

Propagation scheme for nonequilibrium dynamics of electron transport in nanoscale devices

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A closed set of coupled equations of motion for the description of time-dependent electron transport is derived. It provides the time evolution of energy-resolved quantities constructed from nonequilibrium Green's functions. By means of an auxiliary-mode expansion a viable propagation scheme for finite temperatures is obtained, which allows to study arbitrary time dependences and structured reservoirs. Two illustrative examples are presented.

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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 dots³ 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 nonequilibrium Green's 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^{9–11} combining Floquet theory and NEGF formalism have been developed and allow going beyond WBL. In order to overcome the limitations of the special form of driving and of the WBL, schemes based on the traditional approach,⁷ but working directly in the time domain have been put forward.^{12,13} All time convolutions, which result from the projection onto the device states, are transformed into matrix-matrix multiplications using a time-discretization scheme. In contrast, the formalism presented in Refs. 14 and 15 is based on propagating the wave function of the full system (device and reservoirs). This is accomplished by using the Cayley propagator and then projecting on the subsystem of interest. This formalism provides a natural way to work within the so-called partition-free approach, where the time-dependent voltage pulse is considered to act on the total system.

In this paper we present a general propagation scheme which is also based on the NEGF formalism⁷ and allows to obtain device-related observables and the electric current as a function of time. Our formulation, however, relies on a set of coupled equations of motion for quantities with only *one* time argument. In this way we can avoid time convolutions and standard methods for integrating the equations may be applied. As with the standard formulation, the key issue consists in performing integrals over reservoir states which

eventually lead to tunneling self-energies. In this context we propose using an auxiliary-mode expansion which allows to treat finite temperatures. We provide a numerical implementation of our scheme for two relevant cases—the wide-band limit and a level-width function given by a sum of Lorentzians. The methods are applied to transport through a randomly fluctuating level and the transient response of a DQD to a voltage pulse.

In the remaining part of the introduction we briefly discuss the general setup (Sec. I A) and then repeat the findings of the standard NEGF formalism in the context of our propagation scheme (Sec. I B).

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 noninteracting electrons and the Hamiltonian reads

$$H_R = \sum_{\alpha \in L, R} \sum_k \varepsilon_{\alpha k}(t) b_{\alpha k}^\dagger b_{\alpha k} \quad (3)$$

with single-particle energies of the form $\varepsilon_{\alpha k}(t) = \varepsilon_{\alpha k}^0 + \Delta_{\alpha k}(t)$. Finally, the coupling Hamiltonian is

$$H_{DR} = \sum_n \sum_{\alpha k} T_{kn}^\alpha(t) b_{\alpha k}^\dagger c_n + \text{H.c.} \quad (4)$$

with $\{T_{kn}^\alpha\}$ denoting the couplings between device and reservoir $\alpha = L, R$; $\{b_{\alpha k}^\dagger\}$ and $\{b_{\alpha k}\}$ are electron creation and annihilation operators for reservoir states, respectively.

Regarding the time dependence of the reservoirs and the device we adopt the Caroli partition scheme,¹⁶ i.e., all subsystems are separated at $t = -\infty$ and in their respective equilibrium state. Any time dependence only sets in after even-

tually coupling the different parts. Consequently, the single-particle occupation probability in the reservoirs is determined by $\varepsilon_{\alpha k}^0$; 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 nonequilibrium Green's functions

By applying the Keldysh formalism to nonequilibrium Green's functions it is possible to obtain a general formula for the time-dependent current in the setup introduced in Sec. I A. The current J_α through the barrier connecting lead α and the device is given by^{7,8}

$$J_\alpha(t) = 2e \operatorname{Re} \operatorname{Tr} \left\{ \int_{-\infty}^{\infty} dt_1 [\mathbf{G}^<(t, t_1) \mathbf{\Sigma}_\alpha^a(t_1, t) + \mathbf{G}^r(t, t_1) \mathbf{\Sigma}_\alpha^<(t_1, t)] \right\}. \quad (5)$$

Throughout the paper we adopt units with $\hbar=1$. In Eq. (5) $\mathbf{G}^<$ and \mathbf{G}^r are lesser and retarded Green's functions and $\mathbf{\Sigma}^a$ and $\mathbf{\Sigma}^<$ are advanced and lesser self-energies, respectively. All boldface quantities are matrices related to the device states, e.g., $\mathbf{G}^<(t, t_1) \equiv G_{nm}^<(t, t_1)$. Products are to be understood as matrix multiplications. The greater and lesser self-energies are explicitly given by

$$\mathbf{\Sigma}_\alpha^>(t_1, t) = -i \int \frac{d\varepsilon}{2\pi} \bar{f}_\alpha(\varepsilon) e^{-i\varepsilon(t_1-t)} \Gamma_\alpha(\varepsilon, t_1, t), \quad (6a)$$

$$\mathbf{\Sigma}_\alpha^<(t_1, t) = i \int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon) e^{-i\varepsilon(t_1-t)} \Gamma_\alpha(\varepsilon, t_1, t). \quad (6b)$$

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 α with the chemical potential μ_α and inverse temperature $\beta = (k_B T)^{-1}$ at $t_0 = -\infty$. It is $\bar{f}_\alpha(\varepsilon) = 1 - f_\alpha(\varepsilon)$. Using a relation for two-time functions

$$X^{r,a}(t, t') = \pm \Theta(\pm t \mp t') [X^>(t, t') - X^<(t, t')], \quad (7)$$

which applies to Green's 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 Γ_α in Eqs. (6) depends on the density of states $\rho_\alpha(\varepsilon)$ of reservoir α and the coupling $T_{\alpha n}(\varepsilon)$ of device level n and the reservoir state at energy ε

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

Replacing the advanced and retarded quantities in Eq. (5) by using Eq. (7) one can rewrite the expression for the current in a very compact form

$$J_\alpha(t) = 2e \operatorname{Re} \operatorname{Tr} \{ \mathbf{\Pi}_\alpha(t) \}. \quad (9)$$

