Time-dependent quantum transport far from equilibrium: An exact nonlinear response theory

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In this work, we present a theory to calculate the time-dependent current flowing through an arbitrary noninteracting nanoscale phase-coherent device connected to arbitrary noninteracting external leads, in response to sharp step- and square-shaped voltage pulses. Our analysis is based on the Keldysh nonequilibrium Green's-functions formalism, and provides an exact analytical solution to the transport equations in the far from equilibrium, nonlinear response regime. However, the essential feature of our solution is that it does not rely on the commonly used wideband approximation where the coupling between device scattering region and leads is taken to be independent of energy, and as such provides a way to perform transient transport calculations from first principles on realistic systems, taking into account the detailed electronic structure of the device scattering region and the leads. We then perform a model calculation for a quantum dot with Lorentzian linewidth and show how interesting finite-bandwidth effects arise in the time-dependent current dynamics.

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I. INTRODUCTION

Due to the industrial efforts and achievements in device miniaturization, modern electronic devices in present-day computer technology have already entered the nanometer era. For the past four decades, the electronics industry has followed, to a very good degree, the so-called "Moore's law" which observes a steady decrease of device sizes by roughly a factor of 2 every 18 months. The *International Technology Roadmap for Semiconductors* (ITRS) predicts a continued device scaling to the 22-nm technology at year 2016 when the projected minimum device features will be less than 10 nm and computer chips will have more than six billion transistors.[1] Such a relentless device miniaturization has brought electronic device technology into a new realm where quantum phenomena of charge and spin transport become important physical factors. Another important reality of tiny devices is that the discrete properties of materials are playing increasingly dominant roles in device operation. Indeed, ample experimental evidence has demonstrated that the operation of nanoelectronics crucially depends on the close coupling of quantum transport phenomena with the atomic structure of the device material. Such a coupling poses new challenges to both experimental and theoretical understanding of nanoelectronic device physics.

The simplest nanoelectronic device structure is the two-probe lead-device-lead (LDL) configuration, where "device" is the scattering region which is connected to the outside world by the "leads," schematically shown in Fig. 1. The theoretical interest is to predict the quantum transport properties of such devices including all the atomic details of the device material. In the past several years, very good theoretical progress has been achieved for first-principles modeling of *steady-state* quantum transport in these systems from an atomic point of view, by carrying out density-functional theory (DFT) calculations within the Keldysh nonequilibrium Green's-functions formalism (NEGF). The basic idea of the NEGF-DFT formalism[2,3] is to calculate the device Hamiltonian and electronic structure by DFT, populate this electronic structure using NEGF theory which properly takes into account nonequilibrium quantum statistics, and deal with open device boundaries directly using real-space techniques. So far, several implementations of the NEGF-DFT formalism have appeared in the literature[2–10] and many steady-state quantum transport properties of nanoscale conductors have been analyzed using these codes. The fact that the NEGF-DFT formalism works for steady-state transport has been demonstrated by direct quantitative comparison to experimental data,[11–14] as well as by recent literature which puts this formalism onto more rigorous theoretical footing.[15,16]

While good progress has been achieved for *steady-state* quantum transport analysis from an atomic point of view, a very serious challenge to nanoelectronics device theory has been the understanding and prediction of *transient transport dynamics* in these devices. Indeed, an important issue which has yet to be resolved is to predict how fast or how slow a nanoelectronic device can turn on or off a current from quantum-mechanical first principles. One cannot develop an electronic technology unless the operational speed of the device can be designed and controlled. This issue is closely related to the transient transport phenomenon, which is becoming an extremely important problem of nanoelectronic

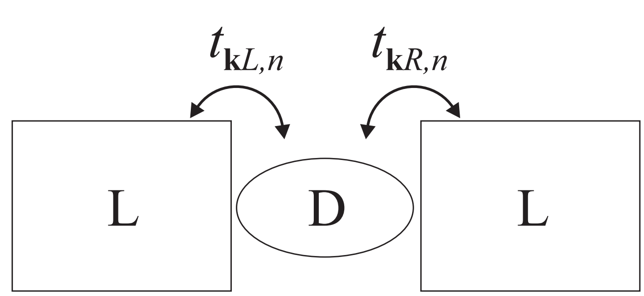

FIG. 1. Schematic diagram of a nanoscale device in the LDL configuration.

device physics, as can be observed in such effects as photon-assisted tunneling,[17] electron turnstiles,[18] and ringing behavior in the time-dependent current.[19,20] Recent real-time measurements of electron dynamics[21] have further raised interest for the study of transient quantum transport. Therefore a very important theoretical problem is to formulate a proper theoretical formalism which can be applied to analyze transient quantum transport in LDL systems.

It is the purpose of this paper to report a time-dependent quantum transport theory far from equilibrium and to derive an exact nonlinear response solution for the time-dependent current $J_{L/R}(t)$ flowing through the left (L) or right (R) lead of the LDL device in response to external time-dependent bias voltage pulses. We will present solutions for three different pulses: a downward step, an upward step, and a square pulse. Because the analysis is rather complicated, detailed derivations will be given so that interested readers can follow without difficulty. Importantly, our exact solution for $J_{L/R}(t)$ is expressed in terms of the steady-state Green's functions of the device (when there are no time-dependent fields) which, as discussed above, are solvable numerically for nanoelectronic devices using the NEGF-DFT formalism. This way, our theory provides a possible solution to the problem of estimating the switching speed of nanoscale electronic devices.

Before moving on to our theory, we note that many different theoretical approaches have been used to tackle time-dependent quantum transport problems. These include the time-dependent Schrödinger equation,[22] the transfer Hamiltonian formalism,[23] path-integral techniques,[24] the Wigner distribution function,[25] the time-dependent numerical renormalization group,[26] evolution operator techniques,[27,28] time-dependent density-functional theory,[15,29–31] and the NEGF technique.[19,20,32–37] In particular, our formalism for calculating $J_{L/R}(t)$ driven by a voltage pulse will be based on NEGF. The main reason for this choice is due to the fact that the *steady-state* Green's functions for any LDL device can be straightforwardly calculated by the well-documented NEGF-DFT formalism,[2–10] and these steady-state Green's functions provide an excellent starting point for analyzing the time-dependent current $J_{L/R}(t)$ as will be seen below.

Nonequilibrium Green's functions[38–42] have so far been used extensively in the study of phase-coherent electronic transport; indeed, both steady-state[2,43–45] and time-dependent[19,20,36,37] problems can be analyzed within this formalism. Apart from numerical studies,[27,46] most investigations of time-dependent transport problems within NEGF have relied on the so-called wideband limit[43] (WBL), which is an approximation that amounts to neglecting the energy dependence of the coupling between the leads and the central scattering region of the LDL device. It can be shown that in this limit, the two-time retarded self-energy function $\Sigma^R(t,t')$ becomes proportional to a delta function[47] $\delta(t-t')$. This results in a tremendous simplification of the transport problem since the retarded single-particle Green's function $G^R(t,t')$ can then be obtained exactly in closed form[48] (in the absence of interactions). Beyond the WBL, however, $G^R(t,t')$ is given by the solution of a double integral equation which is not generally solvable, even in the absence of interactions. Numerical approaches based on discretization[46] require the manipulation of four-dimensional arrays $G^R_{nm}(t_i,t_j)$ that become increasingly large with increasing cutoff and decreasing step size in the time domain. In that sense, it is desirable to be able to exactly solve the transient dynamics analytically and perform the remaining work numerically with the usual three-dimensional arrays $G^R_{nm}(\omega_i)$.

The wideband approximation is valid if the density of states in the leads varies slowly with energy in the vicinity of the levels of the device scattering region. However, in nanoscale systems, most electrode materials are characterized by complicated band structures which lead to nontrivial features in the density of states such as peaks, dips, gaps, and van Hove singularities.[27] Hence if a realistic first-principles description of time-dependent electronic transport in nanoscale devices is to be achieved, one needs to take into account the detailed electronic structure of the leads. Indeed, different electrodes such as metals, semiconductors, superconductors, nanotubes, and nanowires have qualitatively different features in their density of states, and are known to have very different transport properties as a result thereof.

In the following, we present an exact solution, without invoking the WBL approximation, of the nonlinear, far from equilibrium, time-dependent current driven by an external voltage pulse, for nanoscale devices in the LDL configuration. Our solution applies to the cases of sharp step-shaped voltage pulses and square voltage pulses, and is valid for an arbitrary noninteracting scattering region connected to arbitrary noninteracting leads. Our main result is an exact formula for the time-dependent current $J_{L/R}(t)$ flowing through the left (L) or right (R) lead, given in terms of the steady-state Green's functions and self-energies.

Because the theoretical derivation is rather involved due to the complexity of the problem, here we list for convenience the main results of this work. (i) The time-dependent current $J_\alpha(t)$ through lead $\alpha=L,R$ is given by the general formula Eq. (10), valid for any type of pulse. It is expressed in terms of the functions $A_\alpha(\epsilon,t)$ and $\Psi_\alpha(\epsilon,t)$ that need to be found for each specific type of pulse. (iia) For a downward step pulse, $A_\alpha(\epsilon,t)$ is given in Eq. (22) and $\Psi_\alpha(\epsilon,t)$ is given in Eq. (27); (iib) for an upward step pulse, $A_\alpha(\epsilon,t)$ is given in Eq. (47) and $\Psi_\alpha(\epsilon,t)$ is given in Eq. (50); and (iic) for a square pulse, $A_\alpha(\epsilon,t)$ is given in Eq. (58) and $\Psi_\alpha(\epsilon,t)$ is given in Eq. (60).

The paper is structured as follows. In Sec. II we briefly review the Keldysh nonequilibrium Green's-functions formalism applied to the transport problem as put forward in Refs. 19 and 20, and introduce several new definitions needed to solve the time-dependent problem beyond the WBL. In Sec. III we derive an exact solution for a downward step pulse, and validate this solution with sum rule checks for the initial and asymptotic currents. The same is done in Sec. IV for an upward step pulse and in Sec. V for a square pulse. In Sec. VI, we apply these general results to the simplest model capable of exhibiting finite-bandwidth effects, a single-level quantum dot with Lorentzian linewidth. We also show how these results reduce to previously known results obtained by Jauho *et al.*[19,20] under the WBL approximation, in the case we take the linewidth to be independent of energy. Finally, in Appendix A, we present a derivation of the time-dependent Dyson equation based on the path-integral formulation of the Keldysh technique, and in Appendix B we have included a longer derivation belonging to Sec. VI.

II. KELDYSH FORMULATION OF QUANTUM TRANSPORT

Throughout this work, we shall work in units where $\hbar=1$. For a general LDL two-probe device (Fig. 1), the Hamiltonian can be written as

$$H=\sum_{\mathbf{k}\alpha}\epsilon_{\mathbf{k}\alpha}(t)c^{\dagger}_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}+\sum_{mn}\epsilon_{mn}(t)d^{\dagger}_{m}d_{n}+\sum_{\mathbf{k}\alpha,n}(t_{\mathbf{k}\alpha,n}c^{\dagger}_{\mathbf{k}\alpha}d_{n}+t^{*}_{\mathbf{k}\alpha,n}d^{\dagger}_{n}c_{\mathbf{k}\alpha}),\qquad(1)$$

where $c^{\dagger}_{\mathbf{k}\alpha}$ ($c_{\mathbf{k}\alpha}$) with $\alpha=L,R$ is a Fermionic creation (annihilation) operator for a single-particle momentum state $\mathbf{k}$ in the left (L) or right (R) metallic lead, and $d^{\dagger}_{n}$ (d_n) is a Fermionic creation (annihilation) operator for a single-particle state labeled by n in the scattering region. The first two terms in Eq. (1) describe the isolated (unconnected) leads and scattering region. The last term describes hopping processes between the leads and the scattering region with strength $t_{\mathbf{k}\alpha,n}$. We set from the start chemical potentials in both leads to zero, so that the connected system without the time-dependent perturbation is in equilibrium with zero chemical potential everywhere. In order to specify the time-dependent perturbation, we assume that the single-particle energies follow adiabatically the time dependence of the external fields.[19,20,36,37] As pointed out by Jauho *et al.*,[20] this assumption assigns an upper limit ν_c of roughly tens of terahertz to the spectral content of the time-dependent perturbation. In our case, since we will be considering external fields with a step function time dependence, this corresponds roughly to a pulse rise time[49] $\tau\sim\pi/\omega_c$ which is on the order of tens of femtoseconds. With electron dynamics usually in the picosecond range, the approximation of a perfectly sharp step is seen to be reasonable.

In the adiabatic approximation therefore the single-particle energies acquire a rigid time-dependent shift: $\epsilon_{\mathbf{k}\alpha}(t)=\epsilon^{0}_{\mathbf{k}\alpha}+\Delta_{\alpha}(t)$ and $\epsilon_{mn}(t)=\epsilon^{0}_{mn}+\Delta_{mn}(t)$ where $\epsilon^{0}_{\mathbf{k}\alpha}$ and ϵ^{0}_{mn} are the energies in the time-independent unperturbed system. The energy shift in the leads $\Delta_{\alpha}(t)$ is assumed to be uniform throughout the lead, which is reasonable since the above-mentioned frequency limit, being smaller than usual metallic plasma frequencies, ensures that the external electric field is effectively screened.[20] We, however, allow for a spatial dependence of the time-dependent potential $\Delta(\mathbf{x},t)$ in the scattering region, which translates into a matrix $\Delta_{mn}(t)$ in the basis defined by the set of states $\{|n\rangle\}$. Indeed, the electric field is not screened in the small scattering region where the bias drop occurs.

A. Time-dependent current

A Keldysh nonequilibrium Green's-functions analysis[19,20] of the time-dependent current through lead α defined by $J_{\alpha}(t)\equiv-e\langle dN_{\alpha}/dt\rangle$, where $e>0$ is the elementary charge and $N_{\alpha}=\Sigma_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}$ is the number operator for lead α, yields the following formula:

$$J_{\alpha}(t)=-2e\int_{-\infty}^{t}dt'\int\frac{d\epsilon}{2\pi}\,\mathrm{Im\,Tr}\{e^{i\epsilon(t-t')}e^{i\int_{t'}^{t}dt_1\Delta_{\alpha}(t_1)}\times\Gamma_{\alpha}(\epsilon)[G^{<}(t,t')+f(\epsilon)G^{R}(t,t')]\},\qquad(2)$$

where $f(\epsilon)\equiv(e^{\beta\epsilon}+1)^{-1}$ is the Fermi function, the linewidth function $\Gamma_{\alpha}(\epsilon)$ has matrix elements $\Gamma_{\alpha,mn}(\epsilon)\equiv2\pi\rho_{\alpha}(\epsilon)t^{*}_{\alpha,m}(\epsilon)t_{\alpha,n}(\epsilon)$ where $\rho_{\alpha}(\epsilon)=\Sigma_{\mathbf{k}}\delta(\epsilon-\epsilon_{\mathbf{k}\alpha})$ is the density of states in lead α, and we define two nonequilibrium one-particle propagators, the lesser Green's function $G^{<}(t,t')$,

$$G^{<}_{nm}(t,t')\equiv i\langle d^{\dagger}_{m}(t')d_{n}(t)\rangle,$$

and the retarded Green's function $G^{R}(t,t')$,

$$G^{R}_{nm}(t,t')\equiv-i\theta(t-t')\langle\{d_n(t),d^{\dagger}_{m}(t')\}\rangle.$$

The lesser Green's function satisfies the Keldysh equation,[37]

$$G^{<}(t,t')=\int dt_1\int dt_2G^{R}(t,t_1)\Sigma^{<}(t_1,t_2)G^{A}(t_2,t'),\qquad(3)$$

where $G^{A}(t,t')=[G^{R}(t',t)]^{\dagger}$ is the advanced Green's function and $\Sigma^{<}(t_1,t_2)$ is the lesser self-energy given by[20]

$$\Sigma^{<}(t_1,t_2)=i\sum_{\alpha}\int\frac{d\omega}{2\pi}e^{-i\omega(t_1-t_2)}e^{i\int_{t_1}^{t_2}dt_3\Delta_{\alpha}(t_3)}f(\omega)\Gamma_{\alpha}(\omega).$$

We thus see from Eqs. (2) and (3) that since the Keldysh equation in this case is an explicit expression for the lesser Green's function in terms of the retarded Green's function, solving the transport problem amounts to solving for the retarded Green's function. The retarded Green's function satisfies the Dyson equation,[37,50]

$$G^{R}(t,t')=G^{R}_{0}(t,t')+\int dt_1\int dt_2G^{R}_{0}(t,t_1)\times\Sigma^{R}(t_1,t_2)G^{R}(t_2,t'),\qquad(4)$$

where $\Sigma^{R}(t_1,t_2)$ is the retarded self-energy given by

$$\Sigma^{R}(t_1,t_2)=-i\theta(t_1-t_2)\sum_{\alpha}\int\frac{d\omega}{2\pi}e^{-i\omega(t_1-t_2)}\times e^{i\int_{t_1}^{t_2}dt_3\Delta_{\alpha}(t_3)}\Gamma_{\alpha}(\omega),$$

and $G^{R}_{0}(t,t')$ is the retarded Green's function for the isolated scattering region, that is, considering only the second term in the Hamiltonian (1).

For time-dependent problems, instead of working directly with the retarded Green's function, we will work with the quantity $A_{\alpha}(\epsilon,t)$ defined[20] as

$$A_{\alpha}(\epsilon,t)\equiv\int_{-\infty}^{t}dt'\,e^{i\epsilon(t-t')}e^{i\int_{t'}^{t}dt_1\Delta_{\alpha}(t_1)}G^{R}(t,t').\qquad(5)$$

We separate the current into two contributions $J_{\alpha}(t)=J^{R}_{\alpha}(t)+J^{<}_{\alpha}(t)$, where $J^{R,<}_{\alpha}(t)$ is the contribution to the current (2) from $G^{R,<}(t,t')$, respectively. It is easily seen from Eq. (2) that the retarded current is given by

$$J_\alpha^R(t) = -2e \int \frac{d\epsilon}{2\pi} \text{Im Tr}\{f(\epsilon)\Gamma_\alpha(\epsilon)A_\alpha(\epsilon,t)\}. \tag{6}$$

Using Eq. (5) in the Keldysh equation (3), we obtain the following expression for the lesser Green's function,

$$G^<(t,t') = i\sum_\beta \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} e^{i\int_t^{t'} dt_1 \Delta_\beta(t_1)} \times f(\omega)A_\beta(\omega,t)\Gamma_\beta(\omega)A_\beta^\dagger(\omega,t'), \tag{7}$$

so that the lesser current $J_\alpha^<(t)$ is given by

$$J_\alpha^<(t) = -2e \int \frac{d\epsilon}{2\pi} \text{Im Tr}\{\Gamma_\alpha(\epsilon)\Psi_\alpha(\epsilon,t)\}, \tag{8}$$

where in analogy with Eq. (5), we have defined $\Psi_\alpha(\epsilon,t) \equiv \int_{-\infty}^t dt'\, e^{i\epsilon(t-t')} e^{i\int_{t'}^t dt_1\, \Delta_\alpha(t_1)} G^<(t,t')$ for the lesser Green's function, so that we have

$$\Psi_\alpha(\epsilon,t) = i\sum_\beta \int \frac{d\epsilon'}{2\pi} e^{i(\epsilon-\epsilon')t} f(\epsilon')A_\beta(\epsilon',t)\Gamma_\beta(\epsilon') \times \int_{-\infty}^t dt'\, e^{-i(\epsilon-\epsilon')t'} e^{i\int_{t'}^t dt_1[\Delta_\alpha(t_1)-\Delta_\beta(t_1)]} A_\beta^\dagger(\epsilon',t'). \tag{9}$$

The total current, given by the sum of Eqs. (6) and (8),

$$J_\alpha(t) = -2e \int \frac{d\epsilon}{2\pi} \text{Im Tr}\{\Gamma_\alpha(\epsilon)[\Psi_\alpha(\epsilon,t) + f(\epsilon)A_\alpha(\epsilon,t)]\}, \tag{10}$$

is therefore entirely determined by $A_\alpha(\epsilon,t)$. The main objective of our analysis will thus be to obtain an exact solution for $A_\alpha(\epsilon,t)$. As one can expect from Eq. (4), to obtain $A_\alpha(\epsilon,t)$ one needs to solve a particularly difficult integral equation since it contains both an inhomogeneous term arising from $G_0^R(t,t')$ and a double integral over two time variables t_1 and t_2. In equilibrium[50] or steady-state nonequilibrium, Green's functions and self-energies depend only on the time difference $t-t'$ because of the time-translational invariance of the Hamiltonian. In this case, Eq. (4) is a Fourier convolution product that can be reduced to an algebraic equation by a Fourier transformation from the time domain to the frequency domain. In time-dependent transport, however, explicitly time-dependent terms in the Hamiltonian break time-translational invariance and the Green's functions and self-energies depend on both arguments t and t' separately; Fourier transform techniques cannot be applied to solve the problem. However, we will see that it is possible to obtain an exact solution for $A_\alpha(\epsilon,t)$ in the physically relevant cases of a step function pulse and a square pulse using other techniques. In view of doing this, we will need an alternate form of the Dyson equation (4).

