keldysh L V 1965 Sov. Phys. JETP 20 1018
[17] Landauer R 1957 IBM J. Res. Dev. 1 233
[18] Landauer R 1970 Phil. Mag. 21 863
[19] Buttiker M 1986 Phys. Rev. Lett. 57 1761
[20] Chetcuti W J, Sanavio C, Lorenzo S and Apollaro T J G 2020 New J. Phys. 22 033030
[21] Kolovsky A R 2020 Phys. Rev. E 101 062116