I. INTRODUCTION

The investigation of time-resolved currents in mesoscopic devices has gained a lot of interest over the past few years. This is not only because of the potential application to quantum computing but also due to the advent of new experiments specifically looking into time-dependent electron transport [1, 2]. For example, manipulation of quantum dot systems is performed by using pump-probe schemes with a single voltage pulse. The rising and the falling edge of the pulse lead to pumping and probing the device, respectively. The experiments include transient-current spectroscopy of single quantum dots [3] and coherent manipulation of charge [4] and spin [5, 6] qubits in double quantum dots (DQDs).

The theoretical description of the electric current through a device coupled to two-electron reservoirs is usually based on Keldysh non-equilibrium Green function (NEGF) techniques [7, 8]. Within this approach the description of piecewise constant and sinusoidal voltage pulses is readily possible in the wide-band limit (WBL). For harmonic modulations more sophisticated methods [9, 10, 11] combining Floquet theory and NEGF formalism have been developed and allow going beyond WBL. In the remaining part of the introduction we briefly discuss the general setup [Sec. IA] and then repeat the findings of the standard NEGF formalism in the context of our propagation scheme [Sec. IB].

A. Setup

We take the usual threefold setup consisting of a device (system) which is coupled to two electron reservoirs. The coupling is due to tunneling through a barrier. The total Hamiltonian is

$$H = H_D + H_R + H_{DR}. \quad (1)$$

The device is described in terms of discrete energy levels $$\varepsilon_n(t)$$ which may be coupled through $$V_{nm}(t),$$

$$H_D = \sum_n \varepsilon_n(t)c_n^\dagger c_n + \sum_{n \neq m} V_{nm}(t)c_n^\dagger c_m. \quad (2)$$

The operators $$\{c_n^\dagger\}$$ and $$\{c_n\}$$ denote the creation and annihilation of an electron in state $$n.$$ The reservoirs are described by non-interacting electrons and the Hamiltonian reads

$$H_R = \sum_{n \in \{L, R\}} \sum_k \varepsilon_{nk}(t)b_{nk}^\dagger b_{nk}. \quad (3)$$
functions, It is \( \bar{\alpha} \) equilibrium state of reservoir \( \alpha \).

As indicated at the end of the previous section the Fermi level, i.e. all sub-systems are separated at \( t = -\infty \) and in their respective equilibrium state. Any time dependence only sets in after eventually coupling the different parts. Consequently, the single-particle occupation probability in the reservoirs is determined by \( \varepsilon_{\alpha k} \); the time dependence \( \Delta_{\alpha k}(t) \) of the reservoir energies appears as a phase-factor only. The situation where the chemical potentials and therefore the occupation probabilities are time-dependent has been critically discussed before [7].

### B. Time-Dependent Current and Non-Equilibrium Green Functions

By applying the Keldysh formalism to non-equilibrium Green functions it is possible to obtain a general formula for the time-dependent current in the setup introduced in Sec. [A]. The current \( J_\alpha \) through the barrier connecting lead \( \alpha \) and the device is given by [7, 8]

\[
J_\alpha(t) = 2e \text{Re} \text{Tr} \left\{ \int_{-\infty}^{\infty} dt_1 \left[ \mathcal{G}_<(t, t_1) \Sigma^\alpha_>(t_1, t) + \mathcal{G}^\dagger(t, t_1) \Sigma^\alpha_<(t_1, t) \right] \right\}.
\]

Here, \( \mathcal{G}_< \) and \( \mathcal{G}^\dagger \) are lesser and retarded Green functions, \( \Sigma^\alpha_\geq \) and \( \Sigma^\alpha_< \) are advanced and lesser self-energies, respectively. All boldface quantities are matrices related to the device states, e.g., \( \mathcal{G}_<(t, t_1) \equiv G_{nm}^<(t, t_1) \). Products are to be understood as matrix multiplications. The greater and lesser self-energies are explicitly given by

\[
\Sigma^\alpha_>(t_1, t) = -i \int \frac{d\varepsilon}{2\pi} \tilde{f}_\alpha(\varepsilon) e^{-i(\varepsilon-t_1-t)} \Gamma_\alpha(\varepsilon, t_1, t) \tag{6a}
\]

\[
\Sigma^\alpha_< (t_1, t) = i \int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon) e^{-i(\varepsilon-t_1-t)} \Gamma_\alpha(\varepsilon, t_1, t) \tag{6b}
\]

As indicated at the end of the previous section the Fermi distribution, \( f_\alpha(\varepsilon) \equiv f(\beta(\varepsilon - \mu_\alpha)) \), characterizes the equilibrium state of reservoir \( \alpha \) with the chemical potential \( \mu_\alpha \) and inverse temperature \( \beta = (k_B T)^{-1} \) at \( t_0 = -\infty \). It is \( f_\alpha(\varepsilon) = 1 - f_\alpha(\varepsilon) \). Using a relation for two-time functions,

\[
X^{\geq<}(t, t') = \pm \Theta(\pm t \mp t') \left[ X^{\geq<}(t, t') - X^{\geq<}(t, t') \right] , \tag{7}
\]

which applies to Green functions as well as to self energies, one can find advanced (retarded) self-energies in Eq. [5] in terms of greater and lesser functions. The level-width function \( \Gamma_\alpha \) in Eqs. [10] depends on the density of states \( \rho_\alpha(\varepsilon) \) of reservoir \( \alpha \) and the coupling \( T_{\alpha, n}(\varepsilon) \) of device level \( n \) and the reservoir state at energy \( \varepsilon \).

\[
\left[ \Gamma_\alpha(\varepsilon, t_1, t) \right]_{mn} = 2\pi \rho_\alpha(\varepsilon) T_{\alpha, n}(\varepsilon) T^*_{\alpha, m}(\varepsilon, t_1) \times \exp \left\{ i \int_{t_1}^{t} dt_2 \Delta_\alpha(\varepsilon, t_2) \right\} . \tag{8}
\]