The *current matrices* $\mathbf{\Pi}_\alpha(t)$ are given by the following expression:

$$\mathbf{\Pi}_\alpha(t) = \int_{t_0}^t dt_2 [\mathbf{G}^>(t, t_2) \mathbf{\Sigma}_\alpha^<(t_2, t) - \mathbf{G}^<(t, t_2) \mathbf{\Sigma}_\alpha^>(t_2, t)], \quad (10)$$

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 particular approach presented in this paper consists in considering $\mathbf{\Pi}_\alpha(t)$ as an independent entity. In particular, opposed to correlation functions such as $\mathbf{G}^\cong(t, t_2)$ the current matrices $\mathbf{\Pi}_\alpha(t)$ 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, $\boldsymbol{\sigma}(t) = \operatorname{Im} \mathbf{G}^<(t, t)$. The expectation value is then given by

$$\langle O_D(t) \rangle = \operatorname{Tr}_D \{ O_D \boldsymbol{\sigma}(t) \}. \quad (11)$$

Similar to the current matrices $\mathbf{\Pi}_\alpha(t)$ the density matrix only depends on a single time argument and one has the following equation of motion:

$$i \frac{\partial}{\partial t} \boldsymbol{\sigma}(t) = [\mathbf{H}(t), \boldsymbol{\sigma}(t)]_- + i \sum_\alpha [\mathbf{\Pi}_\alpha(t) + \mathbf{\Pi}_\alpha^\dagger(t)], \quad (12)$$

which depends on the current matrices $\mathbf{\Pi}_\alpha(t)$. The boldface Hamiltonian $\mathbf{H}(t) \equiv [H_D]_{nm}$ is obtained from the device Hamiltonian in Eq. (2). Equation (12) is found by using $\mathbf{G}^<(t', t) = -[\mathbf{G}^<(t, t')]^\dagger$ and from the equations of motion for greater and lesser Green's functions $\mathbf{G}^>$ and $\mathbf{G}^<$

$$\begin{aligned} i \frac{\partial}{\partial t} \mathbf{G}^\cong(t, t') &= \mathbf{H}(t) \mathbf{G}^\cong(t, t') + \int dt_2 \mathbf{\Sigma}_{\text{tot}}^r(t, t_2) \mathbf{G}^\cong(t_2, t') \\ &+ \int dt_2 \mathbf{\Sigma}_{\text{tot}}^\cong(t, t_2) \mathbf{G}^a(t_2, t'). \end{aligned} \quad (13)$$

The total self-energies $\mathbf{\Sigma}_{\text{tot}}^{\cong,r}$ are sums of the tunneling self-energies for each reservoir. The Green's 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 introducing 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. 7 for the noninteracting resonant-level model. For notational 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

$$\Gamma_{\alpha}(\varepsilon,t_1,t)=u_{\alpha}^*(t_1)u_{\alpha}(t)\Gamma_{\alpha}(\varepsilon)\exp\left\{i\int_{t_1}^t dt_2\Delta_{\alpha}(\varepsilon,t_2)\right\}. \quad (14)$$

Next, we define *energy-resolved self-energies* as

$$\Sigma_{\alpha}^{>}(\varepsilon;t_1,t)=-iu_{\alpha}^*(t_1)\bar{f}_{\alpha}(\varepsilon)e^{-i\varepsilon(t_1-t)}\Gamma_{\alpha}(\varepsilon)\times\exp\left\{i\int_{t_1}^t dt_2\Delta_{\alpha}(\varepsilon,t_2)\right\}, \quad (15a)$$

$$\Sigma_{\alpha}^{<}(\varepsilon;t_1,t)=iu_{\alpha}^*(t_1)f_{\alpha}(\varepsilon)e^{-i\varepsilon(t_1-t)}\Gamma_{\alpha}(\varepsilon)\times\exp\left\{i\int_{t_1}^t dt_2\Delta_{\alpha}(\varepsilon,t_2)\right\}. \quad (15b)$$

In terms of these expressions the full self-energies are given by

$$\Sigma_{\alpha}^{\Xi}(\varepsilon;t_1,t)=u_{\alpha}(t)\int d\varepsilon\Sigma_{\alpha}^{\Xi}(\varepsilon;t_1,t), \quad (16)$$

which follows from Eq. (6). Using the definitions above we introduce *energy-resolved current matrices*

$$\Pi_{\alpha}(\varepsilon;t)=\int_{t_0}^t dt_2[\mathbf{G}^{>}(t,t_2)\Sigma_{\alpha}^{<}(\varepsilon;t_2,t)-\mathbf{G}^{<}(t,t_2)\Sigma_{\alpha}^{>}(\varepsilon;t_2,t)]. \quad (17)$$

From Eq. (17) one finds $\Pi_{\alpha}(\varepsilon;t_0)=\mathbf{0}$. The expression for the current given by Eq. (9) becomes

$$J_{\alpha}(t)=2e\operatorname{Re}\sum_n u_{\alpha}(t)\int d\varepsilon\Pi_{\alpha,nn}(\varepsilon;t). \quad (18)$$

Therefore, the diagonal elements $\Pi_{\alpha,nn}(\varepsilon;t)$ may be interpreted as the current flowing from the reservoir state at energy ε 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 $\boldsymbol{\sigma}$ of the device becomes

$$i\frac{\partial}{\partial t}\boldsymbol{\sigma}(t)=[\mathbf{H}(t),\boldsymbol{\sigma}(t)]_-+i\sum_{\alpha}\int d\varepsilon[u_{\alpha}(t)\Pi_{\alpha}(\varepsilon;t)+u_{\alpha}^*(t)\Pi_{\alpha}^{\dagger}(\varepsilon;t)], \quad (19)$$

which now contains the energy-resolved current matrices.