B. Dyson equation

There are three basic ingredients in the Hamiltonian (1): (i) the isolated central region, (ii) the coupling between central region and external leads, and (iii) the time-dependent external fields. Different but equivalent Dyson equations can be obtained depending on (a) what is chosen as a perturbation in regard to (b) a chosen unperturbed system. In Eq. (4), the unperturbed system consists of the isolated central region together with the external field $\Delta(t)$, and the coupling together with the applied bias $\Delta_\alpha(t)$ give rise to a self-energy correction. In the study of time-dependent transport, it is better to treat the *time-independent*, coupled system at equilibrium as the unperturbed system, and add the time-dependent external fields as a perturbation. Such a partition-free approach[29] is more consistent with the way actual measurements are carried out in practice. As we will see, it also gives rise to a Dyson equation whose mathematical structure is better suited to the study of transport driven by a voltage pulse. However, provided that the problem is solved exactly, both approaches give the same result for the exact, fully resummed propagator $G^R(t,t')$.

Following the derivation given in Appendix A, we will use the following form of the Dyson equation for our analysis:

$$G^R(t,t') = \tilde{G}^R(t-t') + \int dt_1 \tilde{G}^R(t-t_1)\Delta(t_1)G^R(t_1,t') + \int dt_1 \int dt_2 \tilde{G}^R(t-t_1)V^R(t_1,t_2)G^R(t_2,t'), \tag{11}$$

where we define a two-time retarded potential[46] $V^R(t_1,t_2)$ as

$$V^R(t_1,t_2) \equiv \sum_\beta (e^{-i\int_{t_2}^{t_1} dt'\, \Delta_\beta(t')} - 1)\tilde{\Sigma}_\beta^R(t_1-t_2), \tag{12}$$

and $\tilde{G}^R(t-t')$ and $\tilde{\Sigma}_\beta^R(t-t')$ are the time-translationally invariant, equilibrium Green's function and self-energy due to lead β, respectively. They describe the coupled system at equilibrium and are known. Following Eq. (5), it is straightforward to obtain an integral equation for $A_\alpha(\epsilon,t)$ by integrating on both sides of Eq. (11),

$$A_\alpha(\epsilon,t) = \tilde{A}_\alpha(\epsilon,t) + \int dt'\, e^{i\epsilon(t-t')} e^{i\int_{t'}^t dt_1 \Delta_\alpha(t_1)} \times \tilde{G}^R(t-t')\Delta(t')A_\alpha(\epsilon,t') + \int dt_1 \int dt_2 e^{i\epsilon(t-t_2)} \times e^{i\int_{t_2}^t dt_3\, \Delta_\alpha(t_3)} \tilde{G}^R(t-t_1)V^R(t_1,t_2)A_\alpha(\epsilon,t_2), \tag{13}$$

where $\tilde{A}_\alpha(\epsilon,t) \equiv \int_{-\infty}^t dt'\, e^{i\epsilon(t-t')} e^{i\int_{t'}^t dt_1 \Delta_\alpha(t_1)} \tilde{G}^R(t-t')$ is known.

In order to solve Eq. (13), we need to specify the external fields $\Delta(t)$ and $\Delta_\alpha(t)$. We will study three cases: a downward step pulse (Sec. III) given by $\Delta_{(\alpha)}(t) = \Delta_{(\alpha)}\theta(-t)$, an upward step pulse (Sec. IV) given by $\Delta_{(\alpha)}(t) = \Delta_{(\alpha)}\theta(t)$, and a square pulse (Sec. V) given by $\Delta_{(\alpha)}(t) = \Delta_{(\alpha)}$ for $0 < t < s$ and zero otherwise, where $\Delta_{(\alpha)}$ is a constant amplitude and s is the duration of the pulse. We study the dynamics of the system after the pulse is applied at $t=0$.

III. CURRENT DRIVEN BY A DOWNWARD STEP PULSE

In this section, we will be concerned with a device initially out of equilibrium under dc bias Δ, Δ_α for $t<0$, so that a dc current flows. At $t=0$, this bias is suddenly turned off and remains off for subsequent times. We wish to derive an exact expression for the dynamics of the decaying current as the system relaxes to equilibrium at large times.

A. Calculation of $A_\alpha(\epsilon,t)$

For a time-translationally invariant quantity $C(t-t')$, it is useful to introduce the associated quantity in Fourier space $C(\omega)\equiv\int dt e^{i\omega t}C(t)$ such that $C(t-t')=\int(d\omega/2\pi)e^{-i\omega(t-t')}C(\omega)$. The equilibrium Green's function $\tilde{G}^R(\omega)$ and self-energy $\tilde{\Sigma}^R_\beta(\omega)$ are defined in this way from $\tilde{G}^R(t-t')$ and $\tilde{\Sigma}^R_\beta(t-t')$, respectively.

From these definitions, we can readily calculate the inhomogeneous term $\tilde{A}_\alpha(\epsilon,t)$ in Eq. (13) for $t>0$ in the case of the downward step pulse,

$$\tilde{A}_\alpha(\epsilon,t)=\tilde{G}^R(\epsilon)+\int\frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon)t}\Delta_\alpha\tilde{G}^R(\omega)}{(\omega-\epsilon-\Delta_\alpha-i0^+)(\omega-\epsilon-i0^+)},\tag{14}$$

where we used the relation $\int_{-\infty}^{t}dt' e^{i\omega t'}=-ie^{i\omega t}/(\omega-i0^+)$ and the Plemelj formula $1/(\omega\pm i0^+)=P(1/\omega)\mp i\pi\delta(\omega)$, where 0^+ is a positive infinitesimal and P stands for the principal value.

The time integrations in Eq. (13) range, in principle, over the whole real axis. However, certain simplifications occur in the case of a downward step pulse since $\Delta(t'>0)=0$ and $V^R(t_1,t_2)=0$ when both t_1 and t_2 are greater than zero, as can be seen from Eq. (12). Furthermore, $V^R(t_1,t_2)$ vanishes for $t_2>t_1$ since it is a retarded function and $\tilde{G}^R(t-t_1)=0$ for $t_1>t$ for the same reason. We thus obtain the following equation for $t>0$:

$$\begin{aligned}A_\alpha(\epsilon,t)&=\tilde{A}_\alpha(\epsilon,t)+\int_{-\infty}^{0}dt' e^{i\epsilon(t-t')}e^{i\int_{t'}^{t}dt_1\Delta_\alpha(t_1)}\\&\quad\times\tilde{G}^R(t-t')\Delta A_\alpha(\epsilon,t')+\left(\int_{-\infty}^{0}dt_1\int_{-\infty}^{t_1}dt_2\right.\\&\quad\left.+\int_0^t dt_1\int_{-\infty}^{0}dt_2\right)e^{i\epsilon(t-t_2)}e^{i\int_{t_2}^{t}dt_3\Delta_\alpha(t_3)}\\&\quad\times\tilde{G}^R(t-t_1)V^R(t_1,t_2)A_\alpha(\epsilon,t_2),\end{aligned}\tag{15}$$

which is a generalized Wiener-Hopf equation[51,52] relating $A^+_\alpha(\epsilon,t)\equiv A_\alpha(\epsilon,t>0)$ to $A^-_\alpha(\epsilon,t)\equiv A_\alpha(\epsilon,t<0)$. Indeed, on the left-hand side of Eq. (15) we require only $A_\alpha(\epsilon,t)$ for $t>0$ after the pulse is applied, while the limits of integration on the right-hand side are such that only $A_\alpha(\epsilon,t)$ for $t<0$ is involved in the integrals on that side. However, $A_\alpha(\epsilon,t<0)$ is already known since it depends only on $G^R(t,t')$ for $t,t'<0$ as can be seen from Eq. (5), and $G^R(t<0,t'<0)\equiv\bar{G}^R(t-t')$ is a steady-state nonequilibrium Green's function describing the system under dc bias before the voltage is turned off. Considering the Dyson equation (11) for $t,t'<0$, we have

$$\begin{aligned}\bar{G}^R(t-t')&=\tilde{G}^R(t-t')+\int dt_1\tilde{G}^R(t-t_1)\Delta\bar{G}^R(t_1-t')\\&\quad+\int dt_1\int dt_2\tilde{G}^R(t-t_1)\sum_\beta(e^{-i\Delta_\beta(t_1-t_2)}-1)\\&\quad\times\tilde{\Sigma}^R_\beta(t_1-t_2)\bar{G}^R(t_2-t'),\end{aligned}$$

which can be Fourier transformed to yield

$$\begin{aligned}\bar{G}^R(\omega)&=\tilde{G}^R(\omega)+\tilde{G}^R(\omega)\Delta\bar{G}^R(\omega)+\tilde{G}^R(\omega)\sum_\beta[\tilde{\Sigma}^R_\beta(\omega-\Delta_\beta)\\&\quad-\tilde{\Sigma}^R_\beta(\omega)]\bar{G}^R(\omega),\end{aligned}\tag{16}$$

so that $\bar{G}^R(\omega)$ can be solved for by matrix inversion, $\bar{G}^R(\omega)=\{1-\tilde{G}^R(\omega)(\Delta+\Sigma_\beta[\tilde{\Sigma}^R_\beta(\omega-\Delta_\beta)-\tilde{\Sigma}^R_\beta(\omega)])\}^{-1}\tilde{G}^R(\omega)$. Since the equilibrium Green's function is given by $\tilde{G}^R(\omega)=[\omega S-\tilde{H}-\tilde{\Sigma}^R(\omega)]^{-1}$ with $\tilde{H}_{mn}\equiv\epsilon^0_{mn}$ the unperturbed Hamiltonian matrix, $S_{mn}\equiv\langle m|n\rangle$ the overlap matrix for the n basis, and $\tilde{\Sigma}^R(\omega)\equiv\Sigma_\beta\tilde{\Sigma}^R_\beta(\omega)$ the total equilibrium self-energy, we see that the nonequilibrium Green's function is given by $\bar{G}^R(\omega)=[\omega S-\bar{H}-\bar{\Sigma}^R(\omega)]^{-1}$ where $\bar{H}\equiv\tilde{H}+\Delta$ is the nonequilibrium Hamiltonian matrix and $\bar{\Sigma}^R(\omega)\equiv\Sigma_\beta\tilde{\Sigma}^R_\beta(\omega-\Delta_\beta)$ the nonequilibrium total self-energy.

We can then proceed to calculate $A_\alpha(\epsilon,t<0)$ from Eq. (5),

$$A_\alpha(\epsilon,t<0)=\int\frac{d\omega}{2\pi i}\frac{\bar{G}^R(\omega)}{\omega-\epsilon-\Delta_\alpha-i0^+}=\bar{G}^R(\epsilon+\Delta_\alpha),\tag{17}$$

where the last equality follows by residue integration in the upper half plane where the retarded Green's function is analytic.

We now see that Eq. (15) is actually not an integral equation, but an explicit expression for $A_\alpha(\epsilon,t>0)$ in terms of known quantities Eqs. (14) and (17). We now evaluate the integrals in Eq. (15) in terms of the Fourier-transformed quantities $\tilde{G}^R(\omega)$, $\bar{G}^R(\omega)$, and $\tilde{\Sigma}^R(\omega)$. The integral over t' yields

$$\begin{aligned}&\int_{-\infty}^{0}dt' e^{i\epsilon(t-t')}e^{i\int_{t'}^{t}dt_1\Delta_\alpha(t_1)}\tilde{G}^R(t-t')\Delta A_\alpha(\epsilon,t')\\&\quad=\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\frac{\tilde{G}^R(\omega)\Delta\bar{G}^R(\epsilon+\Delta_\alpha)}{\omega-\epsilon-\Delta_\alpha-i0^+}.\end{aligned}\tag{18}$$

In order to evaluate the first double integral in Eq. (15), we notice that for $(t_1,t_2)\in(-\infty,0]\times(-\infty,t_1]$, the retarded potential $V^R(t_1,t_2)$ depends only on the time difference t_1-t_2 as can be checked from the definition (12), and is given by $V^R(t_1-t_2)=\Sigma_\beta[e^{-i\Delta_\beta(t_1-t_2)}-1]\tilde{\Sigma}^R_\beta(t_1-t_2)$. By direct integration we can show that

$$\int_{-\infty}^{0} dt_1 \int_{-\infty}^{t_1} dt_2 e^{i\epsilon(t-t_2)} e^{i\int_{t_2}^{t} dt_3 \Delta_\alpha(t_3)} \tilde{G}^R(t-t_1) V^R(t_1-t_2) A_\alpha(\epsilon,t_2)$$

$$= \int \frac{d\omega}{2\pi i} \frac{e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)}{\omega-\epsilon-\Delta_\alpha - i0^+} \sum_\beta [\tilde{\Sigma}_\beta^R(\epsilon+\Delta_\alpha-\Delta_\beta) - \tilde{\Sigma}_\beta^R(\epsilon+\Delta_\alpha)]\bar{G}^R(\epsilon+\Delta_\alpha). \quad (19)$$

In the second double integral in Eq. (15), the domain of integration is such that the retarded potential becomes $V^R(t_1,t_2)=\Sigma_\beta[e^{i\Delta_\beta t_2}-1]\tilde{\Sigma}_\beta^R(t_1-t_2)$. Performing the integrals over t_1 and t_2, we obtain

$$\int_0^t dt_1 \int_{-\infty}^{0} dt_2 e^{i\epsilon(t-t_2)} e^{i\int_{t_2}^{t} dt_3 \Delta_\alpha(t_3)} \tilde{G}^R(t-t_1) V^R(t_1,t_2) A_\alpha(\epsilon,t_2)$$

$$= \int \frac{d\omega}{2\pi i}\int \frac{d\epsilon'}{2\pi i} \frac{e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)}{\omega-\epsilon'+i0^+}\sum_\beta \tilde{\Sigma}_\beta^R(\epsilon') \times\left(\frac{1}{\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta+i0^+} - \frac{1}{\epsilon-\epsilon'+\Delta_\alpha+i0^+}\right)\bar{G}^R(\epsilon+\Delta_\alpha). \quad (20)$$

The integral over ϵ' can be carried out exactly by residue integration in the upper half plane where the retarded self-energy $\tilde{\Sigma}_\beta^R(\epsilon')$ is analytic and the only poles are $\epsilon'=\omega+i0^+$, $\epsilon'=\epsilon+\Delta_\alpha+i0^+$, and $\epsilon'=\epsilon+\Delta_\alpha-\Delta_\beta+i0^+$. Equation (20) then becomes

$$\int \frac{d\omega}{2\pi i} e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\sum_\beta\left(\frac{\tilde{\Sigma}_\beta^R(\omega)-\tilde{\Sigma}_\beta^R(\epsilon+\Delta_\alpha-\Delta_\beta)}{\omega-\epsilon-\Delta_\alpha+\Delta_\beta-i0^+} - \frac{\tilde{\Sigma}_\beta^R(\omega)-\tilde{\Sigma}_\beta^R(\epsilon+\Delta_\alpha)}{\omega-\epsilon-\Delta_\alpha-i0^+}\right)\bar{G}^R(\epsilon+\Delta_\alpha). \quad (21)$$

Adding all the contributions to $A_\alpha(\epsilon,t)$ from Eqs. (14), (18), (19), and (21), we see that the term containing $\tilde{\Sigma}_\beta^R(\epsilon+\Delta_\alpha)$ cancels out from Eqs. (19) and (21), so that we finally obtain

$$A_\alpha(\epsilon,t) = \tilde{G}^R(\epsilon) + \int \frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)}{\omega-\epsilon-\Delta_\alpha-i0^+}\left[\frac{\Delta_\alpha}{\omega-\epsilon-i0^+} + \left(\Delta - \sum_\beta \Delta_\beta \tilde{\Upsilon}_{\alpha\beta}^R(\omega,\epsilon)\right)\bar{G}^R(\epsilon+\Delta_\alpha)\right], \quad (22)$$

where we have defined

$$\tilde{\Upsilon}_{\alpha\beta}^R(\omega,\epsilon) \equiv \frac{\tilde{\Sigma}_\beta^R(\omega)-\tilde{\Sigma}_\beta^R(\epsilon+\Delta_\alpha-\Delta_\beta)}{\omega-\epsilon-\Delta_\alpha+\Delta_\beta \pm i0^+}, \quad (23)$$

where the sign of the infinitesimal imaginary part $i0^+$ is immaterial since it gives a vanishing contribution anyway, as can be easily checked. One can choose either sign for ease of calculation, or get rid of the imaginary part altogether. Equation (22) is the first important result of this work since it entirely determines the time-dependent current (10) for the downward step pulse.

B. Calculation of $\Psi_\alpha(\epsilon,t)$

From the explicit solution (22), we can calculate $\Psi_\alpha(\epsilon,t)$ which is needed to obtain the lesser current (8). We separate the integral over t' in Eq. (9) in two parts, one part over $(-\infty,0]$ involving only $A_\beta^\dagger(\epsilon',t'<0)=\bar{G}^A(\epsilon'+\Delta_\beta)$ and the other part over $[0,t]$ involving the Hermitian conjugate of the solution (22). This way we obtain

$$\int_{-\infty}^{t} dt' e^{-i(\epsilon-\epsilon')t'} e^{i\int_{t'}^{t} dt_1[\Delta_\alpha(t_1)-\Delta_\beta(t_1)]} A_\beta^\dagger(\epsilon',t') = \frac{i\bar{G}^A(\epsilon'+\Delta_\beta)}{\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta+i0^+} + B_\beta^\dagger(\epsilon,\epsilon',t),$$

where we have defined

$$B_\beta(\epsilon,\epsilon',t) \equiv \int_0^t dt' e^{i(\epsilon-\epsilon')t'} A_\beta(\epsilon',t'), \quad (24)$$

which is to be calculated from Eq. (22). Carrying out directly the integral over t', we obtain

$$B_\beta(\epsilon,\epsilon',t) = \mathrm{expc}(\epsilon-\epsilon'|t)\tilde{G}^R(\epsilon') + \int \frac{d\omega}{2\pi i}\frac{\mathrm{expc}(\epsilon-\omega|t)\tilde{G}^R(\omega)}{\omega-\epsilon'-\Delta_\beta-i0^+}\left[\frac{\Delta_\beta}{\omega-\epsilon'-i0^+} + \left(\Delta-\sum_\mu \Delta_\mu \tilde{\Upsilon}_{\beta\mu}^R(\omega,\epsilon')\right)\bar{G}^R(\epsilon'+\Delta_\beta)\right], \quad (25)$$

where by analogy with the sine cardinal function sinc x, we have defined a complex exponential cardinal function $\mathrm{expc}(z|t)$ as

$$\mathrm{expc}(z|t) \equiv \begin{cases} \dfrac{e^{izt}-1}{iz} & \text{for } z \neq 0, \\ t & \text{for } z=0, \end{cases} \quad (26)$$

which can be shown to be an entire function of z by the Riemann removable singularity theorem.[53] Its connection to the sine cardinal function is obvious from the relation $\mathrm{Re}\{\mathrm{expc}(\omega|t)\}=t\,\mathrm{sinc}\,\omega t$ valid for real ω,t.