Replacing the advanced and retarded quantities in Eq. [9] by using Eq. [7] one can rewrite the expression for the current in a very compact form,

\[
J_\alpha(t) = 2e \text{Re} \text{Tr} \left\{ \Pi_\alpha(t) \right\} . \tag{9}
\]

The current matrices \( \Pi_\alpha(t) \) are given by the following expression

\[
\Pi_\alpha(t) = \int_{t_0}^{t} dt_2 \left( \mathcal{G}^>(t, t_2) \Sigma^\alpha_< (t_2, t) - \mathcal{G}_<(t, t_2) \Sigma^\alpha_>(t_2, t) \right) , \tag{10}
\]

where the first and the second term describe electrons tunneling into and out of the device, respectively. Equations [9] and [10] have been discussed in the context of current conserving self-energies [8]. The conceptually new approach presented in this article consists in considering \( \Pi_\alpha(t) \) as an independent entity. In particular, opposed to correlation functions such as \( \mathcal{G}^\leq(t, t_2) \) the current matrices \( \Pi_\alpha(t) \) only depend on a single time argument. Therefore, they are fully determined by a single equation of motion. This circumstance provides the basis of our propagation scheme, which is presented in Sec. [II].

Moreover, in order to calculate the expectation value of any device observable \( O_D \) it is advantageous to use the reduced single-electron density matrix, \( \sigma(t) = \text{Im} \mathcal{G}^<(t, t) \). The expectation value is then given by

\[
\langle O_D(t) \rangle = \text{Tr} \left\{ O_D \sigma(t) \right\} . \tag{11}
\]

Similar to the current matrices \( \Pi_\alpha(t) \) the density matrix only depends on a single time argument and one has the following equation of motion

\[
i \frac{\partial}{\partial t} \sigma(t) = \left[ H(t), \sigma(t) \right] - i \sum_\alpha \left( \Pi_\alpha(t) + \Pi^\dagger_\alpha(t) \right) , \tag{12}
\]

which depends on the current matrices \( \Pi_\alpha(t) \). The boldface Hamiltonian \( H(t) \equiv [H_D]_{mn} \) is obtained from the device Hamiltonian in Eq. [2]. Equation [12] is found by using \( \mathcal{G}^<(t', t) = -[\mathcal{G}^>(t, t')]' \) and from the equations
of motion for greater and lesser Green functions \(G^>\) and \(G^<\),
\[
\frac{1}{\partial t} G^\pm(t, t') = H(t) G^\pm(t, t') + \int dt_2 \Sigma_{\text{tot}}^\pm(t, t_2) G^\pm(t_2, t') + \int dt_2 \Sigma_{\text{tot}}^\pm(t_2, t) G^\pm(t, t'). \tag{13}
\]
The total self-energies \(\Sigma_{\text{tot}}^\pm\) are sums of the tunneling
self-energies for each reservoir. The Green functions may
also be obtained from the Dyson series leading to an
integral equation \[8\].

II. CURRENT MATRICES AND AUXILIARY
MODE EXPANSION

In order to arrive at a viable propagation scheme we
will rewrite the equations of motion given above by intro-
ducing energy-resolved quantities. This form allows for
applying an auxiliary-mode expansion which replaces the
energy integrals by finite sums. The number of (matrix)
equations to be propagated is determined by the size of
the expansion.

A. Energy-Resolved Current Matrices

First we assume factorizing momentum and time
dependence of the tunnel coupling, \(T_{\alpha,n}(\varepsilon, t) = T_{\alpha,n}(\varepsilon)u_{\alpha,n}(t)\). The same ansatz has been used in Ref. \[1\] for the non-interacting resonant-level model. For not-
tational convenience we consider in the following only the
case of a common time dependence of the coupling for all
device states, i.e. \(u_{\alpha,n}(t) = u_{\alpha}(t)\). Equation \[8\]
becomes
\[
\Gamma_{\alpha}(\varepsilon, t_1, t) = u_{\alpha}^*(t_1)u_{\alpha}(t)\Gamma_{\alpha}(\varepsilon) \exp\{i \int_{t_1}^t dt_2 \Delta_{\alpha}(\varepsilon, t_2)\}. \tag{14}
\]

Next, we define energy-resolved self-energies as
\[
\Sigma_{\alpha}^>(\varepsilon; t_1, t) = -iu_{\alpha}^*(t_1)f_{\alpha}(\varepsilon) e^{-i\varepsilon(t_1-t)} \Gamma_{\alpha}(\varepsilon) \times \exp\{i \int_{t_1}^t dt_2 \Delta_{\alpha}(\varepsilon, t_2)\}, \tag{15a}
\]
\[
\Sigma_{\alpha}^<\varepsilon; t_1, t) = iu_{\alpha}^*(t_1)f_{\alpha}(\varepsilon) e^{-i\varepsilon(t_1-t)} \Gamma_{\alpha}(\varepsilon) \times \exp\{i \int_{t_1}^t dt_2 \Delta_{\alpha}(\varepsilon, t_2)\}. \tag{15b}
\]

In terms of these expressions the full self-energies are
given by
\[
\Sigma_{\alpha}^\pm(\varepsilon; t_1, t) = u_{\alpha}(t) \int d\varepsilon u_{\alpha}^*(\varepsilon; t_1, t), \tag{16}
\]
which follows from Eq. \[14\]. Using the definitions above we introduce energy-resolved current matrices,
\[
\Pi_{\alpha}(\varepsilon; t) = \int_{t_1}^t dt_2 \left( G^>(\varepsilon; t_2) \Sigma_{\alpha}^<(\varepsilon; t_2, t) - G^<\varepsilon; t_2) \Sigma_{\alpha}^>(\varepsilon; t_2, t) \right). \tag{17}
\]

From Eq. \[17\] one finds \(\Pi_{\alpha}(\varepsilon; t_0) = 0\). The expression for the current given by Eq. \[14\] becomes
\[
J_{\alpha}(t) = 2e \Re \sum_{\alpha} u_{\alpha}(t) \int d\varepsilon \Pi_{\alpha,\alpha}(\varepsilon; t). \tag{18}
\]

Therefore, the diagonal elements \(\Pi_{\alpha,\alpha}(\varepsilon; t)\) may be in-
terpreted as the current flowing from the reservoir state
at energy \(\varepsilon\) to the system state \(n\). The total current through the barrier is then given by the sum of all possible
currents.