Due to the definitions, Eq. (14), of the energy-resolved self-energies, their time derivatives

$$\frac{\partial}{\partial t}\Sigma_{\alpha}^{\Xi}(\varepsilon;t_1,t)=i[\varepsilon+\Delta_{\alpha}(\varepsilon,t)]\Sigma_{\alpha}^{\Xi}(\varepsilon;t_1,t) \quad (20)$$

and by using Eq. (13), one gets an equation of motion for the energy-resolved current matrices

$$i\frac{\partial}{\partial t}\Pi_{\alpha}(\varepsilon;t)=-\frac{i}{2\pi}u_{\alpha}^*(t)[\boldsymbol{\sigma}(t)-f_{\alpha}(\varepsilon)]\Gamma_{\alpha}(\varepsilon)+\{\mathbf{H}(t)-[\varepsilon+\Delta_{\alpha}(\varepsilon,t)]\}\Pi_{\alpha}(\varepsilon;t)+\sum_{\alpha'}u_{\alpha'}^*(t)\int d\varepsilon'\Omega_{\alpha\alpha'}(\varepsilon,\varepsilon';t), \quad (21)$$

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's functions, which give rise to a double-time integral. Consequently, its definition is

$$\Omega_{\alpha\alpha'}(\varepsilon,\varepsilon';t)=\int_{t_0}^t dt_2\int_{t_0}^t dt_1\Sigma_{\alpha'}^{\dagger}(\varepsilon';t_2,t_1)\times[\mathbf{G}^{>}(t_1,t_2)\Sigma_{\alpha}^{<}(\varepsilon;t_2,t)-\mathbf{G}^{<}(t_1,t_2)\Sigma_{\alpha}^{>}(\varepsilon;t_2,t)]-\int_{t_0}^t dt_2\int_{t_0}^{t_2} dt_1[\Sigma_{\alpha'}^{<}(\varepsilon';t_1,t_1)\mathbf{G}^{\mathbf{a}}(t_1,t_2)\Sigma_{\alpha}^{>}(\varepsilon;t_2,t)-\Sigma_{\alpha'}^{>}(\varepsilon';t_1,t_1)\mathbf{G}^{\mathbf{a}}(t_1,t_2)\Sigma_{\alpha}^{<}(\varepsilon;t_2,t)]. \quad (22)$$

We replace the retarded self-energies and the advanced Green's 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)

$$i\frac{\partial}{\partial t}\Omega_{\alpha\alpha'}(\varepsilon,\varepsilon';t)=\frac{1}{2\pi}[u_{\alpha'}(t)\Gamma_{\alpha'}(\varepsilon')\Pi_{\alpha}(\varepsilon;t)+\Pi_{\alpha'}^{\dagger}(\varepsilon';t)\Gamma_{\alpha}(\varepsilon)u_{\alpha}^*(t)]+\{[\varepsilon'+\Delta_{\alpha'}(\varepsilon',t)]-[\varepsilon+\Delta_{\alpha}(\varepsilon,t)]\}\Omega_{\alpha\alpha'}(\varepsilon,\varepsilon';t) \quad (23)$$

with the initial conditions $\Omega_{\alpha\alpha'}(\varepsilon,\varepsilon';t_0)=\mathbf{0}$. The equations of motion given by Eqs. (19), (21), and (23) provide a closed description of the nonequilibrium 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

$$\varphi_{\alpha}=-i\Pi_{\alpha} \quad \text{and} \quad \varphi_{\alpha'\alpha}=-i\Omega_{\alpha\alpha'} \quad (24)$$

renders their equations identical to the ones given above. This provides an independent verification of the density-matrix approach¹⁷ and shows that the hierarchy derived therein yields the exact dynamics for noninteracting electrons under the assumptions stated above.

The full single-particle density matrix has a size of $(N_{\text{D}}+N_{\text{R}})^2$, 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 $N_{\text{D}}^2\times(N_{\text{R}}+1)^2$

quantities with $\mathbf{\Pi}$ and $\mathbf{\Pi}^\dagger$ 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 section 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 bosonic¹⁸ 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 $\mathbf{\Omega}_{\alpha\alpha'}$. 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

$$f_\alpha(\varepsilon) \approx \frac{1}{2} - \frac{1}{\beta} \sum_{p=1}^{N_F} \left(\frac{1}{\varepsilon - \chi_{\alpha p}^+} + \frac{1}{\varepsilon - \chi_{\alpha p}^-} \right) \quad (25)$$

with $\chi_{\alpha p}^\pm = \mu_\alpha \pm x_p/\beta$ and $\text{Im } x_p > 0$. The well-known Matsubara expansion²⁰ 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 [Eq. (6)] and the expansion of the Fermi function [Eq. (25)] one obtains for $t > t_1$

$$\begin{aligned} \Sigma_\alpha^>(t_1, t) &= -i \frac{1}{2} \Gamma_\alpha |u_\alpha(t)|^2 \delta(t - t_1) \\ &+ u_\alpha(t) \sum_p \frac{1}{\beta} \Gamma_\alpha u_\alpha^*(t_1) e^{i \int_{t_1}^t dt_2 \chi_{\alpha p}^+(t_2)}, \end{aligned} \quad (26)$$

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

$$\begin{aligned} \Sigma_\alpha^<(t_1, t) &= i \frac{1}{2} \Gamma_\alpha |u_\alpha(t)|^2 \delta(t - t_1) \\ &+ u_\alpha(t) \sum_p \frac{1}{\beta} \Gamma_\alpha u_\alpha^*(t_1) e^{i \int_{t_1}^t dt_2 \chi_{\alpha p}^+(t_2)}. \end{aligned} \quad (27)$$

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.,

$$\Sigma_\alpha^{\approx}(t_1, t) = \mp i \frac{1}{2} \Gamma_\alpha |u_\alpha(t)|^2 \delta(t - t_1) + u_\alpha(t) \sum_p \Sigma_{\alpha p}(t_1, t), \quad (28a)$$

$$\Sigma_{\alpha p}(t_1, t) = \frac{1}{\beta} \Gamma_\alpha u_\alpha^*(t_1) e^{i \int_{t_1}^t dt_2 \chi_{\alpha p}^+(t_2)}, \quad (28b)$$