The function $\Psi_\alpha(\epsilon,t)$ is thus given by

$$\Psi_\alpha(\epsilon,t) = i\sum_\beta \int \frac{d\epsilon'}{2\pi} e^{i(\epsilon-\epsilon')t} f(\epsilon') A_\beta(\epsilon',t)\Gamma_\beta(\epsilon') \times\left(\frac{i\bar{G}^A(\epsilon'+\Delta_\beta)}{\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta+i0^+} + B_\beta^\dagger(\epsilon,\epsilon',t)\right), \quad (27)$$

with $B_\beta(\epsilon,\epsilon',t)$ given in Eq. (25).

C. Initial and asymptotic currents

We now show that the current calculated from Eqs. (10), (22), and (27) satisfies two limits, namely the initial $t=0$ current which can be calculated otherwise from a standard dc transport nonequilibrium Green's-functions analysis, and the asymptotic $t\to\infty$ current which we expect to be zero.

1. Initial current (t=0)

We first show that $A_\alpha(\epsilon,0)=\bar{G}^R(\epsilon+\Delta_\alpha)$, that is, the solution (22) satisfies the boundary condition (17). Setting $t=0$ in Eq. (22), the integral over ω can be carried out by residue integration in the upper half plane. Choosing a minus sign for the infinitesimal imaginary part in Eq. (23), we see that $\omega=\epsilon+\Delta_\alpha-\Delta_\beta+i0^+$ is not a pole of $\tilde{Y}^R_{\alpha\beta}(\omega,\epsilon)$ since the residue vanishes. Summing over the only poles $\omega=\epsilon+\Delta_\alpha+i0^+$ and $\omega=\epsilon+i0^+$, we see that $\tilde{G}^R(\epsilon)$ cancels out and we obtain

$$A_\alpha(\epsilon,0)=\tilde{G}^R(\epsilon+\Delta_\alpha)+\tilde{G}^R(\epsilon+\Delta_\alpha)\Delta\bar{G}^R(\epsilon+\Delta_\alpha)$$
$$-\tilde{G}^R(\epsilon+\Delta_\alpha)\sum_\beta\Delta_\beta\tilde{Y}^R_{\alpha\beta}(\epsilon+\Delta_\alpha+i0^+,\epsilon)\bar{G}^R(\epsilon+\Delta_\alpha).$$

From Eq. (23), this is seen to be precisely the Dyson equation (16) for the steady-state nonequilibrium Green's function $\bar{G}^R(\omega)|_{\omega=\epsilon+\Delta_\alpha}$, so that we obtain $A_\alpha(\epsilon,0)=\bar{G}^R(\epsilon+\Delta_\alpha)$ as claimed.

We now turn to $\Psi_\alpha(\epsilon,0)$. From the definition (24), it is obvious that $B_\beta(\epsilon,\epsilon',0)=0$. Setting $t=0$ in Eq. (27) gives

$$\Psi_\alpha(\epsilon,0)=\sum_\beta\int\frac{d\epsilon'}{2\pi}f(\epsilon')\frac{\bar{G}^R(\epsilon'+\Delta_\beta)\Gamma_\beta(\epsilon')\bar{G}^A(\epsilon'+\Delta_\beta)}{\epsilon'-\epsilon-\Delta_\alpha+\Delta_\beta-i0^+},$$

so that upon substitution in Eq. (8), we obtain for the initial lesser current

$$J^<_\alpha(0)=-2e\sum_\beta\int\frac{d\epsilon}{2\pi}\int\frac{d\epsilon'}{2\pi}f(\epsilon')$$
$$\times\text{Im}\left\{\frac{\text{Tr}[\Gamma_\alpha(\epsilon)\bar{G}^R(\epsilon'+\Delta_\beta)\Gamma_\beta(\epsilon')\bar{G}^A(\epsilon'+\Delta_\beta)]}{\epsilon'-\epsilon-\Delta_\alpha+\Delta_\beta-i0^+}\right\}. \quad (28)$$

Since $\Gamma_\alpha(\epsilon)=i[\tilde{\Sigma}^R_\alpha(\epsilon)-\tilde{\Sigma}^A_\alpha(\epsilon)]$ is a Hermitian matrix and $\bar{G}^A(\epsilon)=[\bar{G}^R(\epsilon)]^\dagger$, one can easily show by cyclic invariance and using the property $(\text{Tr}[A])^*=\text{Tr}[A^\dagger]$ that the trace in Eq. (28) is a real quantity. Taking the imaginary part in Eq. (28) generates a delta function $\delta(\epsilon'-\epsilon-\Delta_\alpha+\Delta_\beta)$ so that the integral over ϵ' can be carried out trivially, and we obtain

$$J^<_\alpha(0)=-2e\int\frac{d\epsilon}{2\pi}\frac{1}{2i}\text{Tr}\{\bar{\Gamma}_\alpha(\epsilon)\bar{G}^<(\epsilon)\}, \quad (29)$$

where $\bar{G}^<(\epsilon)=\bar{G}^R(\epsilon)\bar{\Sigma}^<(\epsilon)\bar{G}^A(\epsilon)$ is the nonequilibrium lesser Green's function and $\bar{\Sigma}^<(\epsilon)=i\Sigma_\beta f_\beta(\epsilon)\bar{\Gamma}_\beta(\epsilon)$ is the nonequilibrium lesser self-energy, with the corresponding nonequilibrium quantities $f_\beta(\epsilon)\equiv f(\epsilon-\Delta_\beta)$ and $\bar{\Gamma}_\beta(\epsilon)\equiv\Gamma_\beta(\epsilon-\Delta_\beta)$.

From Eq. (6) and the previously shown relation $A_\alpha(\epsilon,0)=\bar{G}^R(\epsilon+\Delta_\alpha)$, we obtain for the retarded current

$$J^R_\alpha(0)=-2e\int\frac{d\epsilon}{2\pi}\text{Im Tr}\{f_\alpha(\epsilon)\bar{\Gamma}_\alpha(\epsilon)\bar{G}^R(\epsilon)\}=$$
$$-2e\int\frac{d\epsilon}{2\pi}\frac{1}{2i}\text{Tr}\{f_\alpha(\epsilon)\bar{\Gamma}_\alpha(\epsilon)[\bar{G}^R(\epsilon)-\bar{G}^A(\epsilon)]\}, \quad (30)$$

so that the total current is given by the sum of the lesser [Eq. (29)] and retarded [Eq. (30)] currents:

$$J_\alpha(0)=ie\int\frac{d\epsilon}{2\pi}\text{Tr}(\bar{\Gamma}_\alpha(\epsilon)\{\bar{G}^<(\epsilon)+f_\alpha(\epsilon)[\bar{G}^R(\epsilon)-\bar{G}^A(\epsilon)]\}),$$

a known result[20,44] from dc transport theory that can be rewritten as the more familiar Landauer-type expression,[2,45,54]

$$J_\alpha(0)=e\sum_\beta\int d\epsilon[f_\alpha(\epsilon)-f_\beta(\epsilon)]$$
$$\times\text{Tr}\{\bar{\Gamma}_\alpha(\epsilon)\bar{G}^R(\epsilon)\bar{\Gamma}_\beta(\epsilon)\bar{G}^A(\epsilon)\}, \quad (31)$$

using the Green's function relation[55] $\bar{G}^R(\epsilon)-\bar{G}^A(\epsilon)=-i\bar{G}^R(\epsilon)\bar{\Gamma}(\epsilon)\bar{G}^A(\epsilon)$ where $\bar{\Gamma}(\epsilon)=\Sigma_\beta\bar{\Gamma}_\beta(\epsilon)$. Our time-dependent solution therefore yields the correct initial current.

2. Asymptotic current (t→∞)

The proof that the asymptotic current $J_\alpha(\infty)$ vanishes proceeds along similar lines. We start by investigating the first contribution to the lesser current, arising from the term in $\Psi_\alpha(\epsilon,t)$ that contains $\bar{G}^A(\epsilon'+\Delta_\beta)$ [see Eq. (27)],

$$J^{<(1)}_\alpha(\infty)=\lim_{t\to\infty}2e\,\text{Im Tr}\sum_\beta\int\frac{d\epsilon}{2\pi}\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon')t}f(\epsilon')$$
$$\times\frac{\Gamma_\alpha(\epsilon)A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')\bar{G}^A(\epsilon'+\Delta_\beta)}{\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta+i0^+}.$$

By virtue of the Riemann-Lebesgue lemma,[56] the Fourier integral over ϵ vanishes and $J^{<(1)}_\alpha(\infty)=0$. The second contribution is given by

$$J^{<(2)}_\alpha(\infty)=\lim_{t\to\infty}2e\,\text{Im Tr}\sum_\beta\int\frac{d\epsilon}{2\pi i}\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon')t}f(\epsilon')$$
$$\times\Gamma_\alpha(\epsilon)A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')B^\dagger_\beta(\epsilon,\epsilon',t). \quad (32)$$

In this expression, the Riemann-Lebesgue lemma must be applied with care since factors of $e^{i\epsilon' t}$ or $e^{-i\epsilon t}$ hidden inside $A_\alpha(\epsilon',t)$ and $B^\dagger_\beta(\epsilon,\epsilon',t)$ can cancel out the $e^{i(\epsilon-\epsilon')t}$ factor in front of the Fermi function, yielding a nonvanishing contribution to the integral in the $t\to\infty$ limit. From Eq. (22), we know that $A_\beta(\epsilon',t)$ is the sum of a constant term plus a term with a time dependence of the form $e^{-i(\omega-\epsilon')t}$ under an integral over ω. As for $B^\dagger_\beta(\epsilon,\epsilon',t)$, we first notice from Eq. (26) that $\text{expc}^*(\omega|t)=\text{expc}(-\omega|t)$for real ω,t. Then from Eq. (25), we observe that $B^\dagger_\beta(\epsilon,\epsilon,t')$ consists of a first term with a time dependence of the form $e^{-i(\epsilon-\epsilon')t}-1$, hence a time-dependent term plus a constant term, plus a second term with a time dependence of the form $e^{-i(\epsilon-\omega)t}-1$ under an integral over ω, hence a time-dependent term plus another constant term. After having investigated the time dependence of the product $e^{i(\epsilon-\epsilon')t}A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')B^\dagger_\beta(\epsilon,\epsilon',t)$, a careful analysis of the cancellations mentioned above reveals that under the application of the Riemann-Lebesgue lemma to the Fourier integrals over ϵ and ϵ', the only nonvanishing contribution to Eq. (32) in the $t\to\infty$ limit is

$$J_\alpha^{<(2)}(\infty) = -2e\sum_\beta \int \frac{d\epsilon}{2\pi}\int \frac{d\epsilon'}{2\pi} f(\epsilon') \times \mathrm{Im}\left\{\frac{\mathrm{Tr}[\Gamma_\alpha(\epsilon)\tilde{G}^R(\epsilon')\Gamma_\beta(\epsilon')\tilde{G}^A(\epsilon')]}{\epsilon'-\epsilon-i0^+}\right\},$$

where we have exploited the analyticity of $\mathrm{expc}(z|t)$ to add a small imaginary part to ϵ and write $\mathrm{expc}(\epsilon'-\epsilon|t)=[e^{i(\epsilon'-\epsilon)t}-1]/i(\epsilon'-\epsilon-i0^+)$, a necessary step to ensure the integrability of the integrand over the real axis (a condition of applicability of the Riemann-Lebesgue lemma) as we express $\mathrm{expc}(\epsilon'-\epsilon|t)$ as the difference of a time-dependent part $\sim e^{i(\epsilon'-\epsilon)t}$ and a constant part. Following the same steps that lead from Eq. (28) to Eq. (29), we obtain

$$J_\alpha^<(\infty) = -2e\int \frac{d\epsilon}{2\pi}\frac{1}{2i}\mathrm{Tr}\{\Gamma_\alpha(\epsilon)\tilde{G}^<(\epsilon)\},$$

since $J_\alpha^<(\infty)=J_\alpha^{<(1)}(\infty)+J_\alpha^{<(2)}(\infty)$, and $\tilde{G}^<(\epsilon)=\tilde{G}^R(\epsilon)\tilde{\Sigma}^<(\epsilon)\tilde{G}^A(\epsilon)$ is the equilibrium lesser Green's function, with $\tilde{\Sigma}^<(\epsilon)=i\Sigma_\beta f(\epsilon)\Gamma_\beta(\epsilon)$ the equilibrium lesser self-energy. In the $t\to\infty$ limit, the Fourier integral over ω in Eq. (22) vanishes by the Riemann-Lebesgue lemma, so that we have $A_\alpha(\epsilon,\infty)=\tilde{G}^R(\epsilon)$. The retarded current is then given by

$$J_\alpha^R(\infty) = -2e\int \frac{d\epsilon}{2\pi}\frac{1}{2i}\mathrm{Tr}\{f(\epsilon)\Gamma_\alpha(\epsilon)[\tilde{G}^R(\epsilon)-\tilde{G}^A(\epsilon)]\},$$

so that the total asymptotic current is

$$J_\alpha(\infty) = ie\int \frac{d\epsilon}{2\pi}\mathrm{Tr}(\Gamma_\alpha(\epsilon)\{\tilde{G}^<(\epsilon)+f(\epsilon)[\tilde{G}^R(\epsilon)-\tilde{G}^A(\epsilon)]\}),$$

and vanishes as a result of the fluctuation-dissipation theorem[37] $\tilde{G}^<(\epsilon)=if(\epsilon)\tilde{a}(\epsilon)$ with the spectral function $\tilde{a}(\epsilon)=i[\tilde{G}^R(\epsilon)-\tilde{G}^A(\epsilon)]$, valid in equilibrium. Our time-dependent solution therefore correctly predicts that the current decays to zero as $t\to\infty$.

IV. CURRENT DRIVEN BY AN UPWARD STEP PULSE

In this section, we consider a system initially in equilibrium with zero bias. At $t=0$, a dc bias is suddenly applied and remains on for $t>0$, driving the system out of equilibrium. We study the transient current for $t>0$.

A. Calculation of $A_\alpha(\epsilon,t)$

As in Sec. III A, we first calculate the inhomogeneous term $\tilde{A}_\alpha(\epsilon,t)$ in Eq. (13). For an upward step pulse we obtain

$$\tilde{A}_\alpha(\epsilon,t) = \tilde{G}^R(\epsilon+\Delta_\alpha) - \int \frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon-\Delta_\alpha)t}\Delta_\alpha\tilde{G}^R(\omega)}{(\omega-\epsilon-\Delta_\alpha-i0^+)(\omega-\epsilon-i0^+)}, \quad (33)$$

for $t>0$.

In Eq. (13) the integration over t' ranges only over $[0,t]$ since $\Delta(t'<0)=0$ and $\tilde{G}^R(t<t')=0$. In addition, the retarded potential $V^R(t_1,t_2)$ vanishes when t_1 and t_2 are both less than zero, as can be seen from Eq. (12). Finally, $V^R(t_1<t_2)=0$ as before from causality so that the integration range for the double integral changes from $\mathbb{R}^2$ to $[0,t]\times(-\infty,t_1]$. Splitting the t_2 integration into two parts $(-\infty,0]\cup[0,t_1]$, we obtain the following integral equation for $A_\alpha(\epsilon,t)$:

$$A_\alpha(\epsilon,t) = A'_\alpha(\epsilon,t) + \int_0^t dt'\, e^{i(\epsilon+\Delta_\alpha)(t-t')}\tilde{G}^R(t-t')\Delta A_\alpha(\epsilon,t') + \int_0^t dt_1\int_0^{t_1} dt_2 e^{i(\epsilon+\Delta_\alpha)(t-t_1)} \times\tilde{G}^R(t-t_1)e^{i(\epsilon+\Delta_\alpha)(t_1-t_2)}V^R(t_1-t_2)A_\alpha(\epsilon,t_2), \quad (34)$$

where the retarded potential $V^R(t_1,t_2)$ is seen to depend only on the time difference t_1-t_2 over the integration domain $[0,t]\times[0,t_1]$, and $A'_\alpha(\epsilon,t)$ is defined as

$$A'_\alpha(\epsilon,t) = \tilde{A}_\alpha(\epsilon,t) + \int_0^t dt_1\int_{-\infty}^0 dt_2 e^{i\epsilon(t-t_2)}e^{i\Delta_\alpha t} \times\tilde{G}^R(t-t_1)V^R(t_1,t_2)A_\alpha(\epsilon,t_2), \quad (35)$$

and is known since it involves only $A_\alpha(\epsilon,t_2<0)$ and $\tilde{A}_\alpha(\epsilon,t)$ which is given in Eq. (33). From the definition (5), $A_\alpha(\epsilon,t<0)$ involves only $G^R(t<0,t'<0)$ which is equal to the equilibrium Green's function $\tilde{G}^R(t-t')$ in the case of the upward step, and describes the system before the pulse is applied. Since $\Delta_\alpha(t<0)=0$, Eq. (5) is simply the Fourier transform of $\tilde{G}^R(t-t')$ and we have $A_\alpha(\epsilon,t<0)=\tilde{G}^R(\epsilon)$. A calculation very similar to that of Eq. (21) yields

$$\int_0^t dt_1\int_{-\infty}^0 dt_2 e^{i\epsilon(t-t_2)}e^{i\Delta_\alpha t}\tilde{G}^R(t-t_1)V^R(t_1,t_2)A_\alpha(\epsilon,t_2) = \int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon-\Delta_\alpha)t}\tilde{G}^R(\omega)\sum_\beta\left(\frac{\tilde{\Sigma}^R_\beta(\omega-\Delta_\beta)-\tilde{\Sigma}^R_\beta(\epsilon)}{\omega-\Delta_\beta-\epsilon-i0^+} - \frac{\tilde{\Sigma}^R_\beta(\omega)-\tilde{\Sigma}^R_\beta(\epsilon)}{\omega-\epsilon-i0^+}\right)\tilde{G}^R(\epsilon). \quad (36)$$

Returning to Eq. (34), we see that unlike for the downward step pulse, $A_\alpha(\epsilon,t>0)$ is involved on both sides of the equation, so that we have a genuine integral equation. We, however, observe that it has the form of a Laplace convolution product,

$$A_\alpha(\epsilon,t) = A'_\alpha(\epsilon,t) + \int_0^t dt' F_\alpha(\epsilon,t-t')\Delta A_\alpha(\epsilon,t') + \int_0^t dt_1 \int_0^{t_1} dt_2 F_\alpha(\epsilon,t-t_1)U_\alpha(\epsilon,t_1-t_2)A_\alpha(\epsilon,t_2), \tag{37}$$

with the definitions $F_\alpha(\epsilon,t) \equiv e^{i(\epsilon+\Delta_\alpha)t}\tilde{G}^R(t)$ and $U_\alpha(\epsilon,t) \equiv e^{i(\epsilon+\Delta_\alpha)t}V^R(t)$. Equation (37) is therefore a Volterra equation of the second kind[57] and can be solved with Laplace transform techniques. Applying the Laplace transform operator $\mathcal{L}_{t\to\sigma}: \phi(t) \mapsto \phi(\sigma)$ where σ is the Laplace variable to both sides of Eq. (37), we obtain

$$A_\alpha(\epsilon,\sigma) = A'_\alpha(\epsilon,\sigma) + F_\alpha(\epsilon,\sigma)\Delta A_\alpha(\epsilon,\sigma) + F_\alpha(\epsilon,\sigma)U_\alpha(\epsilon,\sigma)A_\alpha(\epsilon,\sigma), \tag{38}$$

since the Laplace transform of a convolution product is the ordinary product of the Laplace transforms of the convoluted functions. Equation (38) is a Dyson-like algebraic matrix equation for $A_\alpha(\epsilon,\sigma)$ that can be readily solved by matrix inversion,

$$A_\alpha(\epsilon,\sigma) = \{1 - F_\alpha(\epsilon,\sigma)[\Delta + U_\alpha(\epsilon,\sigma)]\}^{-1}A'_\alpha(\epsilon,\sigma),$$

where 1 is to be understood as the unit matrix. The function $A_\alpha(\epsilon,t)$ is given by the inverse Laplace transform $\mathcal{L}^{-1}_{\sigma\to t}\{A_\alpha(\epsilon,\sigma)\}$ which is obtained from the Bromwich integral,[57]

$$A_\alpha(\epsilon,t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} d\sigma e^{\sigma t}A_\alpha(\epsilon,\sigma), \tag{39}$$

where $\gamma > 0$ is chosen so that all the singularities of $A_\alpha(\epsilon,\sigma)$ in the complex σ plane lie to the left of the Bromwich integration contour $C: \gamma - i\infty \to \gamma + i\infty$, but is otherwise arbitrary.