The equation of motion [Eq. \[12\]] for the reduced
single-electron density matrix \(\sigma\) of the device becomes
\[
\frac{i}{\partial t} \sigma(t) = [H(t), \sigma(t)] - i \sum_{\alpha} \int d\varepsilon \left( u_{\alpha}(t)\Pi_{\alpha}(\varepsilon; t) + u_{\alpha}^*(t)\Pi_{\alpha}^\dagger(\varepsilon; t) \right), \tag{19}
\]
which now contains the energy-resolved current matrices.

Due to the definitions \[16\] of the energy-resolved self-
energies, their time derivatives,
\[
\frac{\partial}{\partial t} \Sigma_{\alpha}^\pm(\varepsilon; t_1, t) = i(\varepsilon + \Delta_{\alpha}(\varepsilon, t)) \Sigma_{\alpha}^\pm(\varepsilon; t_1, t), \tag{20}
\]
and by using Eq. \[13\], one gets an equation of motion for the energy-resolved current matrices,
\[
\frac{\partial}{\partial t} \Pi_{\alpha}(\varepsilon; t) = -\frac{i}{2\pi} u_{\alpha}^*(t)(\sigma(t) - f_{\alpha}(\varepsilon)) \Pi_{\alpha}(\varepsilon) + \{H(t) - (\varepsilon + \Delta_{\alpha}(\varepsilon, t))\} \Pi_{\alpha}(\varepsilon) + \sum_{\alpha'} u_{\alpha'}^*(t) \int d\varepsilon' \Omega_{\alpha\alpha'}(\varepsilon, \varepsilon'; t), \tag{21}
\]
where a new quantity \(\Omega_{\alpha\alpha'}\) has to be introduced. It
contains all contributions from the time derivative of the
greater and lesser Green functions, which give rise to a
double time integral. Consequently, its definition is
\[
\Omega_{\alpha\alpha'}(\varepsilon, \varepsilon'; t) = \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_1 \Sigma_{\alpha\alpha'}(\varepsilon; t, t_1) \left[ G^R(t_1, t_2) \Sigma_{\alpha\alpha'}^<(\varepsilon; t_2, t) - G^<_{\alpha}(t_1, t_2) \Sigma_{\alpha\alpha'}(\varepsilon; t_2, t) \right] \\
- \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1 \left[ \Sigma_{\alpha\alpha'}^<(\varepsilon'; t, t_1) G^R(t_1, t_2) \Sigma_{\alpha\alpha'}(\varepsilon; t_2, t) - \Sigma_{\alpha\alpha'}^>(\varepsilon'; t, t_1) G^<_{\alpha}(t_1, t_2) \Sigma_{\alpha\alpha'}(\varepsilon; t_2, t) \right].
\]

(22)

We replace the retarded self-energies and the advanced Green function again using Eq. (7), but instead of showing the result we rather give the equation of motion, which is easily obtained from Eq. (22),

\[
\frac{d}{dt} \Omega_{\alpha\alpha'}(\varepsilon, \varepsilon'; t) = \frac{1}{2\pi} \left\{ u_{\alpha'}(t) \Gamma_{\alpha'}(\varepsilon') \Pi_{\alpha}(\varepsilon; t) + \Pi_{\alpha'}^I(\varepsilon'; t) \Gamma_{\alpha}(\varepsilon) u_{\alpha}(t) \right\} \\
+ \left\{ (\varepsilon' + \Delta_{\alpha'}(\varepsilon', t)) - (\varepsilon + \Delta_{\alpha}(\varepsilon, t)) \right\} \Omega_{\alpha\alpha'}(\varepsilon, \varepsilon'; t),
\]

(23)

with the initial conditions \(\Omega_{\alpha\alpha'}(\varepsilon, \varepsilon'; t_0) = 0\). The equations of motion given by Eqs. (19, 21) and (23) provide a closed description of the non-equilibrium dynamics of the device. A similar set of equations has been found recently [17], where it was derived from a hierarchy for the many-body density matrix. The identification of

\[
\varphi_{\alpha} = -i \Pi_{\alpha} \quad \text{and} \quad \varphi_{\alpha'\alpha} = -i \Omega_{\alpha\alpha'},
\]

(24)

renders their equations identical to the ones given above. This provides an independent verification of the density-matrix approach [17] and shows that the hierarchy derived therein yields the exact dynamics for non-interacting electrons under the assumptions stated above.

The full single-particle density matrix has a size of \((N_D + N_R)^2\), where \(N_D\) and \(N_R\) are the number of single-particle states in the device and the reservoirs, respectively. In the present case we have to propagate \(N_D^2 \times (N_R + 1)^2\) quantities with \(\Pi\) and \(\Pi^I\) counting independently. Therefore, the complexity of Eqs. (19), (21) and (23) is at least the same compared to calculating the full single-particle density matrix. In particular one has to deal with a continuum of states and consequently the utility of the method depends on finding an efficient strategy for performing the energy integral. In the following subsection we will provide such a method based on the expansion of the Fermi function and making use of the residue theorem. The same strategy has been successfully applied to the propagation of non-Markovian quantum master equations involving bosonic [18] and fermionic reservoirs [17, 19]. The formulation in terms of energy-resolved quantities depending on a single time argument turns out to be beneficial in this context. In order to propagate each matrix only the value of the previous time step has to be known. References to past times [12, 13] are not necessary. This comes at the cost of having to propagate the two-energy quantity \(\Omega_{\alpha\alpha'}\). However, as we will show in the next section one can effectively reduce the associated numerical costs by using an auxiliary-mode expansion.