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 [Eq. (10)]

$$\mathbf{\Pi}_\alpha(t) = \frac{1}{4} |u_\alpha(t)|^2 [1 - 2\sigma(t)] \Gamma_\alpha + u_\alpha(t) \sum_p \mathbf{\Pi}_{\alpha p}(t) \quad (29)$$

and obtain an expansion in terms of *auxiliary current matrices*

$$\mathbf{\Pi}_{\alpha p}(t) = \int_{t_0}^t dt_2 [\mathbf{G}^<(t, t_2) \Sigma_{\alpha p}(t_2, t) - \mathbf{G}^>(t, t_2) \Sigma_{\alpha p}(t_2, t)]. \quad (30)$$

Their equation of motion is easily found

$$i \frac{\partial}{\partial t} \mathbf{\Pi}_{\alpha p}(t) = \frac{1}{\beta} \Gamma_\alpha u_\alpha^*(t) + \left[\mathbf{H}(t) - \frac{i}{2} \Gamma(t) - \chi_{\alpha p}^+(t) 1 \right] \mathbf{\Pi}_{\alpha p}(t), \quad (31)$$

where $\Gamma(t) = \sum_{\alpha'} |u_{\alpha'}(t)|^2 \Gamma_{\alpha'}$. The coupled equations of motion Eqs. (12) and (31) allow with Eq. (29) for a complete description of the nonequilibrium dynamics of the device. Comparing Eqs. (21) and (31) suggests that $\mathbf{\Omega}_{\alpha p, \alpha' p'}(t) = -\frac{i}{2} u_{\alpha'}(t) \Gamma_{\alpha'} \mathbf{\Pi}_{\alpha p}(t) \delta_{pp'}$. Thus, an additional equation of motion for $\mathbf{\Omega}$ 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

$$\Gamma_\alpha(\varepsilon) = \sum_{\ell=1}^{N_L} \left(\frac{\Gamma_{\alpha\ell}^+}{\varepsilon - \varepsilon_{\alpha\ell} - iW_{\alpha\ell}} + \frac{\Gamma_{\alpha\ell}^-}{\varepsilon - \varepsilon_{\alpha\ell} + iW_{\alpha\ell}} \right) \quad (32)$$

with $W_{\alpha\ell} > 0$ and $\Gamma_{\alpha\ell}^\pm = \mp \frac{i}{2} \Gamma_{\alpha\ell} W_{\alpha\ell}$. Equation (32) might be used as a parametrization of an arbitrary level-width function.^{18,19} 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 $t > t_1$

$$\begin{aligned} \Sigma_{\alpha}^{>}(t_1, t) = & + u_{\alpha}^*(t_1) u_{\alpha}(t) \left[\sum_{\ell} \Gamma_{\alpha\ell}^+ \bar{f}_{\alpha\ell}^P e^{-i(\varepsilon_{\alpha\ell} + iW_{\alpha\ell})(t_1 - t)} \right. \\ & \left. + \sum_p \frac{1}{\beta} \Gamma_{\alpha}(\chi_{ap}^+) e^{-i\chi_{ap}^+(t_1 - t)} \right] \\ & \times \exp \left[i \int_{t_1}^t dt_2 \Delta_{\alpha}(\varepsilon, t_2) \right], \end{aligned} \quad (33a)$$

$$\begin{aligned} \Sigma_{\alpha}^{<}(t_1, t) = & - u_{\alpha}^*(t_1) u_{\alpha}(t) \left[\sum_{\ell} \Gamma_{\alpha\ell}^+ f_{\alpha\ell}^P e^{-i(\varepsilon_{\alpha\ell} + iW_{\alpha\ell})(t_1 - t)} \right. \\ & \left. - \sum_p \frac{1}{\beta} \Gamma_{\alpha}(\chi_{ap}^+) e^{-i\chi_{ap}^+(t_1 - t)} \right] \\ & \times \exp \left[i \int_{t_1}^t dt_2 \Delta_{\alpha}(\varepsilon, t_2) \right], \end{aligned} \quad (33b)$$

where $f_{\alpha\ell}^P = f_{\alpha}(\varepsilon_{\alpha\ell} + iW_{\alpha\ell})$ indicates that the expansion given in Eq. (25) should be used to calculate the Fermi function at the position of the pole ℓ . 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 ℓ yielding a single index $x = \{\ell, p\}$. The coefficients and exponents are combined in a similar way

$$\Gamma_{\alpha x}^{>,\pm} = \left\{ \pm \Gamma_{\alpha\ell}^{\pm} \bar{f}_{\alpha}(\varepsilon_{\alpha\ell} \pm iW_{\alpha\ell}), \pm \frac{1}{\beta} \Gamma_{\alpha}(\chi_{ap}^{\pm}) \right\}, \quad (34a)$$

$$\Gamma_{\alpha x}^{<,\pm} = \left\{ \mp \Gamma_{\alpha\ell}^{\pm} f_{\alpha}(\varepsilon_{\alpha\ell} \pm iW_{\alpha\ell}), \pm \frac{1}{\beta} \Gamma_{\alpha}(\chi_{ap}^{\pm}) \right\}, \quad (34b)$$

$$\chi_{\alpha x}^{\pm} = \{\varepsilon_{\alpha\ell} \pm iW_{\alpha\ell}, \chi_{ap}^{\pm}\}. \quad (34c)$$

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

$$\Sigma_{\alpha}^{\cong}(t_1, t) = u_{\alpha}(t) \sum_x \Sigma_{\alpha x}^{\cong}(t_1, t), \quad (35a)$$

$$\Sigma_{\alpha x}^{\cong}(t_1, t) = u_{\alpha}^*(t_1) \Gamma_{\alpha x}^{\cong,+} e^{i \int_{t_1}^t dt_2 \chi_{\alpha x}^+(t_2)}, \quad (35b)$$