The quantity $F_\alpha(\epsilon,\sigma) = \int_0^\infty dt\, e^{-\sigma t}e^{i(\epsilon+\Delta_\alpha)t}\tilde{G}^R(t)$ is easily seen to be

$$F_\alpha(\epsilon,\sigma) = \int \frac{d\omega}{2\pi i}\frac{\tilde{G}^R(\omega)}{\omega - \epsilon - \Delta_\alpha - i\sigma} = \tilde{G}^R(\epsilon + \Delta_\alpha + i\sigma), \tag{40}$$

by residue integration in the upper half plane, since $\mathrm{Re}\,\sigma = \gamma > 0$ implies that $\mathrm{Im}\{\epsilon+\Delta_\alpha+i\sigma\} > 0$. Similarly, from Eq. (12) one has $V^R(t) = \sum_\beta[e^{-i\Delta_\beta t} - 1]\tilde{\Sigma}^R_\beta(t)$, so that we have

$$U_\alpha(\epsilon,\sigma) = \sum_\beta \int \frac{d\omega}{2\pi i}\tilde{\Sigma}^R_\beta(\omega) \times \left(\frac{1}{\omega - \epsilon - \Delta_\alpha + \Delta_\beta - i\sigma} - \frac{1}{\omega - \epsilon - \Delta_\alpha - i\sigma}\right) = \sum_\beta [\tilde{\Sigma}^R_\beta(\epsilon + \Delta_\alpha - \Delta_\beta + i\sigma) - \tilde{\Sigma}^R_\beta(\epsilon + \Delta_\alpha + i\sigma)]. \tag{41}$$

We now turn to the calculation of $A'_\alpha(\epsilon,\sigma)$. From Eqs. (35), (33), and (36), we have

$$A'_\alpha(\epsilon,\sigma) = \frac{\tilde{G}^R(\epsilon+\Delta_\alpha)}{\sigma} + \int \frac{d\omega}{2\pi i}\frac{\tilde{G}^R(\omega)}{\sigma + i(\omega - \epsilon - \Delta_\alpha)} \times \left[\sum_\beta \left(\frac{\tilde{\Sigma}^R_\beta(\omega - \Delta_\beta) - \tilde{\Sigma}^R_\beta(\epsilon)}{\omega - \Delta_\beta - \epsilon - i0^+} - \frac{\tilde{\Sigma}^R_\beta(\omega) - \tilde{\Sigma}^R_\beta(\epsilon)}{\omega - \epsilon - i0^+}\right) \times \tilde{G}^R(\epsilon) - \frac{\Delta_\alpha}{(\omega - \epsilon - \Delta_\alpha - i0^+)(\omega - \epsilon - i0^+)}\right], \tag{42}$$

from the Laplace transforms $\mathcal{L}_{t\to\sigma}\{e^{-i\lambda t}\} = 1/(\sigma + i\lambda)$ and $\mathcal{L}_{t\to\sigma}\{1\} = 1/\sigma$. The ω integral can be performed using Jordan's lemma and closing the contour in the upper half plane. As mentioned previously, the $\tilde{\Upsilon}$ functions are analytic in the upper half plane and the only poles are $\omega = \epsilon + \Delta_\alpha + i\sigma$ as well as $\omega = \epsilon + i0^+$ and $\omega = \epsilon + \Delta_\alpha + i0^+$ arising from the last term in Eq. (42). Summing over the poles, one obtains after some algebra

$$A'_\alpha(\epsilon,\sigma) = \frac{i[\tilde{G}^R(\epsilon) + \Delta_\alpha\tilde{G}^R(\epsilon + \Delta_\alpha + i\sigma)/i\sigma]}{\Delta_\alpha + i\sigma} + i\tilde{G}^R(\epsilon+\Delta_\alpha+i\sigma) \times \sum_\beta \left(\frac{\tilde{\Sigma}^R_\beta(\epsilon + \Delta_\alpha + i\sigma) + \Delta_\beta\tilde{\Sigma}^R_\beta(\epsilon)/(\Delta_\alpha - \Delta_\beta + i\sigma)}{\Delta_\alpha + i\sigma} - \frac{\tilde{\Sigma}^R_\beta(\epsilon + \Delta_\alpha - \Delta_\beta + i\sigma)}{\Delta_\alpha - \Delta_\beta + i\sigma}\right)\tilde{G}^R(\epsilon), \tag{43}$$

from which $A_\alpha(\epsilon,t)$ can be calculated according to Eq. (39). The structure of $A_\alpha(\epsilon,\sigma) = K_\alpha(\epsilon,\sigma)A'_\alpha(\epsilon,\sigma)$ where $K_\alpha(\epsilon,\sigma) \equiv \{1 - F_\alpha(\epsilon,\sigma)[\Delta + U_\alpha(\epsilon,\sigma)]\}^{-1}$ can, however, be somewhat simplified prior to evaluating the Bromwich integral. Indeed, we first notice from Eqs. (40) and (41) that

$$K_\alpha(\epsilon,\sigma) = \bar{G}^R(\epsilon + \Delta_\alpha + i\sigma)[\tilde{G}^R]^{-1}(\epsilon + \Delta_\alpha + i\sigma), \tag{44}$$

from the Dyson equation (16) which can be analytically continued in the upper half plane $\omega + i0^+ \to z$, $\mathrm{Im}\, z > 0$ since it involves only retarded quantities. Pulling a factor $1/(\Delta_\alpha + i\sigma)$ in front of $A'_\alpha(\epsilon,\sigma)$ in Eq. (43) and using the relation $[\tilde{G}^R]^{-1}(\epsilon+\Delta_\alpha+i\sigma) + \sum_\beta[\tilde{\Sigma}^R_\beta(\epsilon+\Delta_\alpha+i\sigma) - \tilde{\Sigma}^R_\beta(\epsilon+\Delta_\alpha-\Delta_\beta+i\sigma)] = \Delta + [\bar{G}^R]^{-1}(\epsilon+\Delta_\alpha+i\sigma)$ from the Dyson equation, it is possible to show that $A'_\alpha(\epsilon,\sigma)$ can be written as

$$A'_\alpha(\epsilon,\sigma) = \frac{i\tilde{G}^R(\epsilon+\Delta_\alpha+i\sigma)}{\Delta_\alpha + i\sigma}\left[\frac{\Delta_\alpha}{i\sigma} + \left(\Delta + [\bar{G}^R]^{-1}(\epsilon + \Delta_\alpha + i\sigma) + \sum_\beta \frac{\Delta_\beta[\tilde{\Sigma}^R_\beta(\epsilon) - \tilde{\Sigma}^R_\beta(\epsilon + \Delta_\alpha - \Delta_\beta + i\sigma)]}{\Delta_\alpha - \Delta_\beta + i\sigma}\right)\tilde{G}^R(\epsilon)\right].$$

Forming the product $K_\alpha(\epsilon,\sigma)A'_\alpha(\epsilon,\sigma)$, we see from Eq. (44) that the factor of $\tilde{G}^R(\epsilon+\Delta_\alpha+i\sigma)$ cancels, and we obtain

$$A_\alpha(\epsilon,\sigma)=\frac{i}{i\sigma+\Delta_\alpha}\left\{\tilde{G}^R(\epsilon)+\bar{G}^R(i\sigma+\epsilon+\Delta_\alpha)\left[\frac{\Delta_\alpha}{i\sigma}+\left(\Delta+\sum_\beta\frac{\Delta_\beta[\tilde{\Sigma}^R_\beta(\epsilon)-\tilde{\Sigma}^R_\beta(i\sigma+\epsilon+\Delta_\alpha-\Delta_\beta)]}{i\sigma+\Delta_\alpha-\Delta_\beta}\right)\tilde{G}^R(\epsilon)\right]\right\}.$$

In order to see more clearly the similarity with the solution for the downward step Eq. (22), we now perform a change of variables $i\sigma\to z$ so that the vertical contour $C_\sigma:\gamma-i\infty\to\gamma+i\infty$ is rotated by $\pi/2$ counterclockwise into $C'_z:\infty+i\gamma\to-\infty+i\gamma$ which runs antiparallel to the real axis. The Bromwich integral (39) thus becomes

$$A_\alpha(\epsilon,t)=\int_{\infty+i\gamma}^{-\infty+i\gamma}\frac{dz}{2\pi i}\frac{e^{-izt}}{z+\Delta_\alpha}\times\left\{\tilde{G}^R(\epsilon)+\bar{G}^R(z+\epsilon+\Delta_\alpha)\left[\frac{\Delta_\alpha}{z}+\left(\Delta+\sum_\beta\frac{\Delta_\beta[\tilde{\Sigma}^R_\beta(\epsilon)-\tilde{\Sigma}^R_\beta(z+\epsilon+\Delta_\alpha-\Delta_\beta)]}{z+\Delta_\alpha-\Delta_\beta}\right)\tilde{G}^R(\epsilon)\right]\right\}. \tag{45}$$

The first term is easily evaluated by closing the contour in the lower half plane and picking up the contribution of the only pole at $z=-\Delta_\alpha$, so that $\int_{C'_z}(dz/2\pi i)e^{-izt}\tilde{G}^R(\epsilon)/(z+\Delta_\alpha)=e^{i\Delta_\alpha t}\tilde{G}^R(\epsilon)$. Note that since the closed contour runs counterclockwise, there is no minus sign. Furthermore, the analytic structure of the integrand in Eq. (45) is now clear: the only singularities are the poles at $z=-\Delta_\alpha$ and $z=0$ on the real axis arising from the factors $1/(z+\Delta_\alpha)$ and $1/z$, as well as the poles of the nonequilibrium Green's function $\bar{G}^R(z+\epsilon+\Delta_\alpha)$ and the self-energy $\tilde{\Sigma}^R_\beta(z+\epsilon+\Delta_\alpha-\Delta_\beta)$, which lie in the lower half of the complex z plane. Note however that the poles $z=z^i_{\alpha\beta}(\epsilon)$ of $\tilde{\Sigma}^R_\beta(z+\epsilon+\Delta_\alpha-\Delta_\beta)$ yield a vanishing contribution to the integral, since $\bar{G}^R(z^i_{\alpha\beta}(\epsilon)+\epsilon+\Delta_\alpha)=0$. Indeed, the Green's function vanishes wherever the self-energy becomes infinite because the self-energy appears in the denominator of the Green's function, as can be seen from the explicit solution to the Dyson equation that follows Eq. (16).

In any case, since all the singularities are on or below the real axis, we can set $\gamma\to 0^+$ to bring down the contour to just infinitesimally above the real axis. With the change of variables $z\to\omega-\epsilon+i0^+$, Eq. (45) can then be rewritten as an integral over the real axis from $-\infty$ to ∞,

$$\begin{aligned}A_\alpha(\epsilon,t)&=e^{i\Delta_\alpha t}\tilde{G}^R(\epsilon)\\&\quad-\int\frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon)t}\bar{G}^R(\omega+\Delta_\alpha)}{\omega-\epsilon+\Delta_\alpha+i0^+}\left[\frac{\Delta_\alpha}{\omega-\epsilon+i0^+}\right.\\&\quad\left.+\left(\Delta-\sum_\beta\Delta_\beta\tilde{\Upsilon}^R_{\alpha\beta}(\epsilon,\omega)\right)\tilde{G}^R(\epsilon)\right].\end{aligned}\tag{46}$$

In order to exhibit more clearly the similarity between the upward and downward step pulses, we use the identity $1/(\omega+i0^+)=1/(\omega-i0^+)-2\pi i\delta(\omega)$ to reverse the sign of the infinitesimal imaginary parts in Eq. (46). It is then easily shown by making use of the Dyson equation (16) that the additional terms resulting from the delta functions cancel exactly with the first term $e^{i\Delta_\alpha t}\tilde{G}^R(\epsilon)$. We finally obtain

$$\begin{aligned}A_\alpha(\epsilon,t)&=\bar{G}^R(\epsilon+\Delta_\alpha)\\&\quad-\int\frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon)t}\bar{G}^R(\omega+\Delta_\alpha)}{\omega-\epsilon+\Delta_\alpha-i0^+}\left[\frac{\Delta_\alpha}{\omega-\epsilon-i0^+}\right.\\&\quad\left.+\left(\Delta-\sum_\beta\Delta_\beta\tilde{\Upsilon}^R_{\alpha\beta}(\epsilon,\omega)\right)\tilde{G}^R(\epsilon)\right],\end{aligned}\tag{47}$$

which is to be compared with the solution for the downward step pulse (22). One sees that $\tilde{G}^R(\omega)$ and $\bar{G}^R(\omega+\Delta_\alpha)$ play a somewhat symmetric role in the two solutions. Equation (47) is the second important result of this work since it entirely determines the time-dependent current (10) for the upward step pulse.

An important remark is in order at this point, which will aid to justify the seemingly arbitrary choice of the sign of the infinitesimal imaginary part in Eqs. (22) and (47). Both solutions contain an integral over all frequencies ω. Because of the Fourier factor $e^{-i(\omega-\epsilon)t}$ with $t>0$, these integrals along the real axis can be performed by adding an infinite semicircle in the lower half plane to close the contour. One sees that the integral is then entirely determined by the singularities enclosed by this contour. By choosing a negative infinitesimal imaginary part as we did, we ensure that the poles at $\omega=\epsilon+i0^+$ and $\omega=\epsilon\pm\Delta_\alpha+i0^+$ lie in the upper half plane and do not contribute to the integral. As a result, the integral is entirely determined by the poles of the Green's functions, $\tilde{G}^R(\omega)$ for the downward step and $\bar{G}^R(\omega+\Delta_\alpha)$ for the upward step. In other words, only the poles with a physical meaning (renormalized energy level and quasiparticle lifetime) contribute to the dynamics of the time-dependent current. The other poles are spurious and give canceling contributions as has been seen.

B. Calculation of $\Psi_\alpha(\epsilon,t)$

As before, we need to calculate $\Psi_\alpha(\epsilon,t)$ from Eq. (9). Since $A^\dagger_\beta(\epsilon',t'<0)=\tilde{G}^A(\epsilon')$, we have

$$\int_{-\infty}^t dt'\,e^{-i(\epsilon-\epsilon')t'}e^{i\int_{t'}^t dt_1[\Delta_\alpha(t_1)-\Delta_\beta(t_1)]}A^\dagger_\beta(\epsilon',t')$$

$$=e^{i(\Delta_\alpha-\Delta_\beta)t}\left(\frac{i\tilde{G}^A(\epsilon')}{\epsilon-\epsilon'+i0^+}+B^\dagger_{\alpha\beta}(\epsilon,\epsilon',t)\right),$$

where we have defined

$$B_{\alpha\beta}(\epsilon,\epsilon',t)\equiv\int_0^t dt'\,e^{i(\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta)t'}A_\beta(\epsilon',t'), \tag{48}$$

which is to be calculated from Eq. (47). Performing the integral over t' yields

$$\begin{aligned}B_{\alpha\beta}(\epsilon,\epsilon',t)&=\mathrm{expc}(\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta|t)\bar{G}^R(\epsilon'+\Delta_\beta)\\&-\int\frac{d\omega}{2\pi i}\frac{\mathrm{expc}(\epsilon-\omega+\Delta_\alpha-\Delta_\beta|t)\bar{G}^R(\omega+\Delta_\beta)}{\omega-\epsilon'+\Delta_\beta-i0^+}\\&\times\left[\frac{\Delta_\beta}{\omega-\epsilon'-i0^+}\right.\\&\left.+\left(\Delta-\sum_\mu\Delta_\mu\tilde{\Upsilon}^R_{\beta\mu}(\epsilon',\omega)\right)\tilde{G}^R(\epsilon')\right].\end{aligned} \tag{49}$$

The function $\Psi_\alpha(\epsilon,t)$ is thus given by

$$\begin{aligned}\Psi_\alpha(\epsilon,t)&=i\sum_\beta\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta)t}f(\epsilon')A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')\\&\times\left(\frac{i\tilde{G}^A(\epsilon')}{\epsilon-\epsilon'+i0^+}+B^\dagger_{\alpha\beta}(\epsilon,\epsilon',t)\right).\end{aligned} \tag{50}$$

C. Initial and asymptotic currents

In this section we show that the time-dependent current calculated from Eqs. (10), (47), and (50) satisfies two boundary conditions: the initial current at $t=0$ is zero and the asymptotic $t\to\infty$ current is the same current that can be calculated from a steady-state Green's function analysis for a system under dc bias. In particular, it is equal to the initial current for the downward step, Eq. (31).

1. Initial current $(t=0)$

Setting $t=0$ in the solution (47), we can close the integration contour in the upper half plane since the Fourier factor $e^{-i(\omega-\epsilon)t}$ is absent. Picking up the two poles at $\omega=\epsilon-\Delta_\alpha+i0^+$ and $\omega=\epsilon+i0^+$ and using the Dyson equation (16) as in Sec. III C 1, we obtain $A_\alpha(\epsilon,0)=\tilde{G}^R(\epsilon)$.