B. Auxiliary-Mode Expansion

The general idea of the auxiliary-mode expansion consists in making use of contour integration and the residue theorem. To this end the Fermi function is expanded in a sum over \(N_F\) simple poles,

\[
f_{\alpha}(\varepsilon) \approx \frac{1}{2} - \frac{1}{\beta} \sum_{p=1}^{N_F} \left( \frac{1}{\varepsilon - \chi_{\alpha p}^+} + \frac{1}{\varepsilon - \chi_{\alpha p}^-} \right)
\]

(25)

with \(\chi_{\alpha p}^\pm = \mu_{\alpha} \pm x_p / \beta\) and \(\text{Im} \ x_p > 0\). The well-known Matsubara expansion [20] is an example for such a decomposition. Its major disadvantage consists in a poor convergence behavior especially for low temperatures. A particular efficient alternative is presented in appendix A.

1. Wide-Band Limit

As a first application we consider the WBL, i.e. \(\Gamma_{\alpha}(\varepsilon) = \text{const}\). From the definition of the self-energies [6] and the expansion of the Fermi function [Eq. (25)] one obtains for \(t > t_1\),

\[
\Sigma_{\alpha}(t_1, t) = -\frac{i}{2} \Gamma_{\alpha} |u_{\alpha}(t)|^2 \delta(t - t_1)
\]

(26)

\[+ u_{\alpha}(t) \sum_p \frac{1}{\beta} \Gamma_{\alpha} u_{\alpha}^*(t_1) \chi_{\alpha p}^+ dt_2 \chi_{\alpha p}^-(t_2),\]

where \(\chi_{\alpha p}^\pm(t) = \chi_{\alpha p}^\pm + \Delta_{\alpha}(t)\). Analogously, one finds for the lesser self-energy

\[
\Sigma_{\alpha}^<(t_1, t) = \frac{i}{2} \Gamma_{\alpha} |u_{\alpha}(t)|^2 \delta(t - t_1)
\]

(27)

\[+ u_{\alpha}(t) \sum_p \frac{1}{\beta} \Gamma_{\alpha} u_{\alpha}^*(t_1) \chi_{\alpha p}^+ dt_2 \chi_{\alpha p}^-(t_2).\]

Thus, the expansion of the Fermi function leads to an expansion of the self-energies into a sum of exponentials.
Due to the WBL one also gets one term proportional to a delta function. We introduce auxiliary self-energies $\Sigma_{\alpha p}$, which incorporate the exponentials, i.e.

$$
\Sigma_{\alpha}(t_1,t) = \mp i \frac{1}{2} \Gamma_{\alpha} u_{\alpha}(t) e^{2i(t-t_1)} + u_{\alpha}(t) \sum_p \Pi_{\alpha p}(t_1,t),
$$

$$
\Sigma_{\alpha p}(t_1,t) = \frac{1}{\beta} \Gamma_{\alpha} u_{\alpha}(t_1) e^{i f_{\alpha} dt_2 \chi_{\alpha p}(t_2)},
$$

which implies $\Sigma_{\alpha p}(t, t_+)=\frac{1}{\beta} \Gamma_{\alpha} u_{\alpha}(t)$. Next, we insert the expanded self-energies into the definition of the current matrices $\Pi_{\alpha p}$,

$$
\Pi_{\alpha}(t) = \frac{1}{4} |u_{\alpha}(t)|^2 \left( 1 - 2 \sigma(t) \right) \Gamma_{\alpha}
+ u_{\alpha}(t) \sum_p \Pi_{\alpha p}(t),
$$

and obtain an expansion in terms of auxiliary current matrices,

$$
\Pi_{\alpha p}(t) = \int_{t_0}^{t} dt_2 \left( G^< (t, t_2) \Sigma_{\alpha p}(t_2, t) - G^> (t, t_2) \Sigma_{\alpha p}(t_2, t) \right).
$$

Their equation of motion is easily found,

$$
i \frac{\partial}{\partial t} \Pi_{\alpha p}(t) = \frac{1}{\beta} \Gamma_{\alpha} u_{\alpha}(t) e^{i f_{\alpha} dt_2 \chi_{\alpha p}(t_2)} + \left( H(t) - \frac{1}{2} \Gamma(t) - \chi_{\alpha p}(t) \right) \Pi_{\alpha p}(t),
$$

where $\Gamma(t) = \sum_{\alpha'} |u_{\alpha'}(t)|^2 \Gamma_{\alpha'}$. The coupled equations of motion (12) and (31) allow with Eq. (29) for a complete description of the non-equilibrium dynamics of the device. Comparing Eqs. (12) and (31) suggests that $\Pi_{\alpha p,\alpha' p'}(t) = \mp \frac{1}{\beta} u_{\alpha}(t) \Gamma_{\alpha'} \Pi_{\alpha p}(t) \delta_{p p'}$. Thus, an additional equation of motion for $\Pi_{\alpha p}$ is not needed for the WBL.