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

$$\mathbf{\Pi}_{\alpha x}(t) = \int_{t_0}^t dt_2 [\mathbf{G}^{>}(t, t_2) \Sigma_{\alpha x}^{<}(t_2, t) - \mathbf{G}^{<}(t, t_2) \Sigma_{\alpha x}^{>}(t_2, t)]. \quad (36)$$

Their equation of motion is then given by

$$\begin{aligned} i \frac{\partial}{\partial t} \mathbf{\Pi}_{\alpha x}(t) = & u_{\alpha}^*(t) \Gamma_{\alpha x}^{<,+} + u_{\alpha}^*(t) \boldsymbol{\sigma}(t) (\Gamma_{\alpha x}^{>,+} - \Gamma_{\alpha x}^{<,+}) \\ & + [\mathbf{H}(t) - \chi_{\alpha x}^+(t)] \mathbf{\Pi}_{\alpha x}(t) + \sum_{\alpha' x'} u_{\alpha'}^*(t) \boldsymbol{\Omega}_{\alpha x, \alpha' x'}(t). \end{aligned} \quad (37)$$

The initial condition $\mathbf{\Pi}_{\alpha x}(t_0) = \mathbf{0}$ follows from Eq. (36). Notice the similarity to the energy-resolved current matrices given by Eq. (21). In particular, we also have a two-mode quantity $\boldsymbol{\Omega}_{\alpha x, \alpha' x'}$ appearing in the equation of motion. Its definition is again in full analogy to the energy-resolved case given in Eq. (22) but with $\Sigma_{\alpha'}^{\cong}(\varepsilon'; t, t_1)$ replaced by $\Sigma_{\alpha' x'}^{\cong}(t, t_1)$. Also the equation of motion is similar to the energy-resolved case [Eq. (23)]

$$\begin{aligned} i \frac{\partial}{\partial t} \boldsymbol{\Omega}_{\alpha x, \alpha' x'}(t) = & i u_{\alpha'}(t) (\Gamma_{\alpha' x'}^{>,-} - \Gamma_{\alpha' x'}^{<,-}) \mathbf{\Pi}_{\alpha x}(t) + i \mathbf{\Pi}_{\alpha' x'}^{\dagger}(t) \\ & \times (\Gamma_{\alpha x}^{>,+} - \Gamma_{\alpha x}^{<,+}) u_{\alpha}^*(t) \\ & + [\chi_{\alpha' x'}^-(t) - \chi_{\alpha x}^+(t)] \boldsymbol{\Omega}_{\alpha x, \alpha' x'}(t). \end{aligned} \quad (38)$$

At $t = t_0$ one finds $\boldsymbol{\Omega}_{\alpha x, \alpha' x'}(t_0) = \mathbf{0}$. It is interesting to notice that for $x = p$ and $x' = p'$, i.e., both indices represent an auxiliary mode resulting from the Fermi-function expansion [Eq. (25)], one gets $\frac{\partial}{\partial t} \boldsymbol{\Omega}_{\alpha p, \alpha' p'}(t) \propto \boldsymbol{\Omega}_{\alpha p, \alpha' p'}(t)$. Taking the initial condition into account it follows that $\boldsymbol{\Omega}_{\alpha p, \alpha' p'}(t) \equiv \mathbf{0}$ for all times. This is consistent with the energy-resolved expression [Eq. (23)] where any reference to the Fermi function is absent. Consequently, instead of propagating $(N_L + N_F) \times (N_L + N_F)$ $\boldsymbol{\Omega}$ matrices we only need to consider $N_L \times (N_L + 2N_F)$ matrices for each reservoir index α . 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.²¹ An analytic expression for the current is given in Appendix B.

The device Hamiltonian [Eq. (2)] is simply

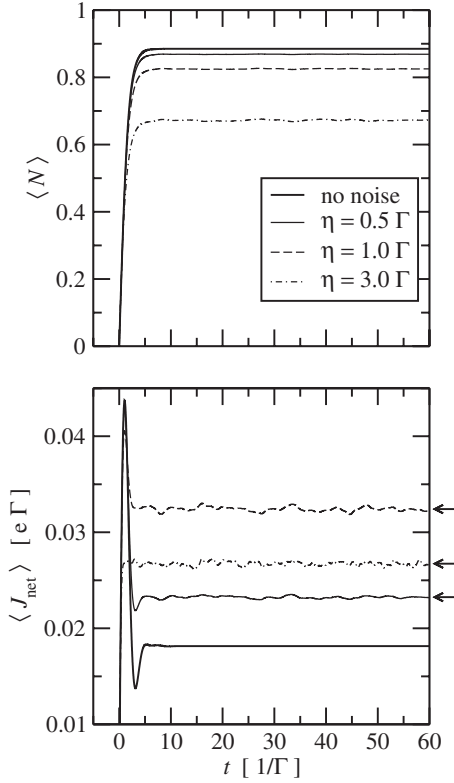


FIG. 1. Time-resolved occupation $\langle N \rangle$ and net current $\langle J_{\text{net}} \rangle$ for different values of the noise amplitude. Noise averages are obtained from 20 000 realizations and $\kappa = 0.5\Gamma$. The arrows indicate the time-averaged values $\langle J_{\text{net}} \rangle$ obtained by sampling the current for times $t > 10/\Gamma$.

$$H_D = \varepsilon_d(t)c_d^\dagger c_d, \quad (39)$$

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

$$\langle \varepsilon_d(t) \rangle = 0, \quad (40a)$$

$$\langle \varepsilon_d(t)\varepsilon_d(t') \rangle = c(t-t'). \quad (40b)$$

Here, we take $\varepsilon_d(t)$ as realization of an Ornstein-Uhlenbeck (OU) process, which yields for the correlation function $c(t-t') = \frac{\eta^2}{2\kappa} \exp[-\kappa(t-t')]$. The OU process is characterized by two parameters, the inverse correlation time κ and the noise amplitude η .²²