We now turn to investigate $\Psi_\alpha(\epsilon,0)$. From Eq. (48), we have $B_{\alpha\beta}(\epsilon,\epsilon',0)=0$. Setting $t=0$ in Eq. (50) gives

$$\Psi_\alpha(\epsilon,0)=\sum_\beta\int\frac{d\epsilon'}{2\pi}f(\epsilon')\frac{\tilde{G}^R(\epsilon')\Gamma_\beta(\epsilon')\tilde{G}^A(\epsilon')}{\epsilon'-\epsilon-i0^+}.$$

Following the same line of reasoning that led to Eq. (29), we get

$$J^<_\alpha(0)=-2e\int\frac{d\epsilon}{2\pi}\frac{1}{2i}\,\mathrm{Tr}\{\Gamma_\alpha(\epsilon)\tilde{G}^<(\epsilon)\},$$

and since $A_\alpha(\epsilon,0)=\tilde{G}^R(\epsilon)$, we get from Eq. (6)

$$J^R_\alpha(0)=-2e\int\frac{d\epsilon}{2\pi}\,\mathrm{Im}\,\mathrm{Tr}\{f(\epsilon)\Gamma_\alpha(\epsilon)\tilde{G}^R(\epsilon)\},$$

so that we recover exactly the results of Sec. III C 2 for the asymptotic current under a downward step pulse. As a result of the fluctuation-dissipation theorem, the total initial current vanishes, $J_\alpha(0)=J^R_\alpha(0)+J^<_\alpha(0)=0$.

2. Asymptotic current $(t\to\infty)$

We investigate the lesser current $J^<_\alpha(\infty)$ first. The contribution to the lesser current that arises from the term in $\Psi_\alpha(\epsilon,t)$ that contains $\tilde{G}^A(\epsilon')$ is [see Eq. (50)]

$$\begin{aligned}J^{<(1)}_\alpha(\infty)&=\lim_{t\to\infty}2e\,\mathrm{Im}\,\mathrm{Tr}\sum_\beta\int\frac{d\epsilon}{2\pi}\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon')t}f(\epsilon')\\&\times e^{i(\Delta_\alpha-\Delta_\beta)t}\frac{\Gamma_\alpha(\epsilon)A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')\tilde{G}^A(\epsilon')}{\epsilon-\epsilon'+i0^+},\end{aligned}$$

and is zero by virtue of the Riemann-Lebesgue lemma as applied to the Fourier integral over ϵ. The second contribution is

$$\begin{aligned}J^{<(2)}_\alpha(\infty)&=\lim_{t\to\infty}2e\,\mathrm{Im}\,\mathrm{Tr}\sum_\beta\int\frac{d\epsilon}{2\pi i}\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon')t}f(\epsilon')\\&\times e^{i(\Delta_\alpha-\Delta_\beta)t}\Gamma_\alpha(\epsilon)A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')B^\dagger_{\alpha\beta}(\epsilon,\epsilon',t),\end{aligned}$$

and requires a more thoughtful analysis as explained in Sec. III C 2. A careful investigation of the cancellations among time-dependent phase factors shows that the only surviving contribution is

$$\begin{aligned}J^{<(2)}_\alpha(\infty)&=-2e\sum_\beta\int\frac{d\epsilon}{2\pi}\int\frac{d\epsilon'}{2\pi}f(\epsilon')\\&\times\mathrm{Im}\left(\frac{\mathrm{Tr}[\Gamma_\alpha(\epsilon)\bar{G}^R(\epsilon'+\Delta_\beta)\Gamma_\beta(\epsilon')\bar{G}^A(\epsilon'+\Delta_\beta)]}{\epsilon'-\epsilon-\Delta_\alpha+\Delta_\beta-i0^+}\right),\end{aligned}$$

which is exactly the result of Eq. (28) for the initial lesser current in the case of the downward step pulse. Consequently, we have

$$J^<_\alpha(\infty)=-2e\int\frac{d\epsilon}{2\pi}\frac{1}{2i}\,\mathrm{Tr}[\bar{\Gamma}_\alpha(\epsilon)\bar{G}^<(\epsilon)],$$

since $J^{<(1)}_\alpha(\infty)=0$.

We now turn to the retarded current $J^R_\alpha(\infty)$. By the Riemann-Lebesgue lemma, the integral over ω in Eq. (47) vanishes in the $t\to\infty$ limit and we are left with $A_\alpha(\epsilon,\infty)=\bar{G}^R(\epsilon+\Delta_\alpha)$. Hence $J^R_\alpha(\infty)$ is given by Eq. (30). As shown before, summing the two contributions $J_\alpha(\infty)=J^R_\alpha(\infty)+J^<_\alpha(\infty)$ yields the Landauer formula (31). We have thus shown that the asymptotic current for the upward step is the same as the initial current for the downward step.

V. CURRENT DRIVEN BY A SQUARE PULSE

In this section, we consider a system initially in equilibrium, subject to the following time-dependent square voltage pulse of finite length s,

$$\Delta_{(\alpha)}(t) = \begin{cases} \Delta_{(\alpha)} & \text{for } 0 < t < s, \\ 0 & \text{for } t < 0 \text{ and } t > s. \end{cases} \quad (51)$$

After the voltage is turned on at $t=0$, we expect the time-dependent current for $0<t<s$ to be the same as that for the upward step pulse, by causality. However, because of the finite duration of the square pulse, the current for $t>s$ is *not* the same as that for the downward pulse, since the current does not have the time to reach its steady-state value before the voltage is turned off.

A. Calculation of $A_\alpha(\epsilon,t)$

The causality requirement implies by Eq. (5) that we know $A_\alpha(\epsilon,t<s)$. Our analysis will therefore focus on finding $A_\alpha(\epsilon,t>s)$. As in previous sections, we first obtain the integral equation satisfied by $A_\alpha(\epsilon,t>s)$. In the case of a square pulse, we have from Eqs. (51) and (12) that $V^R(t_1,t_2)=0$ for $t_1,t_2<0$ and $t_1,t_2>s$. Furthermore, $\Delta(t')=0$ outside the interval $[0,s]$. Equation (13) then becomes

$$A_\alpha(\epsilon,t) = \widetilde{A}_\alpha(\epsilon,t) + \int_0^s dt' e^{i\epsilon(t-t')} e^{i\Delta_\alpha(s-t')} \widetilde{G}^R(t-t')\Delta A_\alpha(\epsilon,t') + \left(\int_0^s dt_1 \int_{-\infty}^{t_1} dt_2 + \int_s^t dt_1 \int_{-\infty}^{s} dt_2\right) e^{i\epsilon(t-t_2)} \times e^{i\int_{t_2}^t dt_3 \Delta_\alpha(t_3)} \widetilde{G}^R(t-t_1) V^R(t_1,t_2) A_\alpha(\epsilon,t_2), \quad (52)$$

for $t>s$. Equation (52) is again seen to be of the Wiener-Hopf type and requires only the knowledge of $A_\alpha(\epsilon,t<s)$. From Eq. (5), we have $A_\alpha(\epsilon,t<0)=\widetilde{G}^R(\epsilon)$ before the pulse, as has been shown in Sec. IV A. In the interval $0<t<s$, we are in the upward step case and $A_\alpha(\epsilon,0<t<s)$ is given by Eqs. (46) or (47). For convenience however, we will use Eq. (46) since it involves only singularities in the lower half plane, which eases the calculations.

The inhomogeneous term $\widetilde{A}_\alpha(\epsilon,t) = \int_{-\infty}^t dt' e^{i\epsilon(t-t')} e^{i\int_{t'}^t dt_1 \Delta_\alpha(t_1)} \widetilde{G}^R(t-t')$ is given by

$$\widetilde{A}_\alpha(\epsilon,t) = \left(\int_{-\infty}^0 dt' e^{i\Delta_\alpha s} + \int_0^s dt' e^{i\Delta_\alpha(s-t')} + \int_s^t dt'\right) e^{i\epsilon(t-t')} \widetilde{G}^R(t-t') = \widetilde{G}^R(\epsilon) + e^{i\Delta_\alpha s} \int \frac{d\omega}{2\pi i} e^{-i(\omega-\epsilon)t} \widetilde{G}^R(\omega) \chi_\alpha^{(-)}(\omega,\epsilon), \quad (53)$$

where we have defined

$$\chi_\alpha^{(\pm)}(\omega,\epsilon) \equiv \frac{\Delta_\alpha[e^{i(\omega-\epsilon\pm\Delta_\alpha)s}-1]}{(\omega-\epsilon\pm\Delta_\alpha-i0^+)(\omega-\epsilon-i0^+)}. \quad (54)$$

The second term in Eq. (52) is given by

$$\int_0^s dt' e^{i\epsilon(t-t')} e^{i\Delta_\alpha(s-t')} \widetilde{G}^R(t-t') \Delta A_\alpha(\epsilon,t') = e^{i\Delta_\alpha s} \int \frac{d\omega}{2\pi i} e^{-i(\omega-\epsilon)t} \widetilde{G}^R(\omega) \Delta \left[\left(\frac{e^{i(\omega-\epsilon)s}-1}{\omega-\epsilon-i0^+}\right) \widetilde{G}^R(\epsilon) - \int \frac{d\omega'}{2\pi i} Q_\alpha(\omega,\omega',\epsilon)\right], \quad (55)$$

where we have defined

$$Q_\alpha(\omega,\omega',\epsilon) \equiv \frac{e^{i(\omega-\omega'-\Delta_\alpha)s} \widetilde{G}^R(\omega'+\Delta_\alpha)}{(\omega'-\epsilon+\Delta_\alpha+i0^+)(\omega-\omega'-\Delta_\alpha-i0^+)} \left[\frac{\Delta_\alpha}{\omega'-\epsilon+i0^+} + \left(\Delta - \sum_\mu \Delta_\mu \widetilde{\Upsilon}^R_{\alpha\mu}(\epsilon,\omega')\right) \widetilde{G}^R(\epsilon)\right]. \quad (56)$$

Finally, a lengthy but straightforward calculation of the two double integrals in Eq. (52) yields

$$\left(\int_0^s dt_1 \int_{-\infty}^{t_1} dt_2 + \int_s^t dt_1 \int_{-\infty}^{s} dt_2\right) e^{i\epsilon(t-t_2)} e^{i\int_{t_2}^t dt_3 \Delta_\alpha(t_3)} \times \widetilde{G}^R(t-t_1) V^R(t_1,t_2) A_\alpha(\epsilon,t_2) = e^{i\Delta_\alpha s} \int \frac{d\omega}{2\pi i} e^{-i(\omega-\epsilon)t} \widetilde{G}^R(\omega) \left[\sum_\beta [\chi_\beta^{(-)}(\omega,\epsilon) \widetilde{\Sigma}^R_\beta(\epsilon) - e^{-i\Delta_\beta s} \chi_\beta^{(+)}(\omega,\epsilon) \widetilde{\Sigma}^R_\beta(\omega)] \widetilde{G}^R(\epsilon) + \int \frac{d\omega'}{2\pi i} \sum_\beta \Delta_\beta \left(\widetilde{\Upsilon}^R_{\alpha\beta}(\omega,\omega') Q_\alpha(\omega,\omega',\epsilon) + \frac{\chi_\beta^{(-)}(\omega,\omega') \widetilde{\Sigma}^R_\beta(\omega') \widetilde{G}^R(\epsilon)}{(\omega'-\epsilon+\Delta_\beta+i0^+)(\omega'-\epsilon+i0^+)}\right)\right]. \quad (57)$$

Adding the three contributions Eqs. (53), (55), and (57) yields the solution

$$A_\alpha(\epsilon,t) = \widetilde{G}^R(\epsilon) + e^{i\Delta_\alpha s} \int \frac{d\omega}{2\pi i} e^{-i(\omega-\epsilon)t} \widetilde{G}^R(\omega) \Bigg\{ \chi_\alpha^{(-)}(\omega,\epsilon) + \left[\left(\frac{e^{i(\omega-\epsilon)s}-1}{\omega-\epsilon-i0^+}\right)\Delta + \sum_\beta [\chi_\beta^{(-)}(\omega,\epsilon) \widetilde{\Sigma}^R_\beta(\epsilon) - e^{-i\Delta_\beta s} \chi_\beta^{(+)}(\omega,\epsilon) \widetilde{\Sigma}^R_\beta(\omega)]\right] \widetilde{G}^R(\epsilon)$$

$$+\int\frac{d\omega'}{2\pi i}\Bigg[\sum_\beta\frac{\Delta_\beta\chi_\beta^{(-)}(\omega,\omega')\tilde{\Sigma}_\beta^R(\omega')\tilde{G}^R(\epsilon)}{(\omega'-\epsilon+\Delta_\beta+i0^+)(\omega'-\epsilon+i0^+)} - \Big(\Delta-\sum_\beta\Delta_\beta\tilde{\Upsilon}_{\alpha\beta}^R(\omega,\omega')\Big)Q_\alpha(\omega,\omega',\epsilon)\Bigg]\Bigg\}, \quad (58)$$

for $t>s$. Equation (58) is the third important result of this work, and together with Eq. (47) determines entirely the time-dependent current driven by a square pulse.

B. Calculation of $\Psi_\alpha(\epsilon,t)$

We now calculate $\Psi_\alpha(\epsilon,t)$ from Eq. (9). By causality, $\Psi_\alpha(\epsilon,0<t<s)$ is given by Eq. (50). For $t>s$, we have

$$\int_{-\infty}^t dt' e^{-i(\epsilon-\epsilon')t'}e^{i\int_{t'}^t dt_1[\Delta_\alpha(t_1)-\Delta_\beta(t_1)]}A_\beta^\dagger(\epsilon',t') = e^{i(\Delta_\alpha-\Delta_\beta)s}\Big(\frac{i\tilde{G}^A(\epsilon')}{\epsilon-\epsilon'+i0^+}+B_{\alpha\beta}^\dagger(\epsilon,\epsilon',s) + e^{-i(\Delta_\alpha-\Delta_\beta)s}B_\beta^>(\epsilon,\epsilon',t)^\dagger\Big),$$

where $B_{\alpha\beta}(\epsilon,\epsilon',s)$ is given by Eq. (49), and we define $B_\beta^>(\epsilon,\epsilon',t)$ for $t>s$ as

$$B_\beta^>(\epsilon,\epsilon',t)\equiv\int_s^t dt' e^{i(\epsilon-\epsilon')t'}A_\beta(\epsilon',t'>s),$$

which is to be calculated from the square pulse solution Eq. (58). Performing the integration over t', we obtain

$$B_\beta^>(\epsilon,\epsilon',t) = e^{i(\epsilon-\epsilon')s}\mathrm{expc}(\epsilon-\epsilon'|t-s)\tilde{G}^R(\epsilon') + e^{i\Delta_\beta s}\int\frac{d\omega}{2\pi i}e^{i(\epsilon-\omega)s}\mathrm{expc}(\epsilon-\omega|t-s)\tilde{G}^R(\omega)$$
$$\times\Bigg\{\chi_\beta^{(-)}(\omega,\epsilon')+\Bigg[\Bigg(\frac{e^{i(\omega-\epsilon')s}-1}{\omega-\epsilon'-i0^+}\Bigg)\Delta+\sum_\mu[\chi_\mu^{(-)}(\omega,\epsilon')\tilde{\Sigma}_\mu^R(\epsilon')-e^{-i\Delta_\mu s}\chi_\mu^{(+)}(\omega,\epsilon')\tilde{\Sigma}_\mu^R(\omega)]\Bigg]\tilde{G}^R(\epsilon')$$
$$+\int\frac{d\omega'}{2\pi i}\Bigg[\sum_\mu\frac{\Delta_\mu\chi_\mu^{(-)}(\omega,\omega')\tilde{\Sigma}_\mu^R(\omega')\tilde{G}^R(\epsilon')}{(\omega'-\epsilon'+\Delta_\mu+i0^+)(\omega'-\epsilon'+i0^+)}-\Big(\Delta-\sum_\mu\Delta_\mu\tilde{\Upsilon}_{\beta\mu}^R(\omega,\omega')\Big)Q_\beta(\omega,\omega',\epsilon')\Bigg]\Bigg\}. \quad (59)$$

The function $\Psi_\alpha(\epsilon,t)$ is then given by

$$\Psi_\alpha(\epsilon,t)=i\sum_\beta\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon')t}f(\epsilon')A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')e^{i(\Delta_\alpha-\Delta_\beta)s}\Bigg(\frac{i\tilde{G}^A(\epsilon')}{\epsilon-\epsilon'+i0^+}+B_{\alpha\beta}^\dagger(\epsilon,\epsilon',s)+e^{-i(\Delta_\alpha-\Delta_\beta)s}B_\beta^>(\epsilon,\epsilon',t)^\dagger\Bigg). \quad (60)$$

C. Boundary conditions

Since the solution for $t<s$ is the same as that for the upward step pulse, it follows from Sec. IV C 1 that $J_\alpha(0)=0$. The $t\to\infty$ limit is given as previously by a careful application of the Riemann-Lebesgue lemma. Repeating the analysis in Sec. IV C 2, we see that the contribution to the lesser current $J_\alpha^<(t)$ from the time-independent terms $\tilde{G}^A(\epsilon')$ and $B_{\alpha\beta}^\dagger(\epsilon,\epsilon',s)$ in $\Psi_\alpha(\epsilon,t)$ vanishes in this limit. We are left with

$$J_\alpha^<(\infty)=\lim_{t\to\infty}2e\,\mathrm{Im}\,\mathrm{Tr}\sum_\beta\int\frac{d\epsilon}{2\pi i}\int\frac{d\epsilon'}{2\pi}e^{i(\epsilon-\epsilon')t}f(\epsilon') \times\Gamma_\alpha(\epsilon)A_\beta(\epsilon',t)\Gamma_\beta(\epsilon')B_\beta^>(\epsilon,\epsilon',t)^\dagger.$$

As can be shown from Eqs. (58) and (59), cancelations of the time-dependent phase factors among $e^{i(\epsilon-\epsilon')t}$, $A_\beta(\epsilon',t)$, and $B_\beta^>(\epsilon,\epsilon',t)$ are such that only the first term in $A_\beta(\epsilon',t)$ and the first term in $B_\beta^>(\epsilon,\epsilon',t)$ contribute in the $t\to\infty$ limit. We thus obtain

$$J_\alpha^<(\infty)=-2e\sum_\beta\int\frac{d\epsilon}{2\pi}\int\frac{d\epsilon'}{2\pi}f(\epsilon')\times\mathrm{Im}\Bigg(\frac{\mathrm{Tr}[\Gamma_\alpha(\epsilon)\tilde{G}^R(\epsilon')\Gamma_\beta(\epsilon')\tilde{G}^A(\epsilon')]}{\epsilon'-\epsilon-i0^+}\Bigg),$$

a result that was obtained previously for the downward step. Furthermore, by applying the Riemann-Lebesgue lemma to Eq. (58) we see that $A_\alpha(\epsilon,\infty)=\tilde{G}^R(\epsilon)$, hence we recover exactly the results of Sec. III C 2 and $J_\alpha(\infty)=0$. As expected, the time-dependent current driven by a downward step pulse and a square pulse have the same asymptotic behavior, but may have a different behavior on short time scales after turnoff.