2. Lorentzian Level-Width Function

The next application we consider is the case of a Lorentzian level-width function (LLWF). We take a general ansatz of the form

$$
\Gamma_{\alpha}(\varepsilon) = \sum_{\ell=1}^{N_{\ell}} \left( \frac{\Gamma_{\alpha}^{+}}{\varepsilon - \varepsilon_{\alpha\ell} - iW_{\alpha\ell}} + \frac{\Gamma_{\alpha}^{-}}{\varepsilon - \varepsilon_{\alpha\ell} + iW_{\alpha\ell}} \right),
$$

with $W_{\alpha\ell} > 0$ and $\Gamma_{\alpha}^{\pm} = \mp i \Gamma_{\alpha} W_{\alpha\ell}$. Equation (32) might be used as a parametrization of an arbitrary level-width function (18). Now, we can plug Eq. (32) into the definition of the self-energies (Eq. (6)) and evaluate the energy integral by means of contour integration. This procedure yields for $t > t_1$

$$
\Sigma_{\alpha}^{\pm}(t_1, t) = + u_{\alpha}^{*}(t_1) u_{\alpha}(t) \left( \sum_{\ell} \Gamma_{\alpha}^{\pm} f_{\alpha\ell} e^{-i(\varepsilon_{\alpha\ell} + iW_{\alpha\ell})(t_1 - t)} \right)
+ \sum_{p} \frac{1}{\beta} \Gamma_{\alpha} \chi_{\alpha p}^{\pm} e^{-i\chi_{\alpha p}(t_1 - t)}
\times \exp\{i \int_{t_1}^{t} dt_2 \Delta_{\alpha}(\varepsilon, t_2) \},
$$

$$
\Sigma_{\alpha p}^{\pm}(t_1, t) = - u_{\alpha}^{*}(t_1) u_{\alpha}(t) \left( \sum_{\ell} \Gamma_{\alpha}^{\pm} f_{\alpha\ell} e^{-i(\varepsilon_{\alpha\ell} + iW_{\alpha\ell})(t_1 - t)} \right)
- \sum_{p} \frac{1}{\beta} \Gamma_{\alpha} \chi_{\alpha p}^{\pm} e^{-i\chi_{\alpha p}(t_1 - t)}
\times \exp\{i \int_{t_1}^{t} dt_2 \Delta_{\alpha}(\varepsilon, t_2) \},
$$

where $f_{\alpha\ell} = f_{\alpha}(\varepsilon_{\alpha\ell} + iW_{\alpha\ell})$ indicates that the expansion given in Eq. (25) should be used to calculate the Fermi function at the position of the pole $\ell$. The self-energies are thus given by a finite sum with $N_{L} + N_{F}$ terms. For convenience we combine the two indices $p$ and $\ell$ yielding a single index $x = \{\ell, p\}$. The coefficients and exponents are combined in a similar way.

$$
\Gamma_{\alpha x}^{+} = \{ \pm \frac{1}{\beta} \Gamma_{\alpha} f_{\alpha}(\varepsilon_{\alpha} \pm iW_{\alpha}), \pm \frac{1}{\beta} \Gamma_{\alpha} (\chi_{\alpha p}^{\pm}) \} \{ \varepsilon_{\alpha} \pm iW_{\alpha}, \chi_{\alpha p}^{\pm} \} \}
$$

$$
\Gamma_{\alpha x}^{-} = \{ \mp \frac{1}{\beta} \Gamma_{\alpha} f_{\alpha}(\varepsilon_{\alpha} \pm iW_{\alpha}), \mp \frac{1}{\beta} \Gamma_{\alpha} (\chi_{\alpha p}^{\pm}) \} \{ \varepsilon_{\alpha} \pm iW_{\alpha}, \chi_{\alpha p}^{\pm} \} \}
$$

Using these conventions the self-energies can be written in a compact form, assuming $t > t_1$ we have

$$
\Sigma_{\alpha}^{\pm}(t_1, t) = u_{\alpha}(t) \sum_{x} \Sigma_{\alpha x}^{\pm}(t_1, t),
$$

$$
\Sigma_{\alpha x}^{\pm}(t_1, t) = u_{\alpha}^{*}(t_1) \Sigma_{\alpha x}^{\pm} + e^{i f_{\alpha} dt_2 \chi_{\alpha p}(t_2)},
$$

where $\chi_{\alpha x}^{\pm} = \chi_{\alpha}^{\pm} + \chi_{\alpha x}(t)$. The auxiliary self-energies $\Sigma_{\alpha x}^{\pm}$ are simply exponentials. The respective auxiliary current matrices $\Pi_{\alpha x}^{\pm}$ can be calculated in analogy to the energy-resolved current matrices, i.e.

$$
\Pi_{\alpha x}(t) = \int_{t_0}^{t} dt_2 \left( G^< (t, t_2) \Sigma_{\alpha x}^{<}(t_2, t) - G^> (t, t_2) \Sigma_{\alpha x}^{>}(t_2, t) \right).
$$

Their equation of motion is then given by

$$
i \frac{\partial}{\partial t} \Pi_{\alpha x}(t) = u_{\alpha}^{*}(t) \Gamma_{\alpha x}^{<} + u_{\alpha}(t) \sigma(t) \left( \Gamma_{\alpha x}^{<} - \Gamma_{\alpha x}^{+} \right)
+ \left( H(t) - \chi_{\alpha x}(t) \right) \Pi_{\alpha x}(t)
+ \sum_{\alpha' x'} u_{\alpha'}^{*}(t) \Pi_{\alpha x, \alpha' x'}(t).
$$
The initial condition \( \Pi_{\alpha x}(t_0) = 0 \) follows from Eq. (26). Notice the similarity to the energy-resolved current matrices given by Eq. (21). In particular, we also have a two-mode quantity \( \Omega^{\alpha x, \alpha' x'} \) appearing in the equation of motion. Its definition is again in full analogy to the energy-resolved case given in Eq. (22), but with \( \Sigma^\alpha_\alpha(\varepsilon_t, t, t_1) \) replaced by \( \Pi^\alpha_\alpha(t, t_1) \). Also the equation of motion is similar to the energy-resolved case [Eq. (23)],

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \Omega^{\alpha x, \alpha' x'}(t) = i u_{\alpha'}(t) \left( \Gamma^{\alpha' x'}_\alpha - \Gamma^{\alpha x'}_\alpha \right) \Pi^{\alpha x}(t) \equiv \Omega^{\alpha x, \alpha' x'}(t) \tag{38}
\]