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

The equations of motion obtained in Sec. II B are propagated using a weak second-order Runge-Kutta scheme²³ with a constant time step²⁴ $\delta t = 0.01/\Gamma$. We use $N_F = 240$ auxiliary modes for all calculations. The resulting time-resolved occu-

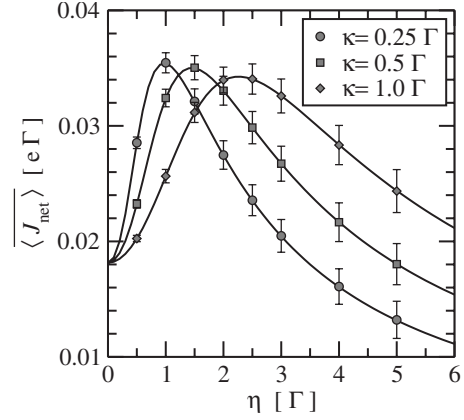


FIG. 2. Time-averaged current vs noise amplitude for different values of the inverse noise correlation time κ . Noise averages are obtained from 20 000 realizations. Error bars indicate 95% confidence interval for the sample mean. Full lines denote the analytical result given by Eq. (B4).

pation, $N(t)$, and net current, $J_{\text{net}}(t) = [J_L(t) - J_R(t)]/2$, are averaged over 20 000 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 $0 \leq t \leq 10/\Gamma$ 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 η is nonmonotonic.

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 η and for various values of the inverse correlation time κ . The time-averaged current exhibits a pronounced maximum as a function of noise strength; the transport through the energy level is stochastically enhanced. This effect reminds of the phenomenon of stochastic resonance.²⁵ The observed behavior is a result of additional broadening due to the stochastic driving.⁸ The current is proportional to the area under the spectral density, $A(\varepsilon) = -2\text{Im} G^r(\varepsilon)$, within the transport window given by $\{\mu_L, \mu_R\}$, cf. Appendix B. 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. (B4)], which is also shown in Fig. 2. 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, Ref. 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

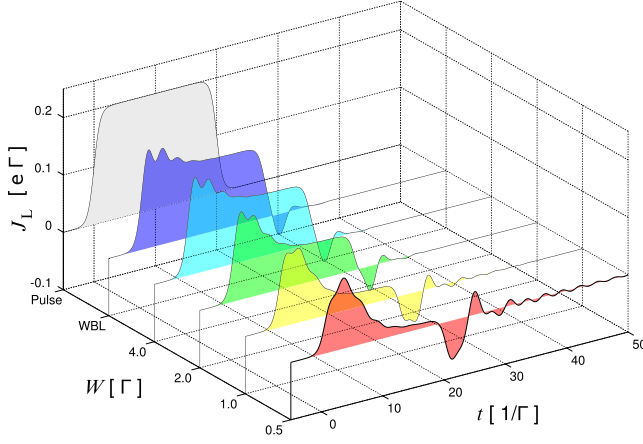


FIG. 3. (Color online) Time-resolved current through left barrier J_L for different values of W in Eq. (42) driven by a bias-voltage pulse according to Eq. (43) with $V_{\text{bias}}=3\Gamma$, $t_s=1/\Gamma$, and $t_p=20/\Gamma$. The WBL corresponds to $W\rightarrow\infty$.

$$H_D = \sum_{d=l,r} \varepsilon_d(t) c_d^\dagger c_d + V c_l^\dagger c_r + \text{H.c.} \quad (41)$$

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 μ_L and μ_R and the QD energies $\varepsilon_{l,r}$ are zero. The temperature is $k_B T=0.1\Gamma$ for both reservoirs. Since the two dots are coupled in series, the level-width functions contain one nonzero element

$$\mathbf{\Gamma}_L = \begin{bmatrix} \Gamma(\varepsilon)/2 & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}_R = \begin{bmatrix} 0 & 0 \\ 0 & \Gamma(\varepsilon)/2 \end{bmatrix}.$$

The matrix element $\Gamma(\varepsilon)$ is either constant in the case of WBL or is taken to be a single Lorentzian²⁶

$$\Gamma(\varepsilon) = \Gamma \frac{W^2}{\varepsilon^2 + W^2}. \quad (42)$$

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

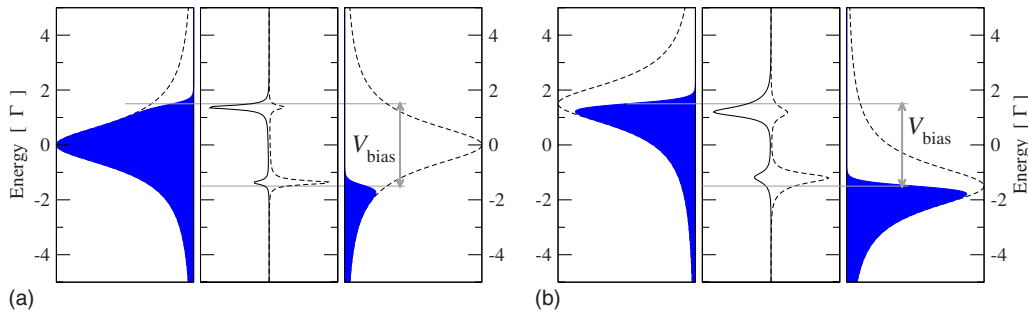


FIG. 4. (Color online) Energy scheme for $W=\Gamma$ at the plateau of the pulse with $V_{\text{bias}}=V_{\text{max}}=3\Gamma$. Outermost parts show $f_\alpha(\varepsilon)\Gamma(\varepsilon)$ for $\alpha=L,R$ (blue/dark-shaded areas). The inner part shows spectral densities of left and right levels. Left panel: $V_{\text{bias}}=\mu_L-\mu_R$ and $\Delta_L=\Delta_R=0$. Right panel: $V_{\text{bias}}=\Delta_L-\Delta_R$ and $\mu_L=\mu_R=0$.

$$V_{\text{bias}}(t) = \frac{V_{\text{max}}}{2} \left[\tanh\left(\frac{t}{t_s}\right) - \tanh\left(\frac{t-t_p}{t_s}\right) \right], \quad (43)$$

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 and 3). In the following calculations we use $t_s=1/\Gamma$ and $V_{\text{max}}=3\Gamma$. The equations of motion obtained in Sect. II for the WBL and the LLWF, respectively, are propagated using a fourth-order Runge-Kutta scheme²⁷ 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. (42)] are shifted with respect to each other. The two distinct situations are illustrated in Fig. 4. We adopt the physical relevant situation shown in the right panel (see also Ref. 7).