D. Causality

We will now provide an additional check on Eq. (58) by showing that we recover the upward step solution (47) if we replace s by t in Eq. (58), which follows from causality.[19]

Upon setting $s=t$ in Eq. (58), the factor $e^{-i\omega t}$ in the integral over ω cancels against the factor $e^{i\omega t}$ in $\chi_\beta^{(\pm)}(\omega,\epsilon)|_{s\to t}$ from Eq. (54), so that some of the integrals can be performed analytically by closing the contour in the upper half plane where the retarded functions are analytic. In this way, we can show that the first integral in Eq. (58) is given by

$$e^{i\Delta_\alpha t}\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\chi_\alpha^{(-)}(\omega,\epsilon)_t=(e^{i\Delta_\alpha t}-1)\tilde{G}^R(\epsilon) - \int\frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon)t}\Delta_\alpha\tilde{G}^R(\omega+\Delta_\alpha)}{(\omega-\epsilon+\Delta_\alpha+i0^+)(\omega-\epsilon+i0^+)},\tag{61}$$

where we use the notation $\chi_\alpha^{(\pm)}(\omega,\epsilon)_t\equiv\chi_\alpha^{(\pm)}(\omega,\epsilon)|_{s\to t}$. Similarly we obtain

$$e^{i\Delta_\alpha t}\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\left(\frac{e^{i(\omega-\epsilon)t}-1}{\omega-\epsilon-i0^+}\right)\Delta\tilde{G}^R(\epsilon) = -\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\frac{\tilde{G}^R(\omega+\Delta_\alpha)\Delta\tilde{G}^R(\epsilon)}{\omega-\epsilon+\Delta_\alpha+i0^+}.\tag{62}$$

The next two terms become

$$e^{i\Delta_\alpha t}\sum_\beta\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\Big[\chi_\beta^{(-)}(\omega,\epsilon)_t\tilde{\Sigma}_\beta^R(\epsilon) - e^{-i\Delta_\beta t}\chi_\beta^{(+)}(\omega,\epsilon)_t\tilde{\Sigma}_\beta^R(\omega)\Big]\tilde{G}^R(\epsilon) = e^{i\Delta_\alpha t}\sum_\beta\Delta_\beta\int\frac{d\omega}{2\pi i}\frac{e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)}{\omega-\epsilon+i0^+}\left(\frac{e^{-i\Delta_\beta t}\tilde{\Sigma}_\beta^R(\omega)}{\omega-\epsilon+\Delta_\beta+i0^+} - \frac{\tilde{\Sigma}_\beta^R(\epsilon)}{\omega-\epsilon-\Delta_\beta+i0^+}\right)\tilde{G}^R(\epsilon).\tag{63}$$

The double integrals can be reduced to simple integrals,

$$e^{i\Delta_\alpha t}\sum_\beta\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\int\frac{d\omega'}{2\pi i}\frac{\Delta_\beta\chi_\beta^{(-)}(\omega,\omega')_t\tilde{\Sigma}_\beta^R(\omega')\tilde{G}^R(\epsilon)}{(\omega'-\epsilon+\Delta_\beta+i0^+)(\omega'-\epsilon+i0^+)} = e^{i\Delta_\alpha t}\sum_\beta\Delta_\beta\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon+\Delta_\beta)t}\frac{\big[\tilde{G}^R(\omega+\Delta_\beta)-\tilde{G}^R(\omega)\big]\tilde{\Sigma}_\beta^R(\omega)\tilde{G}^R(\epsilon)}{(\omega-\epsilon+\Delta_\beta+i0^+)(\omega-\epsilon+i0^+)},\tag{64}$$

where we have used the Dyson equation (16), and we also have

$$e^{i\Delta_\alpha t}\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\int\frac{d\omega'}{2\pi i}\times\left(\Delta-\sum_\beta\Delta_\beta\tilde{Y}_{\alpha\beta}^R(\omega,\omega')\right)Q_\alpha(\omega,\omega',\epsilon)_t = \int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\frac{\tilde{G}^R(\omega+\Delta_\alpha)-\tilde{G}^R(\omega+\Delta_\alpha)}{\omega-\epsilon+\Delta_\alpha+i0^+}\times\left[\frac{\Delta_\alpha}{\omega-\epsilon+i0^+}+\left(\Delta-\sum_\beta\Delta_\beta\tilde{Y}_{\alpha\beta}^R(\epsilon,\omega)\right)\tilde{G}^R(\epsilon)\right],\tag{65}$$

where we have used the notation $Q_\alpha(\omega,\omega',\epsilon)_t\equiv Q_\alpha(\omega,\omega',\epsilon)|_{s\to t}$. As we put together the different contributions Eqs. (61)–(65) as well as the first time-independent term $\tilde{G}^R(\epsilon)$ in Eq. (58), most of the terms cancel out and we are left with the result of Eq. (46), which is equivalent to Eq. (47). Our solution thus satisfies the causality requirement. Alternatively, by setting $t=s$ we have shown that $A_\alpha(\epsilon,t>s)|_{t=s}=A_\alpha(\epsilon,t<s)|_{t=s}$, which means that the two solutions connect continuously at the turnoff point $t=s$.

VI. SINGLE-LEVEL MODEL WITH LORENTZIAN LINEWIDTH

The discussion so far has been quite general and applies to an arbitrary noninteracting central scattering region connected to external leads described by an arbitrary energy-dependent linewidth function $\Gamma_\alpha(\epsilon)$. We will now apply the formal results Eqs. (22), (47), and (58) to the simplest model capable of exhibiting nontrivial finite-bandwidth effects, a single-level quantum dot with Lorentzian linewidth.

A. Lorentzian model

The model is described by the Hamiltonian (1), but the scattering region consists of a single state $|0\rangle$ with on-site energy ϵ_0 and hopping strength $t_{\mathbf{k}\alpha}$,

$$H=\sum_{\mathbf{k}\alpha}\epsilon_{\mathbf{k}\alpha}(t)c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha}+\epsilon_0(t)d^\dagger d+\sum_{\mathbf{k}\alpha}(t_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}^\dagger d+t_{\mathbf{k}\alpha}^* d^\dagger c_{\mathbf{k}\alpha}),$$

where $\epsilon_0(t)=\epsilon_0+\Delta(t)$ and $\epsilon_{\mathbf{k}\alpha}(t)=\epsilon_{\mathbf{k}\alpha}+\Delta_\alpha(t)$. The propagators and self-energies for the scattering region thus become scalars instead of matrices. The linewidth $\Gamma_\alpha(\epsilon)\equiv 2\pi\rho_\alpha(\epsilon)|t_\alpha(\epsilon)|^2$ is chosen to be Lorentzian,

$$\Gamma_\alpha(\epsilon)=\frac{\Gamma_\alpha^0 W^2}{\epsilon^2+W^2},\tag{66}$$

where Γ_α^0 is the linewidth amplitude and W is the bandwidth. Lorentzian linewidths provide a mathematically convenient way to introduce finite-bandwidth effects and have been used in several problems such as in Anderson model calculations,[58,59] where a high-energy cutoff is needed to regularize ultraviolet divergences. The simple analytic properties of Lorentzian linewidths are such that it is often possible to obtain analytical solutions in closed form. Perhaps the best example is a remarkable property of the Hubbard model in infinite dimensions,[60] where the use of a Lorentzian density of states yields an exact solution for a model of strongly correlated particles, which is rather rare.

The linewidth function (66) has two simple poles at $\omega = \pm iW$ with residues

$$R_\alpha^{\Gamma(\pm)} \equiv \operatorname*{Res}_{\omega=\pm iW} \Gamma_\alpha(\omega) = \mp \frac{i\Gamma_\alpha^0 W}{2}.$$

We obtain the self-energies $\widetilde{\Sigma}_\alpha^{R,A}(\omega)$ from their spectral (Lehmann) representations where the spectral density is the linewidth function (66),

$$\widetilde{\Sigma}_\alpha^{R,A}(\omega) = \int \frac{d\epsilon}{2\pi} \frac{\Gamma_\alpha(\epsilon)}{\omega - \epsilon \pm i0^+} = \frac{1}{2} \frac{\Gamma_\alpha^0 W}{\omega \pm iW},$$

where the plus (minus) sign corresponds to the retarded (advanced) self-energy. The equilibrium retarded Green's function is given by

$$\widetilde{G}^R(\omega) = \frac{1}{\omega - \epsilon_0 - \Gamma W/2(\omega + iW)},$$

where $\Gamma \equiv \Sigma_\alpha \Gamma_\alpha^0$ is the total linewidth amplitude. The poles of $\widetilde{G}^R(\omega)$ are the roots of the following second-order algebraic equation:

$$\omega^2 - (\epsilon_0 - iW)\omega - iW\left(\epsilon_0 - \frac{i\Gamma}{2}\right) = 0,$$

and are given by

$$\widetilde{\omega}_\pm = \frac{\epsilon_0 - iW \pm \sqrt{(\epsilon_0 + iW)^2 + 2\Gamma W}}{2},$$

so that the Green's function can be written as

$$\widetilde{G}^R(\omega) = \frac{\omega + iW}{(\omega - \widetilde{\omega}_+)(\omega - \widetilde{\omega}_-)}.$$

The residues are given by

$$\widetilde{R}_\pm \equiv \operatorname*{Res}_{\omega=\widetilde{\omega}_\pm} \widetilde{G}^R(\omega) = \pm \frac{\widetilde{\omega}_\pm + iW}{\delta\widetilde{\omega}},$$

where $\delta\widetilde{\omega} \equiv \widetilde{\omega}_+ - \widetilde{\omega}_- = \sqrt{(\epsilon_0 + iW)^2 + 2\Gamma W}$. From the discussion following Eq. (16), we see that the nonequilibrium retarded Green's function is

$$\bar{G}^R(\omega) = \frac{1}{\omega - \epsilon_0 - \Delta - \frac{1}{2}\sum_\beta \frac{\Gamma_\beta^0 W}{\omega - \Delta_\beta + iW}}.$$

In what follows, we will choose $\Delta_R = 0$ and $\Delta_L \neq 0$ to simplify the algebra, without loss of generality since only relative energy shifts are relevant.[19] The poles of $\bar{G}^R(\omega)$ are now

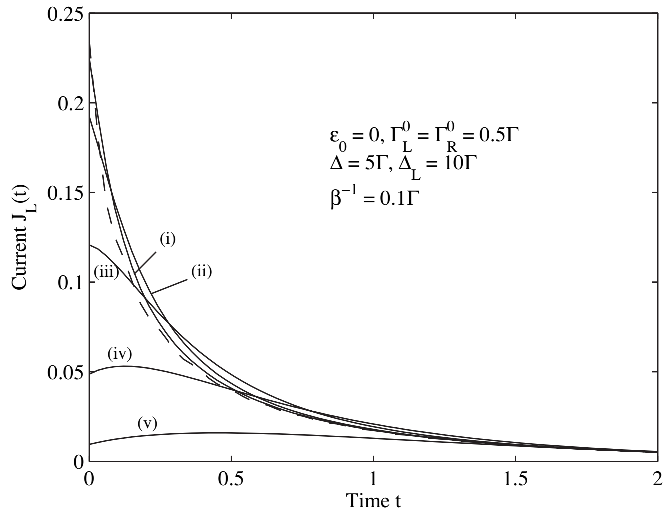

FIG. 2. Time-dependent current $J_L(t)$ through left lead in response to a downward step pulse for different bandwidths: dashed line, WBL ($W=\infty$); (i) $W=20\Gamma$, (ii) $W=10\Gamma$, (iii) $W=5\Gamma$, (iv) $W=2.5\Gamma$, and (v) $W=\Gamma$. The current is in units of $e\Gamma/\hbar$ and the time is in units of $\hbar/\Gamma$ where $\Gamma=\Gamma_L^0+\Gamma_R^0$ is the total linewidth amplitude. Parameters are taken the same as in Ref. 19. When $W=100\Gamma$, the result was found (not shown) to be indistinguishable from the $W=\infty$ curve.

given by the roots of a third-order algebraic equation,

$$\omega^3 + b\omega^2 - c\omega + d = 0, \tag{67}$$

with

$$b \equiv 2iW - \epsilon_0 - \Delta - \Delta_L;$$

$$c \equiv \frac{\Gamma W}{2} + (W + i\Delta_L)W + (\epsilon_0 + \Delta)(2iW - \Delta_L);$$

$$d \equiv (\epsilon_0 + \Delta)(W + i\Delta_L)W + \frac{W}{2}\left(\Gamma_R^0 \Delta_L - i\Gamma W\right).$$

The roots of Eq. (67) are given by

$$\bar{\omega}_1 = -\frac{b}{3} + \left(\frac{2}{Q}\right)^{1/3}\left(c + \frac{b^2}{3}\right) + \frac{1}{3}\left(\frac{Q}{2}\right)^{1/3};$$

$$\bar{\omega}_2 = -\frac{b}{3} - \frac{1 + i\sqrt{3}}{2^{2/3}Q^{1/3}}\left(c + \frac{b^2}{3}\right) - \frac{1 - i\sqrt{3}}{6}\left(\frac{Q}{2}\right)^{1/3};$$

$$\bar{\omega}_3 = -\frac{b}{3} - \frac{1 - i\sqrt{3}}{2^{2/3}Q^{1/3}}\left(c + \frac{b^2}{3}\right) - \frac{1 + i\sqrt{3}}{6}\left(\frac{Q}{2}\right)^{1/3},$$

where we define $Q \equiv -2b^3 - 9bc - 27d + \vartheta$ and $\vartheta \equiv \sqrt{(2b^3 + 9bc + 27d)^2 - 4(b^2 + 3c)^3}$. The Green's function can then be written as

$$\bar{G}^R(\omega) = \frac{(\omega - \Delta_L + iW)(\omega + iW)}{(\omega - \bar{\omega}_1)(\omega - \bar{\omega}_2)(\omega - \bar{\omega}_3)},$$

with the residues given by

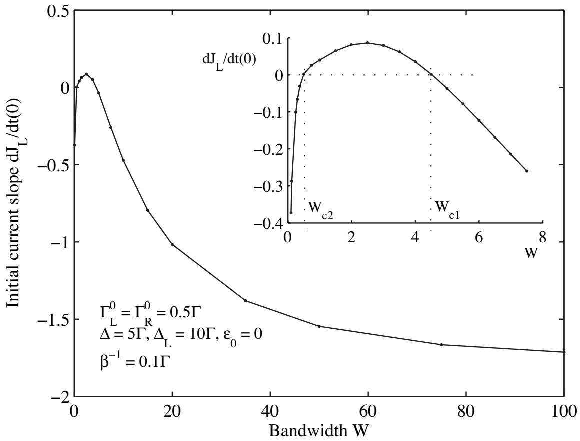

FIG. 3. Time derivative of the current through the left lead $dJ_L(t)/dt$ at $t=0$. The bandwidth W is in units of Γ and the time derivative $\partial_t J_L(0)$ is in units of $e\Gamma^2/\hbar^2$. The inset shows a closeup view of the interval around the critical bandwidths $W_{c1}\sim 4.53\Gamma$ and $W_{c2}\sim 0.49\Gamma$ where the slope changes sign.

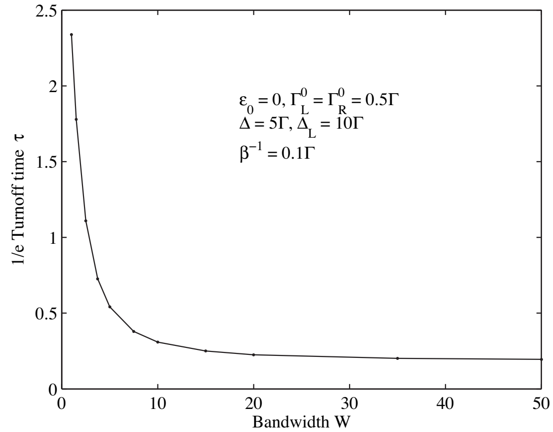

FIG. 4. $1/e$ turnoff time τ (in units of $\hbar/\Gamma$) as a function of bandwidth W (in units of Γ).

$$\bar{R}_i \equiv \operatorname*{Res}_{\omega=\bar{\omega}_i} \bar{G}^R(\omega) = \frac{2(\bar{\omega}_i - \Delta_L + iW)(\bar{\omega}_i + iW)}{\sum_{j,k=1}^{3} |\epsilon_{ijk}|(\bar{\omega}_i - \bar{\omega}_j)(\bar{\omega}_i - \bar{\omega}_k)},$$

for $i=1,2,3$, where ϵ_{ijk} is the usual Levi-Cività symbol.

B. Exact solution

With the poles of the Green's functions explicitly known, it is possible to calculate $A_\alpha(\epsilon,t)$ from Eqs. (22), (47), and (58) by residue integration.

1. Downward step pulse

The integral in Eq. (22) is readily performed by closing the contour in the lower half plane and summing over the poles $\tilde{\omega}_\pm$ of the equilibrium Green's function. No other singularities contribute to the integral as has been previously discussed. We obtain

$$A_\alpha(\epsilon,t) = \tilde{G}^R(\epsilon) - \sum_{i=\pm} \frac{\tilde{R}_i e^{-i(\tilde{\omega}_i-\epsilon)t}}{\tilde{\omega}_i - \epsilon - \Delta_\alpha} \times \left(\frac{\Delta_\alpha}{\tilde{\omega}_i - \epsilon} + [\Delta - \Delta_L \tilde{\Upsilon}^R_{\alpha L}(\tilde{\omega}_i,\epsilon)]\bar{G}^R(\epsilon+\Delta_\alpha) \right), \tag{68}$$

and

$$B_\beta(\epsilon,\epsilon',t) = \operatorname{expc}(\epsilon-\epsilon'|t)\tilde{G}^R(\epsilon') - \sum_{i=\pm} \frac{\tilde{R}_i \operatorname{expc}(\epsilon-\tilde{\omega}_i|t)}{\tilde{\omega}_i - \epsilon' - \Delta_\beta} \times \left(\frac{\Delta_\beta}{\tilde{\omega}_i - \epsilon'} + [\Delta - \Delta_L \tilde{\Upsilon}^R_{\beta L}(\tilde{\omega}_i,\epsilon')]\bar{G}^R(\epsilon'+\Delta_\beta) \right),$$

from Eq. (25). The integral in the expression for the retarded current (6) is then performed numerically. The integral over ϵ in the expression for the lesser current (8) can be performed analytically by closing the contour in the upper half plane, picking up the pole of $\Gamma_\alpha(\epsilon)$ at $\epsilon=iW$. We have

$$\int \frac{d\epsilon}{2\pi} \frac{e^{i\epsilon t}\Gamma_\alpha(\epsilon)}{\epsilon - \epsilon' + \Delta_\alpha - \Delta_\beta + i0^+} = \frac{iR_\alpha^{\Gamma(+)} e^{-Wt}}{iW - \epsilon' + \Delta_\alpha - \Delta_\beta},$$

and

$$\int \frac{d\epsilon}{2\pi} e^{i\epsilon t}\Gamma_\alpha(\epsilon) B_\beta^\dagger(\epsilon,\epsilon',t) = iR_\alpha^{\Gamma(+)} e^{-Wt} B_\beta^\dagger(\epsilon,\epsilon',t)\bigg|_{\epsilon=iW}.$$

The remaining integral over ϵ' is performed numerically as well, so that the total time-dependent current $J_\alpha(t)$ is determined analytically up to one integral.

We show the results of the calculation for a typical choice of parameters in Fig. 2. When the bandwidth W dominates all the other energy scales Γ,Δ,Δ_L of the problem, the WBL result is seen to be correct. The WBL approximation, however, gets poorer as the bandwidth is decreased and becomes comparable to the other energy scales, $W\sim\Gamma,\Delta,\Delta_L$. First of all, the WBL yields the wrong initial current. This is obvious from Eq. (31) which requires that $\Gamma_\alpha(\epsilon)$ be integrated over all energies in order to obtain the right initial current. In addition, interesting finite-bandwidth effects occur that do not show up in the WBL. In the case $W\sim\Gamma$ for example, we see from the curves (iv) and (v) in Fig. 2 that the current can *increase* after the bias is turned off. This effect has also been observed in a previous numerical study[46] for a system with leads described by a one-dimensional tight-binding model.