At \( t = t_0 \) one finds \( \Omega^{\alpha x, \alpha' x'}(t_0) = 0 \). It is interesting to notice that for \( x = p, x' = p' \), i.e. both indices represent an auxiliary mode resulting from the Fermi-function expansion [Eq. (23)], one gets \( \partial_t \Omega^{\alpha p, \alpha' p'}(t) \propto \Omega^{\alpha p, \alpha' p'}(t) \). Taking the initial condition into account it follows that \( \Omega^{\alpha p, \alpha' p'}(t = 0) \equiv 0 \) for all times. This is consistent with the energy-resolved expression [Eq. (23)] where any reference to the Fermi function is absent. Consequently, in the energy-resolved expression \( \Omega^{\alpha x, \alpha' x'}(t) \) matrices we only need to consider \( N_L \times (N_L + 2N_F) \) matrices for each reservoir index \( \alpha \). Since typically \( N_L \ll N_F \) the memory requirement of the proposed method scales with \( N_L \times N_F \) and the computational time requirement scales with \( N_T \times N_L \times N_F \), where \( N_T \) is the number of time steps. Notice that in spite of having to use two-energy quantities, using the auxiliary-mode expansion for the Fermi function yields a scheme, which scales linearly with the number of modes and thus allows for a particularly efficient propagation.

### III. APPLICATIONS

We apply the proposed propagation scheme to two situations: a resonant-level model with a randomly fluctuating energy level and a DQD system driven by finite bias-voltage pulses. These two situations demonstrate that our scheme is especially suited to study a strongly fluctuating driving and realistic experimental pulses including structured reservoirs.

#### A. Fluctuating Energy Level

As a first application we consider a resonant-level model with a single randomly fluctuating energy-level \( \varepsilon_d(t) \), which is given by a Gaussian stochastic process [29]. An analytic expression for the current is given in appendix B. The device Hamiltonian [Eq. (2)] is simply,

\[
H_D = \varepsilon_d(t) \epsilon_d^+ \epsilon_d \tag{39}
\]

with “\( d \)” denoting the single-electron state of the device. All matrices become scalars and the respective equations of motion are scalar equations. The stochastic process \( \varepsilon_d(t) \) is fully characterized by the first and second moments,

\[
\langle \varepsilon_d(t) \rangle = 0, \quad \langle \varepsilon_d(t) \varepsilon_d(t') \rangle = c(t - t'). \tag{40a}
\]

Here, we take \( \varepsilon_d(t) \) as realization of an Ornstein-Uhlenbeck (OU) process, which yields for the correlation function \( c(t - t') \equiv \frac{1}{\tau} \exp[-\kappa(t - t')] \). The OU process is characterized by two parameters, the inverse correlation-time \( \kappa \) and the noise amplitude \( \eta \) [21].

Considering the WBL and using a symmetric coupling to the left and right reservoir, \( \Gamma_L = \Gamma_R = \Gamma_0/2 \), we suddenly connect the device and the reservoirs at \( t = 0 \). The reservoirs are further characterized by chemical potentials \( \mu_L = 2\gamma \), \( \mu_R = \Gamma \) and temperature \( k_B T = 0.1\Gamma \). Thus, without stochastic driving the energy level is not located in the transport window and a non-vanishing current is a result of the broadening due to the coupling to the reservoirs.

The equations of motion obtained in Sect. III B are

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**FIG. 1:** Time-resolved occupation \( \langle N \rangle \) and net-current \( \langle J_{\text{net}} \rangle \) for different values of the noise amplitude. Noise averages are obtained from 20000 realizations and \( \kappa = 0.5\Gamma \). The arrows indicate the time-averaged values \( \langle J_{\text{net}} \rangle \) obtained by sampling the current for times \( t > 10/\Gamma \).
propagated using a weak second-order Runge-Kutta scheme \(^2\) with a constant time step \(\delta t = 0.01/\Gamma\). We use \(N_F = 240\) auxiliary modes for all calculations. The resulting time-resolved occupation, \(N(t)\), and net current, \(J_{\text{net}}(t) = \langle J_L(t) - J_R(t) \rangle / 2\), are averaged over 20000 realizations of the stochastic process. Figure 1 shows the averages \(\langle N(t) \rangle\) and \(\langle J_{\text{net}}(t) \rangle\) for \(\kappa = 0.5\Gamma\) and three selected values of \(\eta = 0.5, 1.0, 3.0\Gamma\). We also show the case of no stochastic driving. One sees a transient response to the sudden coupling for times \(t = 0 \ldots 10/\Gamma\) and the eventual settling to a stationary value. In all cases shown in Fig. 1 the stationary current is larger than for the case without any noise; but the dependence on \(\eta\) is non-monotonic.

In order to quantify the stationary current we take the time average \(\langle J_{\text{net}} \rangle\) for the time interval starting at \(t = 10/\Gamma\). Figure 2 shows the obtained time-averaged current as a function of the noise strength \(\eta\) and for various values of the inverse correlation-time \(\kappa\). The time-averaged current exhibits a pronounced maximum as a function of noise strength; the transport through the energy-level is stochastic. This effect remains of the phenomenon of stochastic resonance \(^2\). The observed behavior is a result of additional broadening due to the stochastic driving \(^3\). The current is proportional to the area under the spectral density, \(A(\varepsilon) = -2\text{Im} G'(\varepsilon)\), within the transport window given by \(\{\mu_L, \mu_R\}\), cf. appendix 1. For increasing noise strength the spectral density becomes broader and has more weight in the transport window. However, the height of \(A(\varepsilon)\) decreases at the same time which eventually leads to a decrease in the area in the transport window. These findings are corroborated by the analytical result [Eq. (B3)], which is also shown in Fig. 3. The numerical results agree very well with those results.