At any rate, the stationary current is found to vanish for $W\rightarrow 0$, which is an artifact of the level-width function given by Eq. (42). The ringing behavior at the beginning and after the pulse is qualitatively similar for all values of W . However, for small W the damping of the current oscillations is weaker. In experiments the direct observation of the ringing may be obscured by capacitive effects or the resolution of the ampere meter. Therefore, one considers the time-averaged or time-integrated current as a function of pulse length.^{3,28} The latter yields the number of pulse-induced tunneling electrons

$$N_p(t_p) = \int_{-\infty}^{\infty} dt [J(t) - J_0], \quad (44)$$

where J_0 is the stationary current without pulse and $J(t)=J_L(t)$. In Fig. 5 we show N_p as a function of pulse length t_p for various values of W . One observes an increase in the number of tunneling electrons with 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,

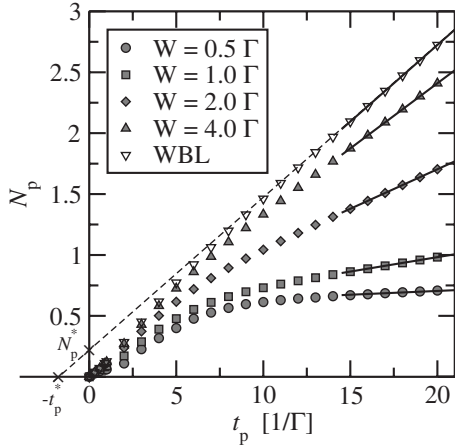


FIG. 5. Number of pulse-induced tunneling electrons N_p vs pulse length t_p . Symbols indicate numerical results for different values of W in Eq. (42). Straight lines show result of linear fit in the respective range. The dashed line gives the two intercepts N_p^* and t_p^* , respectively, for the case of the WBL.

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.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 $N_p = J_{\text{stat}} t_p$ and the N_p -intercept would vanish. Non-vanishing values of N_p^* reflect the additional transient contributions to the current. Figure 6(a) shows a stronger transient response for smaller values of 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, $t_p^* = N_p^* / J_{\text{stat}}$ (cf. dashed line in Fig. 5). This quantity is shown in Fig. 6(b). It gives a measure for the pulse length at which transient and stationary

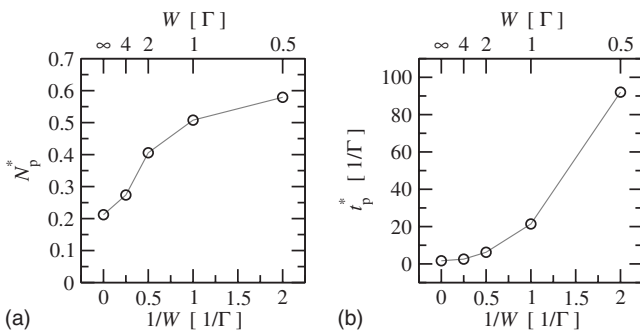


FIG. 6. Results of the linear fit to $N_p(t_p)$ shown in Fig. 5: (a) N_p^* intercept and (b) t_p^* intercept.

contributions are of similar size. Therefore, the transient response for pulses with $t_p \gg t_p^*$ becomes negligible.

IV. SUMMARY

We have presented a propagation scheme for time-dependent electron transport which is based on nonequilibrium Green's 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 expression⁷ 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.²⁹ The matrix equations to be solved are Eqs. (12), (37), and (38), respectively. In the often applied wide-band limit the set of equations simplifies since Ω can be found explicitly in terms of the current matrices, cf. Eq. (31).

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. (44)] 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.

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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. (25). The poles are given by $\chi_{ap}^+ = \mu_\alpha + x_p / \beta = (\chi_{ap}^-)^*$. Instead of using the Matsubara expansion²⁰ with poles $x_p = i\pi(2p-1)$, we use a partial fraction decomposition of the Fermi function,²⁹ which converges much faster than the standard Matsubara expansion. Furthermore, it allows to estimate

the error made by truncating the sum in Eq. (25) at N_F terms. For this decomposition the poles $x_p = \pm 2\sqrt{z_p}$ are given by the eigenvalues z_p of the $N_F \times N_F$ matrix²⁹

$$Z_{ij} = 2i(2i-1)\delta_{j,i+1} - 2N_F(2N_F-1)\delta_{iN_F}. \quad (\text{A1})$$

We take the branch of the root $\sqrt{z_p}$ such that $\text{Im}(x_p) > 0$ for all p . Thus all poles χ_p^+ (χ_p^-) 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 RESONANT-LEVEL MODEL

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. (5)]

$$\langle J_{\text{net}}(t) \rangle = e \text{Re Tr} \left\{ \int_{-\infty}^{\infty} dt_1 \langle G^r(t, t_1) \rangle [\Sigma_L^<(t_1, t) - \Sigma_R^<(t_1, t)] \right\}, \quad (\text{B1})$$

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

$$G^r(t, t_1) = -i\Theta(t-t_1) \exp \left[-i \int_{t_1}^t dt' \varepsilon_d(t') - \frac{\Gamma}{2}(t-t_1) \right]. \quad (\text{B2})$$