In order to further characterize this effect, we calculate the initial slope of the time-dependent current, $\partial_t J_L(0) \equiv dJ_L(t)/dt|_{t=0}$. From Eqs. (10), (27), (24), and (68), we can show that

$$\partial_t J_\alpha(0) = -2e \int \frac{d\epsilon}{2\pi} f(\epsilon) \operatorname{Im}\Bigg[\Gamma_\alpha(\epsilon)\partial_t A_\alpha(\epsilon,0) - R_\alpha^{\Gamma(+)} \times \sum_\beta \Gamma_\beta(\epsilon) \left(\frac{(\Delta_\alpha - \Delta_\beta)\bar{G}^R(\epsilon+\Delta_\beta) + i\partial_t A_\beta(\epsilon,0)}{iW - \epsilon + \Delta_\alpha - \Delta_\beta} \right) \times \bar{G}^A(\epsilon+\Delta_\beta) \Bigg],$$

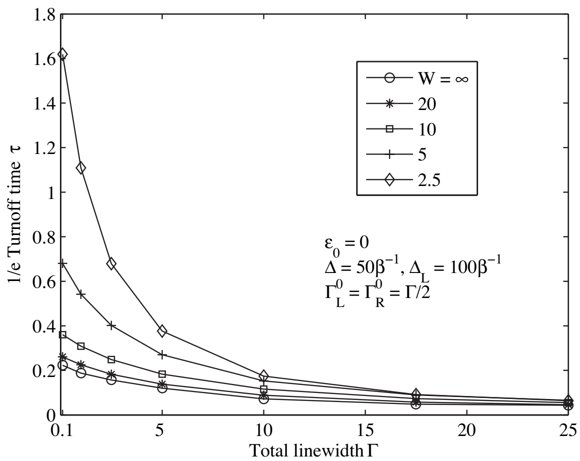

FIG. 5. $1/e$ turnoff time τ as a function of total linewidth Γ. Energies (Γ and W) are in units of $10\beta^{-1}$ and τ is in units of $\hbar/(10\beta^{-1})$.

where $\partial_t A_\alpha(\epsilon,0)\equiv \partial A_\alpha(\epsilon,t)/\partial t|_{t=0}$ is given by

$$\partial_t A_\alpha(\epsilon,0) = i\sum_{i=\pm}\tilde{R}_i\left(1+\frac{\Delta_\alpha}{\tilde{\omega}_i-\epsilon-\Delta_\alpha}\right)\times\left(\frac{\Delta_\alpha}{\tilde{\omega}_i-\epsilon}+[\Delta-\Delta_L\tilde{\Upsilon}^R_{\alpha L}(\tilde{\omega}_i,\epsilon)]\bar{G}^R(\epsilon+\Delta_\alpha)\right).$$

In Fig. 3 we plot the initial slope $\partial_t J_L(0)$ as a function of the bandwidth W. When the bandwidth is large, the initial slope of the current is negative, as we expect. As the bandwidth is reduced, the slope in absolute value decreases and becomes zero when a first critical bandwidth W_{c1} is reached. For $W<W_{c1}$, the slope is positive until W reaches a second critical bandwidth W_{c2}, at which point it changes sign again.

A useful parameter that can be extracted from the calculation for the downward step pulse is the turnoff time of the device. We define a $1/e$ turnoff time τ as the time after which the current has dropped to $1/e$ of its initial value, i.e., $J_L(\tau)/J_L(0)=1/e$. Such a parameter is a natural measure of the "speed" of a nanoscale device. In Fig. 4 we plot the turnoff time τ as a function of the bandwidth W. The turnoff time is seen to increase sharply as the bandwidth is reduced and becomes comparable to the pulse strength Δ,Δ_L. Indeed, a narrow band in the leads means that less states are available for electrons to tunnel and for charge to leak out of the central scattering region. In other words, tunneling electrons see a smaller effective coupling $\Gamma_{\rm eff}<\Gamma$ to the leads and are forced to stay longer in the central region.

In Fig. 5 we plot the dependence of the turnoff time τ on the total linewidth Γ, for different bandwidths W. The turnoff time is seen to increase with decreasing linewidth, as expected from the previous discussion: electrons that are weakly coupled to the external reservoirs have a longer lifetime inside the central scattering region. The turnoff time is also seen to depend more strongly on the linewidth for smaller bandwidths, which is a consequence of the nonlinear dependence of τ on W exhibited in Fig. 4.

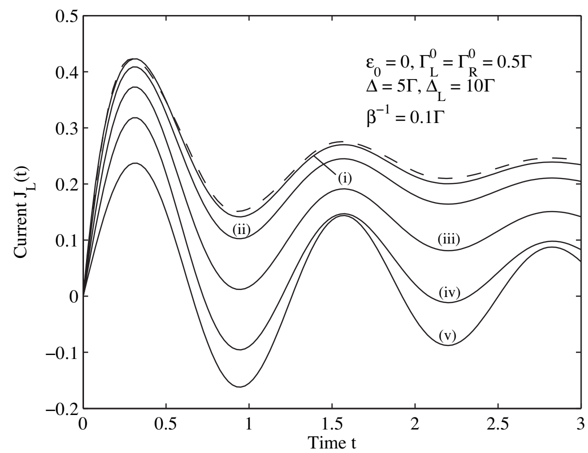

FIG. 6. Time-dependent current $J_L(t)$ through left lead in response to an upward step pulse for different bandwidths: dashed line, WBL ($W=\infty$); (i) $W=20\Gamma$, (ii) $W=10\Gamma$, (iii) $W=5\Gamma$, (iv) $W=2.5\Gamma$, and (v) $W=\Gamma$. Units and parameters are the same as in Fig. 2. Here again, the $W=100\Gamma$ curve (not shown) is indistinguishable from the $W=\infty$ curve.

2. Upward step pulse

In this case, the integral in Eq. (47) is determined by the poles of the nonequilibrium Green's function $\bar{G}^R(\omega+\Delta_\alpha)$ which occur at $\omega=\bar{\omega}_i-\Delta_\alpha$ for $i=1,2,3$. We obtain

$$A_\alpha(\epsilon,t) = \bar{G}^R(\epsilon+\Delta_\alpha)+\sum_{i=1}^{3}\frac{\bar{R}_i e^{-i(\bar{\omega}_i-\epsilon-\Delta_\alpha)t}}{\bar{\omega}_i-\epsilon}\times\left(\frac{\Delta_\alpha}{\bar{\omega}_i-\epsilon-\Delta_\alpha}+[\Delta-\Delta_L\tilde{\Upsilon}^R_{\alpha L}(\epsilon,\bar{\omega}_i-\Delta_\alpha)]\tilde{G}^R(\epsilon)\right), \tag{69}$$

as well as

$$B_{\alpha\beta}(\epsilon,\epsilon',t) = \mathrm{expc}(\epsilon-\epsilon'+\Delta_\alpha-\Delta_\beta|t)\bar{G}^R(\epsilon'+\Delta_\beta)+\sum_{i=1}^{3}\frac{\bar{R}_i\mathrm{expc}(\epsilon-\bar{\omega}_i+\Delta_\alpha|t)}{\bar{\omega}_i-\epsilon'}\times\left(\frac{\Delta_\beta}{\bar{\omega}_i-\epsilon'-\Delta_\beta}+[\Delta-\Delta_L\tilde{\Upsilon}^R_{\beta L}(\epsilon',\bar{\omega}_i-\Delta_\beta)]\tilde{G}^R(\epsilon')\right),$$

from Eq. (49). As in the previous section, we have

$$\int\frac{d\epsilon}{2\pi}\frac{e^{i\epsilon t}\Gamma_\alpha(\epsilon)}{\epsilon-\epsilon'+i0^+} = \frac{iR_\alpha^{\Gamma(+)}e^{-Wt}}{iW-\epsilon'},$$

and

$$\int\frac{d\epsilon}{2\pi}e^{i\epsilon t}\Gamma_\alpha(\epsilon)B^\dagger_{\alpha\beta}(\epsilon,\epsilon',t) = iR_\alpha^{\Gamma(+)}e^{-Wt}B^\dagger_{\alpha\beta}(\epsilon,\epsilon',t)\bigg|_{\epsilon=iW}.$$

In Fig. 6 we plot the time-dependent current for the upward step pulse. As in Fig. 2, the WBL is seen to be essentially correct for large bandwidths. As the bandwidth de-

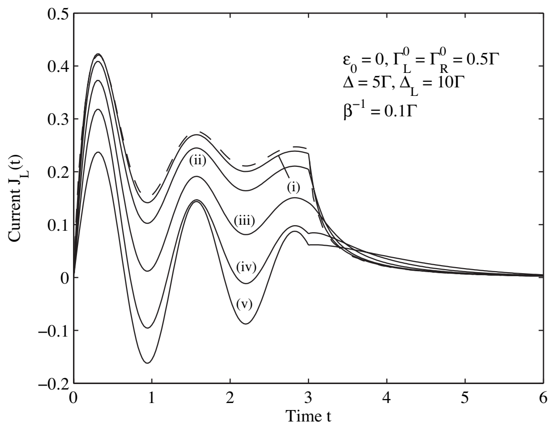

FIG. 7. Time-dependent current $J_L(t)$ through left lead in response to a square pulse of duration $s=3\hbar/\Gamma$ for different bandwidths: dashed line, WBL ($W=\infty$); (i) $W=20\Gamma$, (ii) $W=10\Gamma$, (iii) $W=5\Gamma$, (iv) $W=2.5\Gamma$, and (v) $W=\Gamma$. Units and parameters are the same as in Fig. 2. Here again, the $W=100\Gamma$ curve (not shown) is indistinguishable from the $W=\infty$ curve.

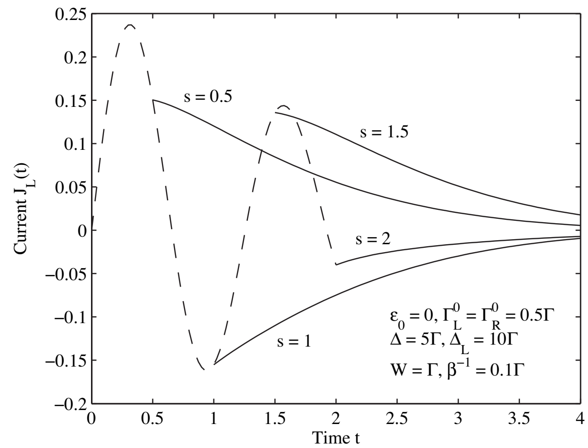

FIG. 8. Time-dependent current $J_L(t)$ through left lead in response to a square pulse, for different pulse lengths s in units of $\hbar/\Gamma$. Other units are the same as in Fig. 2. Dashed line: current during the pulse; solid line: current after the pulse.

creases, the effective coupling Γ_{eff} gets smaller and the asymptotic current is reduced accordingly, corresponding to the decrease in initial current for the downward step, described in the previous section. Another interesting finite-bandwidth effect is the fact that a positive voltage step pulse can instantaneously drive a negative current [curves (iv) and (v) in Fig. 6]. This effect has been observed previously.[46]

3. Square pulse

Starting from Eqs. (58) and (59), calculations in the case of the square pulse are performed by straightforward residue integration as in the two previous cases, but yield rather lengthy and unilluminating results that will not be reproduced here. There are, however, no difficulties of principle and the time-dependent current is still determined analytically up to one integral which is performed numerically.

In Figs. 7 and 8 we plot the time-dependent current for the square pulse. Once again, the WBL is correct for large bandwidths. If the pulse length s is smaller or comparable to the period of oscillations[19] in the current $\Delta t=2\pi\hbar/(\Delta_L-\Delta)$, the current response for $t>s$ may differ from the response to a downward step (Fig. 2), especially for $W\sim\Gamma$ (e.g., Fig. 8) where the current is positive in Fig. 2 but can be either positive or negative in Fig. 8. Indeed, if the bias is turned off before the current can stabilize to its steady-state value, the instantaneous current right after the turnoff can be either positive or negative in the case of narrow bandwidths.

C. Wideband limit

In the WBL, $\Gamma_\alpha(\omega)=\Gamma_\alpha$ is independent of energy and the exact time-dependent nonequilibrium Green's function $G^R(t,t')$ only differs from the equilibrium Green's function $\tilde{G}^R(t-t')$ by a simple time-dependent phase factor:[19,20,43,48]

$$G^R(t,t')=e^{-i\int_{t'}^{t}dt_1\Delta(t_1)}\tilde{G}^R(t-t'),$$

with $\tilde{G}^R(\omega)=(\omega-\epsilon_0+i\Gamma/2)^{-1}$ and $\Gamma=\Sigma_\alpha\Gamma_\alpha$. The function $A_\alpha(\epsilon,t)$ can thus be calculated directly from Eq. (5), and one obtains

$$A_\alpha(\epsilon,t)=\frac{\epsilon-\epsilon_0+i\Gamma/2-(\Delta-\Delta_\alpha)(1-e^{i(\epsilon-\epsilon_0+i\Gamma/2)t})}{(\epsilon-\epsilon_0+i\Gamma/2)(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)} \tag{70}$$

for a downward step pulse,

$$A_\alpha(\epsilon,t)=\frac{\epsilon-\epsilon_0+i\Gamma/2-(\Delta-\Delta_\alpha)e^{i(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)t}}{(\epsilon-\epsilon_0+i\Gamma/2)(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)} \tag{71}$$

for an upward step pulse,[20] and

$$A_\alpha(\epsilon,t)=\frac{\epsilon-\epsilon_0+i\Gamma/2-(\Delta-\Delta_\alpha)[1-e^{i(\epsilon-\epsilon_0+i\Gamma/2)(t-s)}(1-e^{i(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)s})]}{(\epsilon-\epsilon_0+i\Gamma/2)(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)} \tag{72}$$

for $t>s$ in the case of a square pulse.[19] We will now show how these known results can be recovered from our formalism. The Green's functions $\tilde{G}^R(\omega)$ and $\bar{G}^R(\omega)=(\omega-\epsilon_0-\Delta+i\Gamma/2)^{-1}$ now have only one pole respectively at $\tilde{\omega}=\epsilon_0-i\Gamma/2$ with residue $\tilde{R}=1$, and $\bar{\omega}=\epsilon_0+\Delta-i\Gamma/2$ with residue $\bar{R}=1$. Since the self-energy $\tilde{\Sigma}^R_\alpha(\omega)=-i\Gamma_\alpha/2$ is independent of energy, we have $\tilde{\Upsilon}^R_{\alpha\beta}(\omega,\epsilon)=0$ and Eq. (68) becomes

$$A_\alpha(\epsilon,t)=\frac{1}{\epsilon-\epsilon_0+i\Gamma/2}+\frac{e^{i(\epsilon-\epsilon_0+i\Gamma/2)t}}{\epsilon-\epsilon_0+\Delta_\alpha+i\Gamma/2}\times\left(\frac{\Delta}{\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2}-\frac{\Delta_\alpha}{\epsilon-\epsilon_0+i\Gamma/2}\right),$$

which reduces to Eq. (70) after simple algebra. Similarly, Eq. (69) becomes

$$A_\alpha(\epsilon,t)=\frac{1}{\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2}-\frac{e^{i(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)t}}{\epsilon-\epsilon_0-\Delta+i\Gamma/2}\left(\frac{\Delta}{\epsilon-\epsilon_0+i\Gamma/2}-\frac{\Delta_\alpha}{\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2}\right),$$

which reduces to Eq. (71). The case of the square pulse is somewhat more involved and is treated in Appendix B.

VII. CONCLUSIONS

We now summarize the main results of this work. We have derived a solution for the time-dependent current flowing through a nanoscale device in the LDL configuration, driven either by a downward step voltage pulse, an upward step pulse, or a square pulse. This solution is valid for far from equilibrium, nonlinear transport and is exact within the Keldysh nonequilibrium Green's-functions approach to time-dependent transport in the adiabatic approximation as put forward by Jauho *et al.*[20] More importantly, our analysis provides the first analytical solution to the transport equations in closed form [Eqs. (22), (47), and (58)] without invoking the wideband approximation. This solution is valid for noninteracting leads with arbitrary electronic structure, and depends explicitly on steady-state Green's functions and self-energies that appear in the dc transport formalism. As such, we believe that this solution provides a way to study transient transport in nanoelectronic devices within the framework of the usual steady-state NEGF-DFT formalism where these quantities can be calculated self-consistently, without requiring a whole new formalism and its separate implementation such as time-dependent density-functional theory.

As a model application of the general solutions, we have calculated the time-dependent current flowing through a single-level quantum dot connected to external leads described by a Lorentzian linewidth. Such a toy calculation, while being far from a true, realistic first-principles calculation, can still provide some insight into the physics of time-dependent transport in the finite-bandwidth regime, which needless to say has to be considered if one wishes to proceed to realistic calculations. Our model revealed some interesting physics in this regime, such as current increase after a sharp bias turnoff, dependence of device turnoff time on the bandwidth, and instantaneously negative current driven by a positive voltage pulse. In short, our model calculation showed that beyond the wideband limit, the bandwidth emerges as a new energy scale in the problem which gives rise to new phenomena in the transient transport characteristics.

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APPENDIX A: TIME-DEPENDENT DYSON EQUATION

In order to derive Eq. (11), we will first perform a time-dependent unitary transformation $U(t)$ on the Hamiltonian (1),

$$U(t)=\exp\left(i\sum_{\mathbf{k}\alpha}\int_0^t dt'\,\Delta_\alpha(t')c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}\right).$$

From the Baker-Hausdorff lemma, it is straightforward to show that U acts on the annihilation operators as $Uc_{\mathbf{k}\alpha}U^\dagger=e^{-i\int_0^t dt'\Delta_\alpha(t')}c_{\mathbf{k}\alpha}$ so that the transformed Hamiltonian[61] $\hat{H}=U(H-i\partial_t)U^\dagger$ becomes

$$\hat{H}=\sum_{\mathbf{k}\alpha}\epsilon^0_{\mathbf{k}\alpha}c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}+\sum_{mn}\epsilon_{mn}(t)d^\dagger_m d_n+\sum_{\mathbf{k}\alpha,n}(t_{\mathbf{k}\alpha,n}(t)c^\dagger_{\mathbf{k}\alpha}d_n+t^*_{\mathbf{k}\alpha,n}(t)d^\dagger_n c_{\mathbf{k}\alpha}),\quad\text{(A1)}$$

where the hopping elements $t_{\mathbf{k}\alpha,n}(t)\equiv e^{i\int_0^t dt'\Delta_\alpha(t')}t_{\mathbf{k}\alpha,n}$ have acquired a time dependence. Since the operators d_n and $d_n^\dagger$ are unchanged by the unitary transformation, we can use $\hat{H}$ to calculate correlation functions of these operators. The Hamiltonian being quadratic, perturbation theory is unnecessary and we will obtain the Dyson equation directly from a functional integral approach.[62–65] The Keldysh Lagrangian is given by[24]

$$L(\bar{c},c,\bar{d},d)=\sum_{\mathbf{k}\alpha}\bar{c}_{\mathbf{k}\alpha}(i\partial_\tau-\epsilon^0_{\mathbf{k}\alpha})c_{\mathbf{k}\alpha}+\sum_{mn}\bar{d}_m[i\partial_\tau-\epsilon^0_{mn}-\Delta_{mn}(\tau)]d_n-\sum_{\mathbf{k}\alpha,n}[\bar{c}_{\mathbf{k}\alpha}t_{\mathbf{k}\alpha,n}(\tau)d_n+\bar{d}_n t^*_{\mathbf{k}\alpha,n}(\tau)c_{\mathbf{k}\alpha}],\quad\text{(A2)}$$

where $c_{\mathbf{k}\alpha},\bar{c}_{\mathbf{k}\alpha}$ and $d_n,\bar{d}_n$ are Grassmann fields and τ is a variable on the Schwinger-Keldysh contour[38,39] C. The Keldysh generating functional is defined as

$$Z[\bar{\eta},\eta]=\mathrm{Tr}[\rho T_c(e^{-i\oint_C d\tau[:H:-\sum_n(\bar{\eta}_n d_n+d_n^\dagger\eta_n)]})],$$

where :: denotes normal ordering, ρ is the unperturbed equilibrium density matrix, and $\eta_n,\bar{\eta}_n$ are Grassmann sources.