**B. Double Quantum Dot**

As a second application we will now discuss the response of a DQD to a voltage pulse. The device consists of two QDs which are coupled in series. Each dot is also coupled to an electron reservoir. This setup resembles a typical experimental situation (see for example \(^1\)).

The DQD is modeled by a two-level system, i.e., one localized energy-level per dot. The device Hamiltonian [Eq. (2)] is then,

\[
H_D = \sum_{d=L,R} \varepsilon_{d}(t) c_d^\dagger c_d + V c_L^\dagger c_r + \text{h.c.},
\]

with “l” and “r” the localized single-electron states. The time-dependent bias-voltage is assumed to act on the energies in the following way: \(\Delta_L(t) = -\Delta_R(t) = V_{\text{bias}}(t)/2\) and \(\varepsilon_L(t) = -\varepsilon_r(t) = V_{\text{bias}}(t)/4\). Initially, the chemical potentials \(\mu_L\) and \(\mu_R\) and the QD energies \(\varepsilon_{l,r}\) are zero. The temperature is \(T = 0.1\Gamma\) for both reservoirs. Since the two dots are coupled in series, the level-width functions contain one non-zero element,

\[
\Gamma_L = \begin{pmatrix} \Gamma(\varepsilon)/2 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_R = \begin{pmatrix} 0 & 0 \\ 0 & \Gamma(\varepsilon)/2 \end{pmatrix}.
\]

The matrix element \(\Gamma(\varepsilon)\) is either constant in the case of WBL, or is taken to be a single Lorentzian \(^{24}\),

\[
\Gamma(\varepsilon) = \Gamma_L W^2 / \varepsilon^2 + W^2.
\]

The latter is compatible with the general ansatz given in Eq. (32) and is chosen such that WBL is attained for \(W \to \infty\). For the time dependence of the bias voltage we take a rectangular pulse, i.e.,

\[
V_{\text{bias}}(t) = \frac{V_{\text{max}}}{2} \left[ \tanh \left( \frac{t}{t_s} \right) - \tanh \left( \frac{t - t_p}{t_s} \right) \right],
\]

which is characterized by the pulse length \(t_p\). The finite switching time \(t_s\) reflects the experimental situation (e.g. as reported in Refs. \(^1\), \(^2\)). In the following calculations we use \(t_s = 1/\Gamma\) and \(V_{\text{max}} = 3\Gamma\). The equations of motion obtained in Sect. 11 for the WBL and the LLWF, respectively, are propagated using a fourth-order Runge-Kutta scheme \(^{25}\) with constant time step \(\delta t = 0.02/\Gamma\). We use \(N_F = 120\) auxiliary modes for all calculations.

Figure 3 shows the numerically obtained current \(J_L\) as a function of time \(t\) for different widths \(W\) in response to the same pulse of length \(t_p = 20/\Gamma\). The current shows a transient behavior at the beginning and after the end of the pulse. For sufficiently long pulses it settles to a new stationary value according to the plateau bias voltage \(V_{\text{bias}} = V_{\text{max}}\). Notice that this situation for a structured reservoir is different from initially having \(\mu_L - \mu_R = V_{\text{max}}\). In the latter case the chemical potential and the center of the level-width function [Eq. (12)] are shifted with respect to each other. The two distinct
The inner part shows spectral densities of left and right levels. Left panel: $V_{bias} = μL - μR$ and $ΔL = ΔR = 0$. Right panel: $V_{bias} = ΔL - ΔR$ and $μL = μR = 0$. Increasing pulse length. Remembering the time dependence as shown in Fig. 3 it is clear that for short pulses $N_p$ is dominantly determined by the transient part of the current. For sufficiently long pulses, however, the main contribution comes from the new stationary current $J_{stat}$ and one expects $N_p \propto t_p$ with a slope given by $J_{stat}$. This asymptotic behavior is shown in Fig. 5 by the straight lines which have been obtained from a linear fit to the numerical data. The slope was fixed by independently calculating $J_{stat}$ using stationary NEGF formalism \cite{8}. The fitting procedure yields the $N_p$-intercept denoted by $N^*_p$ (cf. dashed line in Fig. 5), which provides a measure of how transient the current response actually was. If the current would instantaneously switch to the new stationary value one would get $N_p = J_{stat}t_p$ and the $N_p$-intercept would vanish. Non-vanishing values of $N^*_p$ reflect the additional transient contributions to the current. Figure 6b shows a stronger transient response for smaller $W$ which is in accordance with the observations for the time-resolved current. In any case the net excess is positive since the transient response following the switching-on outbalances the one after the switching-off.

Using the $N_p$-intercept and the stationary current one can also calculate the pulse length that would be necessary to yield the same number of tunneling electrons if the DQD would switch instantaneously, $t_p^* = N^*_p / J_{stat}$ (cf. dashed line in Fig. 5). This quantity is shown in Fig. 6b. It gives a measure for the pulse length at which transient and stationary contributions are of similar size. Therefore, the transient response for pulses with $t_p \gg t_p^*$ becomes negligible.
We have presented a propagation scheme for time-dependent electron transport which is based on non-equilibrium Green functions. It relies on quantities with a single time argument which allows for a straightforward numerical implementation with standard differential equation solvers.

The basis of our scheme is a reformulation of the well-known expression \( \sigma(t) \) for the current \( J(t) \) by means of the density matrix \( \sigma(t) \) and newly introduced current matrices \( \Pi(t) \), cf. Eq. (10). Decomposing these matrices into energy-resolved expressions allows to obtain a closed set of coupled equations of motion for \( \sigma(t) \) and \( \Pi(\varepsilon, t) \). Thereby, one has to consider another energy-resolved quantity \( \Omega(\varepsilon, \varepsilon'; t) \) given in Eq. (22). The equations of motion are given by Eqs. (19), (21) and (23).