In order to evaluate Eq. (B1) 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.,

$$\begin{aligned} & \left\langle \exp \left[-i \int_{t_1}^t dt' \varepsilon_d(t') \right] \right\rangle \\ &= \exp \left[-\frac{1}{2} \int_{t_1}^t d\tau_1 \int_{t_1}^t d\tau_2 \langle \varepsilon_d(\tau_1) \varepsilon_d(\tau_2) \rangle \right] \\ &= \exp \left[-\frac{1}{2} \int \frac{d\omega}{2\pi} c(\omega) \left| \int_{t_1}^t d\tau e^{-i\omega\tau} \right|^2 \right] \\ &= \exp \left[-\frac{1}{2} \int \frac{d\omega}{2\pi} \frac{c(\omega)}{\omega^2} 4 \sin^2 \left(\frac{\omega(t-t_1)}{2} \right) \right]. \quad (\text{B3}) \end{aligned}$$

In the derivation we have used the properties of the noise [Eqs. (40)] and introduced the Fourier transform of $c(\tau_1 - \tau_2)$ which is denoted by $c(\omega)$.

Thus, the noise-averaged retarded Green's function does only depend on the time difference and the time-averaged current is given by a Landauer-type expression⁷

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

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

$$\begin{aligned} A(\varepsilon) &= -2\text{Im} \int_0^{\infty} d\tau \langle G^r(t, t-\tau) \rangle e^{i\varepsilon\tau} \\ &= \int_{-\infty}^{\infty} d\tau e^{i\varepsilon\tau - \Gamma|\tau|/2} \\ &\quad \times \exp \left[-\frac{1}{2} \int \frac{d\omega}{2\pi} \frac{c(\omega)}{\omega^2} 4 \sin^2 \left(\frac{\omega\tau}{2} \right) \right]. \quad (\text{B5}) \end{aligned}$$

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

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¹T. Fujisawa, T. Hayashi, and S. Sasaki, Rep. Prog. Phys. **69**, 759 (2006).

²L. P. Kouwenhoven, J. M. Elzerman, R. Hanson, L. H. Willems van Beveren, and L. M. K. Vandersypen, Phys. Status Solidi B **243**, 3682 (2006).

³T. Fujisawa, D. G. Austing, Y. Tokura, Y. Hirayama, and S. Tarucha, J. Phys.: Condens. Matter **15**, R1395 (2003).

⁴T. Hayashi, T. Fujisawa, H. D. Cheong, Y. H. Jeong, and Y. Hirayama, Phys. Rev. Lett. **91**, 226804 (2003).

⁵J. R. Petta, A. C. Johnson, J. M. Taylor, E. A. Laird, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Science **309**, 2180 (2005).

⁶F. H. L. Koppens, C. Buizert, K. J. Tielrooij, I. T. Vink, K. C. Nowack, T. Meunier, L. P. Kouwenhoven, and L. M. K. Vandersypen, Nature (London) **442**, 766 (2006).

⁷A.-P. Jauho, N. S. Wingreen, and Y. Meir, Phys. Rev. B **50**, 5528 (1994).

⁸H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors*, 2nd revised ed. (Springer, Berlin, 2007).

⁹C. A. Stafford and N. S. Wingreen, Phys. Rev. Lett. **76**, 1916 (1996).

¹⁰S. Camalet, J. Lehmann, S. Kohler, and P. Hänggi, Phys. Rev. Lett. **90**, 210602 (2003).

¹¹L. Arrachea, Phys. Rev. B **72**, 125349 (2005).

¹²Y. Zhu, J. Maciejko, T. Ji, H. Guo, and J. Wang, Phys. Rev. B **71**, 075317 (2005).

¹³V. Moldoveanu, V. Gudmundsson, and A. Manolescu, Phys. Rev. B **76**, 085330 (2007).

¹⁴S. Kurth, G. Stefanucci, C.-O. Almbladh, A. Rubio, and E. K. U. Gross, Phys. Rev. B **72**, 035308 (2005).

¹⁵G. Stefanucci, E. Perfetto, and M. Cini, Phys. Rev. B **78**, 075425 (2008).

¹⁶C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, J. Phys. C **4**, 916 (1971).

¹⁷J. Jin, X. Zheng, and Y. Yan, J. Chem. Phys. **128**, 234703 (2008).

¹⁸C. Meier and D. J. Tannor, J. Chem. Phys. **111**, 3365 (1999).

¹⁹S. Welack, M. Schreiber, and U. Kleinekathöfer, J. Chem. Phys. **124**, 044712 (2006).

²⁰G. D. Mahan, *Many Particle Physics*, 2nd ed. (Plenum, New

- York, 1990).
- ²¹The more general case of coupling the spin degree of freedom of the tunneling electron to a fluctuating semimagnetic barrier was investigated by Y. G. Rubo, *J. Exp. Theor. Phys.* **77**, 685 (1993).
- ²²C. W. Gardiner, *Handbook of Stochastic Methods: For Physics, Chemistry and the Natural Sciences*, Springer Series in Synergetics (Springer, Berlin, 1996).
- ²³G. N. Milshtein and M. V. Tret'yakov, *J. Stat. Phys.* **77**, 691 (1994).
- ²⁴For one set of parameters, $\kappa=0.25\Gamma$ and $\eta=5.0\Gamma$, we had to use $\delta t=0.005/\Gamma$.
- ²⁵L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, *Rev. Mod. Phys.* **70**, 223 (1998).
- ²⁶N. S. Wingreen and Y. Meir, *Phys. Rev. B* **49**, 11040 (1994).
- ²⁷W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes in C: The Art of Scientific Computing*, 2nd ed. (Cambridge University Press, Cambridge, 1992), p. 994.
- ²⁸N. S. Wingreen, A.-P. Jauho, and Y. Meir, *Phys. Rev. B* **48**, 8487 (1993).
- ²⁹A. Croy and U. Saalman, *Phys. Rev. B* **80**, 073102 (2009).