The chosen normalization is seen to be $Z[0,0]=\mathrm{Tr}\,\rho\equiv Z$, the partition function of the unperturbed system. The following functional integral representation holds:

$$Z[\bar{\eta},\eta]=\int \mathcal{D}[\bar{c},c]\int \mathcal{D}[\bar{d},d]e^{i[S[\bar{c},c,\bar{d},d]+\oint_C d\tau(\bar{\eta}d+\bar{d}\eta)]},$$

where we use a simplified notation for the dot product of the η and d fields, $\bar{\eta}d\equiv\Sigma_n\bar{\eta}_n d_n$ and similarly for $\bar{d}\eta$, and the action S is the integral over the contour C of the Lagrangian (A2), $S=\oint_C d\tau L$. The two-point contour-ordered correlation function $G_{nm}(\tau,\tau')\equiv -i\langle T_c\{d_n(\tau)d_m^\dagger(\tau')\}\rangle$ is then obtained from $Z[\bar{\eta},\eta]$ by functional differentiation[66] with respect to the sources,

$$iG_{nm}(\tau,\tau')=\left.\frac{1}{Z}\frac{\delta^2 Z[\bar{\eta},\eta]}{\delta\bar{\eta}_n(\tau)\delta\eta_m(\tau')}\right|_{\bar{\eta}=0,\,\eta=0}. \tag{A3}$$

We will obtain an effective action for the scattering region by integrating out the degrees of freedom of the leads. In order to do that, we first perform the following change of variables in the Lagrangian (A2),

$$\bar{c}'_{\mathbf{k}\alpha}=\bar{c}_{\mathbf{k}\alpha}-\sum_n \bar{d}_n t^*_{\mathbf{k}\alpha,n}(\tau)(i\partial_\tau-\epsilon^0_{\mathbf{k}\alpha})^{-1},$$

$$c'_{\mathbf{k}\alpha}=c_{\mathbf{k}\alpha}-(i\partial_\tau-\epsilon^0_{\mathbf{k}\alpha})^{-1}\sum_n t_{\mathbf{k}\alpha,n}(\tau)d_n, \tag{A4}$$

so that after substitution the transformed Lagrangian becomes

$$L(\bar{c}',c',\bar{d},d)=\sum_{\mathbf{k}\alpha}\bar{c}'_{\mathbf{k}\alpha}\hat{g}^{-1}_{\mathbf{k}\alpha}(\tau)c'_{\mathbf{k}\alpha}+\sum_{mn}\bar{d}_m\Big(i\partial_\tau-\epsilon^0_{mn}-\Delta_{mn}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,m}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,n}(\tau)\Big)d_n, \tag{A5}$$

where we have defined $\hat{g}_{\mathbf{k}\alpha}(\tau)\equiv(i\partial_\tau-\epsilon^0_{\mathbf{k}\alpha})^{-1}$, the Green's operator of the leads. Since the transformation (A4) is only a shift, the Jacobian is unity[66] and we have $\mathcal{D}[\bar{c}',c']=\mathcal{D}[\bar{c},c]$ so that the Keldysh generating functional becomes

$$Z[\bar{\eta},\eta]=\int \mathcal{D}[\bar{c}',c']e^{iS_{\mathrm{leads}}[\bar{c}',c']}\int \mathcal{D}[\bar{d},d]\exp\left[i\left(S^{\mathrm{eff}}[\bar{d},d]+\oint_C d\tau(\bar{\eta}d+\bar{d}\eta)\right)\right], \tag{A6}$$

where $S_{\mathrm{leads}}[\bar{c}',c']\equiv\oint_C d\tau\Sigma_{\mathbf{k}\alpha}\bar{c}'_{\mathbf{k}\alpha}\hat{g}^{-1}_{\mathbf{k}\alpha}(\tau)c'_{\mathbf{k}\alpha}$ is the action of the isolated leads, and S^{eff} is an effective action for the scattering region,

$$S^{\mathrm{eff}}[\bar{d},d]=\oint_C d\tau\sum_{mn}\bar{d}_m\Big(\hat{g}^{-1}_{mn}(\tau)-\Delta_{mn}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,m}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,n}(\tau)\Big)d_n, \tag{A7}$$

and $\hat{g}^{-1}_{mn}(\tau)\equiv i\partial_\tau-\epsilon^0_{mn}$ defines the Green's operator $\hat{g}(\tau)$ for the isolated scattering region in equilibrium. The c fields have thus been decoupled from the d fields, and can be integrated out exactly as we will see later. To decouple the sources η from the d fields in Eq. (A6), we perform a transformation on the d fields similar to that in Eq. (A4):

$$\bar{d}'_n=\bar{d}_n+\sum_m\bar{\eta}_m\Big(\hat{g}^{-1}_{mn}(\tau)-\Delta_{mn}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,m}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,n}(\tau)\Big)^{-1},$$

$$d'_n=d_n+\sum_m\Big(\hat{g}^{-1}_{nm}(\tau)-\Delta_{nm}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,n}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,m}(\tau)\Big)^{-1}\eta_m. \tag{A8}$$

Subsitution of Eq. (A8) into the effective action (A7) and the source term $\bar{\eta}d+\bar{d}\eta$ yields

$$S^{\mathrm{eff}}[\bar{d},d]+\oint_C d\tau(\bar{\eta}d+\bar{d}\eta)=\sum_{mn}\bar{d}'_m\Big(\hat{g}^{-1}_{mn}(\tau)-\Delta_{mn}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,m}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,n}(\tau)\Big)d'_n-\sum_{mn}\bar{\eta}_m\Big(\hat{g}^{-1}_{mn}(\tau)-\Delta_{mn}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,m}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,n}(\tau)\Big)^{-1}\eta_n, \tag{A9}$$

and the Jacobian of transformation (A8) is again unity, $\mathcal{D}[\bar{d}',d']=\mathcal{D}[\bar{d},d]$, so that Eq. (A6) becomes

$$Z[\bar{\eta},\eta]=\exp\left(-i\oint_C d\tau\sum_{mn}\bar{\eta}_m\hat{G}_{mn}(\tau)\eta_n\right)\times\int \mathcal{D}[\bar{c}',c']e^{iS_{\mathrm{leads}}[\bar{c}',c']}\int \mathcal{D}[\bar{d}',d']e^{iS^{\mathrm{eff}}[\bar{d}',d']}, \tag{A10}$$

where we define the Green's operator $\hat{G}(\tau)$ by its matrix elements,

$$\hat{G}_{mn}(\tau)\equiv\Big(\hat{g}^{-1}_{mn}(\tau)-\Delta_{mn}(\tau)-\sum_{\mathbf{k}\alpha}t^*_{\mathbf{k}\alpha,m}(\tau)\hat{g}_{\mathbf{k}\alpha}(\tau)t_{\mathbf{k}\alpha,n}(\tau)\Big)^{-1}. \tag{A11}$$

The remaining functional integrals can be carried out exactly and simply yield the equilibrium partition function Z according to the chosen normalization, since the nonequilibrium sources $\bar{\eta},\eta$, which are different on different parts of the two-branch Schwinger-Keldysh contour C, have been factored out of the integrals. In other words, as the system evolves along the contour $C=C_+\cup C_-$ according to the action $S_{\mathrm{leads}}+S^{\mathrm{eff}}$ in absence of sources, the evolution on the forward part $C_+=(-\infty,\infty)$ of the contour cancels that on the backward part $C_-=(\infty,-\infty)$ and one simply traces over the initial density matrix ρ at $t=-\infty$. Equation (A10) thus becomes

$$Z[\bar{\eta},\eta]=Z\exp\left(-i\oint_C d\tau\sum_{mn}\bar{\eta}_m\hat{G}_{mn}(\tau)\eta_n\right),$$

so that in Eq. (A3), the factor of Z cancels out and we have

$$iG_{nm}(\tau,\tau')=\frac{\delta^2}{\delta\bar{\eta}_n(\tau)\delta\eta_m(\tau')}\times\exp\left(-i\oint_C ds\oint_C ds'\times\sum_{ij}\bar{\eta}_i(s)\mathcal{G}_{ij}(s,s')\eta_j(s')\right)\Bigg|_{\bar{\eta}=0,\eta=0},\tag{A12}$$

where we have defined the function $\mathcal{G}_{ij}(s,s')$ that describes the action of the operator $\hat{G}_{ij}(s)$ on an arbitrary function $\phi(s)$ defined on the contour, $\hat{G}_{ij}(s)\phi(s)=\oint_C ds'\mathcal{G}_{ij}(s,s')\phi(s')$. By straightforward functional differentiation, paying, however, attention to introduce a minus sign as the derivative $\delta/\delta\eta_m(\tau')$ is moved past the first source field $\bar{\eta}_i(s)$ since both are Grassmann-valued quantities, we obtain from Eq. (A12) that $G_{nm}(\tau,\tau')=\mathcal{G}_{nm}(\tau,\tau')$ as expected. From the operator equation (A11), we can thus write for the associated functions

$$G^{-1}_{nm}(\tau,\tau')=g^{-1}_{nm}(\tau,\tau')-\Delta_{nm}(\tau)\delta(\tau,\tau')-\sum_{\alpha}e^{-i\int_0^{\tau}ds\Delta_\alpha(s)}\tilde{\Sigma}_{\alpha,nm}(\tau,\tau')e^{i\int_0^{\tau'}ds\Delta_\alpha(s)},$$

where $\tilde{\Sigma}_{\alpha,nm}(\tau,\tau')\equiv\sum_{\mathbf{k}}t^*_{\mathbf{k}\alpha,n}g_{\mathbf{k}\alpha}(\tau,\tau')t_{\mathbf{k}\alpha,m}$ defines the equilibrium contour-ordered self-energy of lead α, $g_{\mathbf{k}\alpha}(\tau,\tau')$ being the function associated with the Green's operator $\hat{g}_{\mathbf{k}\alpha}(\tau)$, and $\delta(\tau,\tau')$ is a delta function on the contour C. Defining the equilibrium Green's function $\tilde{G}_{nm}(\tau,\tau')$ of the scattering region by $\tilde{G}^{-1}_{nm}(\tau,\tau')=g^{-1}_{nm}(\tau,\tau')-\tilde{\Sigma}_{nm}(\tau,\tau')$with $\tilde{\Sigma}_{nm}(\tau,\tau')\equiv\sum_\alpha\tilde{\Sigma}_{\alpha,nm}(\tau,\tau')$ the total self-energy, we have

$$G^{-1}_{nm}(\tau,\tau')=\tilde{G}^{-1}_{nm}(\tau,\tau')-\Delta_{nm}(\tau)\delta(\tau,\tau')-\sum_{\alpha}(e^{-i\int_{\tau'}^{\tau}ds\Delta_\alpha(s)}-1)\tilde{\Sigma}_{\alpha,nm}(\tau,\tau'),$$

so that by acting with G from the right and with $\tilde{G}$ from the left, we obtain the desired Dyson equation,

$$G_{nm}(\tau,\tau')=\tilde{G}_{nm}(\tau,\tau')+\sum_{n'm'}\oint_C ds\tilde{G}_{nn'}(\tau,s)\Delta_{n'm'}(s)\times G_{m'm}(s,\tau')+\sum_{n'm'}\oint_C ds_1\oint_C ds_2\tilde{G}_{nn'}(\tau,s_1)\times V_{n'm'}(s_1,s_2)G_{m'm}(s_2,\tau'),\tag{A13}$$

where the two-time potential $V_{n'm'}(s_1,s_2)$,

$$V_{n'm'}(s_1,s_2)\equiv\sum_\alpha(e^{-i\int_{s_2}^{s_1}ds\Delta_\alpha(s)}-1)\tilde{\Sigma}_{\alpha,n'm'}(s_1,s_2),$$

gives rise to the retarded potential (12) when one applies the Langreth analytic continuation rules[67] to Eq. (A13) in order to obtain Eq. (11).

APPENDIX B: SQUARE PULSE IN THE WIDEBAND LIMIT

In the WBL, the self-energy $\tilde{\Sigma}^R_\beta$ is a constant so that we have

$$\sum_\beta\int\frac{d\omega'}{2\pi i}\frac{\Delta_\beta\chi^{(-)}_\beta(\omega,\omega')\tilde{\Sigma}^R_\beta\tilde{G}^R(\epsilon)}{(\omega'-\epsilon-\epsilon+\Delta_\beta+i0^+)(\omega'-\epsilon+i0^+)}=-\sum_\beta\int\frac{d\omega'}{2\pi i}\frac{\Delta_\beta(e^{i(\omega-\omega'-\Delta_\beta)s}-1)}{\omega-\omega'-\Delta_\beta-i0^+}\frac{1}{\omega'-\omega+i0^+}\times\left(\frac{1}{\omega'-\epsilon+i0^+}-\frac{1}{\omega'-\epsilon+\Delta_\beta+i0^+}\right)\tilde{\Sigma}^R_\beta\tilde{G}^R(\epsilon).$$

Making use of the following partial fraction decomposition:

$$\frac{1}{\omega'-\omega+i0^+}\left(\frac{1}{\omega'-\epsilon+i0^+}-\frac{1}{\omega'-\epsilon+\Delta_\beta+i0^+}\right)=\frac{1}{\omega-\epsilon-i0^+}\left(\frac{1}{\omega'-\omega+i0^+}-\frac{1}{\omega'-\epsilon+i0^+}\right)-\frac{1}{\omega-\epsilon+\Delta_\beta-i0^+}\left(\frac{1}{\omega'-\omega+i0^+}-\frac{1}{\omega'-\epsilon+\Delta_\beta+i0^+}\right),$$

and summing over the poles at $\omega'=\omega-i0^+$, $\omega'=\epsilon-i0^+$, and $\omega'=\epsilon-\Delta_\beta-i0^+$ we can show that

$$\sum_\beta\int\frac{d\omega'}{2\pi i}\frac{\Delta_\beta\chi^{(-)}_\beta(\omega,\omega')\tilde{\Sigma}^R_\beta\tilde{G}^R(\epsilon)}{(\omega'-\epsilon-\epsilon+\Delta_\beta+i0^+)(\omega'-\epsilon+i0^+)}=-\sum_\beta[\chi^{(-)}_\beta(\omega,\epsilon)-e^{-i\Delta_\beta s}\chi^{(+)}_\beta(\omega,\epsilon)]\tilde{\Sigma}^R_\beta\tilde{G}^R(\epsilon),$$

which cancels against the corresponding term with a positive sign in Eq. (58). We are left with

$$A_\alpha(\epsilon,t)=\tilde{G}^R(\epsilon)+e^{i\Delta_\alpha s}\int\frac{d\omega}{2\pi i}e^{-i(\omega-\epsilon)t}\tilde{G}^R(\omega)\left[\chi^{(-)}_\alpha(\omega,\epsilon)+\left(\frac{e^{i(\omega-\epsilon)s}-1}{\omega-\epsilon-i0^+}\right)\Delta\tilde{G}^R(\epsilon)-\Delta\int\frac{d\omega'}{2\pi i}Q_\alpha(\omega,\omega',\epsilon)\right].\tag{B1}$$

Considered as a function of ω, the quantity in square brackets in Eq. (B1) only has poles in the upper half plane. We can thus perform the ω integral by closing the contour in the lower half plane so that only the pole of $\tilde{G}^R(\omega)$ at $\tilde{\omega}=\epsilon_0-i\Gamma/2$ is enclosed. We obtain

$$A_\alpha(\epsilon,t) = \widetilde{G}^R(\epsilon) - e^{i\Delta_\alpha s}e^{i(\epsilon-\epsilon_0+i\Gamma/2)t}\left[\chi_\alpha^{(-)}(\epsilon_0 - i\Gamma/2,\epsilon) + \Delta\left(\frac{1-e^{-i(\epsilon-\epsilon_0+i\Gamma/2)s}}{(\epsilon-\epsilon_0+i\Gamma/2)^2} - \int\frac{d\omega'}{2\pi i}Q_\alpha(\epsilon_0 - i\Gamma/2,\omega',\epsilon)\right)\right]. \quad \text{(B2)}$$

We need to calculate

$$\int\frac{d\omega'}{2\pi i}Q_\alpha(\epsilon_0 - i\Gamma/2,\omega',\epsilon) = -\int\frac{d\omega'}{2\pi i}\frac{e^{i(\epsilon_0-\Delta_\alpha-i\Gamma/2-\omega')s}\widetilde{G}^R(\omega'+\Delta_\alpha)}{(\omega'-\epsilon+\Delta_\alpha+i0^+)(\omega'-\epsilon_0+\Delta_\alpha+i\Gamma/2)}\left(\frac{\Delta_\alpha}{\omega'-\epsilon+i0^+}+\Delta\widetilde{G}^R(\epsilon)\right),$$

where we see that $Q_\alpha(\epsilon_0 - i\Gamma/2,\omega',\epsilon)$ has four simple poles in the lower half of the complex ω' plane: $\omega'=\epsilon-i0^+$, $\omega'=\epsilon-\Delta_\alpha-i0^+$, $\omega'=\epsilon_0-\Delta_\alpha-i\Gamma/2$, and $\omega'=\epsilon_0+\Delta-\Delta_\alpha-i\Gamma/2$. After some algebra, we obtain

$$\Delta\int\frac{d\omega'}{2\pi i}Q_\alpha(\epsilon_0 - i\Gamma/2,\omega',\epsilon) = \frac{(1-e^{-i(\epsilon-\epsilon_0+i\Gamma/2)s})\Delta}{(\epsilon-\epsilon_0+i\Gamma/2)^2} - \frac{\Delta_\alpha}{(\epsilon-\epsilon_0+i\Gamma/2)(\epsilon-\epsilon_0+\Delta_\alpha+i\Gamma/2)} + \frac{1}{\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2}\left(\frac{e^{-i(\epsilon-\epsilon_0+\Delta_\alpha+i\Gamma/2)s}\Delta}{\epsilon-\epsilon_0+\Delta_\alpha+i\Gamma/2} - \frac{e^{-i\Delta s}(\Delta-\Delta_\alpha)}{\epsilon-\epsilon_0+i\Gamma/2}\right),$$

where the first term is seen to cancel against the corresponding term in Eq. (B2). Putting the different parts of Eq. (B2) together and using the definition of $\chi_\alpha^{(-)}$ in Eq. (54), we obtain after further cancellations

$$A_\alpha(\epsilon,t) = \frac{1}{\epsilon-\epsilon_0+i\Gamma/2} + e^{i\Delta_\alpha s}e^{i(\epsilon-\epsilon_0+i\Gamma/2)t}(\Delta-\Delta_\alpha)\left(\frac{e^{-i(\epsilon-\epsilon_0+\Delta_\alpha+i\Gamma/2)s} - e^{-i\Delta s}}{(\epsilon-\epsilon_0+i\Gamma/2)(\epsilon-\epsilon_0-\Delta+\Delta_\alpha+i\Gamma/2)}\right),$$

which is easily shown to be equal to Eq. (72).

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