For a numerical implementation of these equations we propose using an expansion of the Fermi function and a parameterization of the level-width function by a set of Lorentzians [18]. The error made by truncating the expansion can be reduced by applying a fast converging decomposition [27]. The matrix equations to be solved are (12), (37) and (38), respectively. In the often applied wide-band limit the set of equations simplifies since \( \Omega \) can be found explicitly in terms of the current matrices, cf. Eq. (33).

Finally, we have applied our scheme to two illustrative examples: the randomly fluctuating energy level and the response of a DQD to a voltage pulse. In both cases a non-trivial driving was involved. For the DQD we demonstrated the influence of structured reservoirs on the transient current response. This transient contribution may be quantified by using the number of pulse-induced tunneling electrons [Eq. (14)] as a function of the pulse-length. For the fluctuating energy level we showed a good agreement of our numerical calculations with analytic results obtained for the stationary current. Moreover, we found an enhancement of the current due to the stochastic driving. The study of this effect in more complex systems might lead to interesting new applications. In general, we expect our method to be a valuable tool for investigating time-resolved electron transport in nanoscale devices.

Acknowledgments

We thank Cenap Ates for his valuable comments during the preparation of the manuscript.

APPENDIX A: EXPANSIONS OF SELF-ENERGIES

In order to perform the energy integration in Eqs. (6) we expand the Fermi function in terms of a finite sum over simple poles. This procedure yields the expression given in Eq. (26). The poles are given by \( \chi_p = \mu_p + x_p/\beta = (\chi_p^*)^\ast \). Instead of using the Matsubara expansion [20], with poles \( x_p = i\pi(2p-1) \), we use a partial fraction decomposition of the Fermi function [27], which converges much faster than the standard Matsubara expansion. Furthermore, it allows to estimate the error made by truncating the sum [Eq. (25)] at \( N_F \) terms. For this decomposition the poles \( x_p = \pm 2\sqrt{\frac{p}{\Gamma}} \) are given by the eigenvalues \( z_p \) of the \( N_F \times N_F \) matrix [27]

\[
Z_{ij} = 2i(2i-1)\delta_{j,i+1} - 2N_F(2N_F-1)\delta_{iN_F}.
\]

We take the branch of the root \( \sqrt{z_p} \) such that \( \text{Im}(x_p) > 0 \) for all \( p \). Thus all poles \( \chi_p^\ast \) are in the upper (lower) complex plane.

Given the expansion [Eq. (25)] one can evaluate the energy integrals by a contour integration in the upper or lower complex plane depending on the sign of \( t - t_1 \). Thereby, the integration becomes a (finite) sum of the residues.

APPENDIX B: NOISE-AVERAGED CURRENT FOR RLM

The noise-averaged net-current, \( \langle J_{\text{net}}(t) \rangle = \langle J_L(t) - J_R(t) \rangle / 2 \), can be obtained from the general expression for the time-dependent current [Eq. (4)],

\[
\langle J_{\text{net}}(t) \rangle = \epsilon \text{Re Tr} \left\{ \int_{-\infty}^{\infty} dt_1 \langle G(t, t_1) \rangle \right\}
\times \left[ \Sigma_L^<(t_1, t) - \Sigma_R^<(t_1, t) \right],
\]

where a symmetric coupling, \( \Gamma_L(\varepsilon, t_1, t) = \Gamma_R(\varepsilon, t_1, t) \), is assumed. For the resonant level model all quantities are scalars and in particular for the setting considered in Sec. III A one has

\[
G^t(t, t_1) = -i\Theta(t-t_1) \exp \left[ -i \int_{t_1}^{t} dt' \varepsilon d(t') - \frac{\Gamma}{2}(t-t_1) \right].
\]
In order to evaluate Eq. (131) we need the average of the fluctuating exponential function in $G^r(t, t_1)$ which is obtained by using the cumulant expansion, i.e.,

$$\langle \exp \left[ -i \int_{t_1}^{t} dt' \varepsilon_d(t') \right] \rangle = \exp \left[ -\frac{1}{2} \int_{t_1}^{t} d\tau_1 \int_{t_1}^{t} d\tau_2 \langle \varepsilon_d(\tau_1) \varepsilon_d(\tau_2) \rangle \right]$$

$$= \exp \left[ -\frac{1}{2} \int d\omega \frac{c(\omega)}{2\pi} \left| \int_{t_1}^{t} d\tau e^{-i\omega\tau} \right|^2 \right]$$

$$= \exp \left[ -\frac{1}{2} \int d\omega \frac{c(\omega)}{2\pi} \frac{4\sin^2\left(\frac{\omega(t-t_1)}{2}\right)}{\omega^2} \right] . \tag{B3}$$

In the derivation we have used the properties of the noise [Eqs. (91)] and introduced the Fourier transform of $c(\tau_1 - \tau_2)$ which is denoted by $c(\omega)$.

Thus, the noise-averaged retarded Green function does only depend on the time difference and the time-averaged current is given by a Landauer-type expression [7]

$$\langle J_{\text{net}}(t) \rangle = \frac{e\Gamma}{2} \int \frac{d\varepsilon}{2\pi} \left[ f_L(\varepsilon) - f_R(\varepsilon) \right] A(\varepsilon) , \tag{B4}$$

where the spectral density $A(\varepsilon)$ is given by the time and noise averaged retarded Green function,

$$A(\varepsilon) = -2 \text{Im} \int_{0}^{\infty} d\tau \langle G^r(t, t-\tau) \rangle e^{i\varepsilon\tau}$$

$$= \int_{-\infty}^{\infty} d\tau e^{i\varepsilon\tau} - \Gamma |\tau|/2 \tag{B5}$$

$$\exp \left[ -\frac{1}{2} \int d\omega \frac{C(\omega)}{2\pi} \frac{4\sin^2\left(\omega|\tau|/2\right)}{\omega^2} \right] .$$

For white noise one has $c(\omega) = \gamma$ and the fluctuations lead to a trivial broadening of the spectral density.