Nonadiabatic electron pumping through interacting quantum dots

Alexander Croy* and Ulf Saalmann
Max-Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D-01187 Dresden, Germany

Alexis R. Hernández
Instituto de Física, Universidade Federal do Rio de Janeiro, 21941-970 Rio de Janeiro, Brazil

Caio H. Lewenkopf
Instituto de Física, Universidade Federal Fluminense, 24210-346 Niterói, Brazil

(Received 25 October 2011; revised manuscript received 15 December 2011; published 11 January 2012)

We study nonadiabatic charge pumping through single-level quantum dots taking into account Coulomb interactions. We show how a truncated set of equations of motion can be propagated in time by means of an auxiliary-mode expansion. This formalism is capable of treating time-dependent electronic transport for arbitrary driving parameters. We verify that the proposed method describes very precisely the well-known limit of adiabatic pumping through quantum dots without Coulomb interactions. As an example we discuss pumping driven by short voltage pulses for various interaction strengths. Such finite pulses are particularly suited to investigation of transient nonadiabatic effects, which may also be important for periodic drivings, where they are much more difficult to reveal.

DOI: 10.1103/PhysRevB.85.035309 PACS number(s): 73.63.Kv, 73.23.Hk, 72.10.Bg

I. INTRODUCTION

In 1983 Thouless[1] proposed a simple pumping mechanism to produce, even in the absence of an external bias, a quantized electron current through a quantum conductor by an appropriate time-dependent variation of the system parameters. Experimental realizations of quantum pumps using quantum dots (QDs) were already reported in the early 1990s.[2,3] More recently, due to the technological advances in nanolithography and control, such experiments have risen to a much higher level of sophistication, making it possible to pump electron[4–6] and spin[7] currents through open nanoscale conductors, as well as through single and double QDs.[8–11]

Early theoretical investigations were devoted to the adiabatic pumping regime within the single-particle approximation.[12–14] This is well justified for experiments with open QDs, where interaction effects are believed to be weak[15] and the typical pumping parameters are slow with respect to the characteristic transport time scales, such as the electron dwell time τ_d. This time-scale separation enormously simplifies the analysis of the two-time evolution of the system. Within the adiabatic regime, inelastic and dissipation[16] effects of currents generated by quantum pumps were analyzed. Furthermore, issues like counting statistics,[17] memory effects,[18] and generalizations of charge pumping to adiabatic quantum spin pumps were also proposed and studied.[19–21]

Nonadiabatic pumping has been theoretically investigated within the single-particle picture, either by use of Keldysh nonequilibrium Green's functions, with an optimal parametrization of the carrier operators inspired by bosonization studies,[22] or by a Floquet analysis of the S matrix obtained from the scattering approach.[23] While the first approach renders complicated integrodifferential equations for the Green's functions associated with transport, the second one gives a set of coupled equations for the Floquet operator. It is worth stressing that, in both cases the single-particle picture is crucial to make the solution possible and it is well established that both methods are equivalent.[24,25]

Several works have provided a quite satisfactory description of quantum pumping for weakly interacting systems. In contrast, the picture is not as clear for situations where interaction effects are important. Different approximation schemes have been proposed to deal with pumping in the presence of interactions and to address charging effects, which are not accounted for in a mean-field approximation. Typically, two limiting regimes have been studied, namely, that of low pumping frequencies Ω, such that $\Omega\tau_d \ll 1$ (adiabatic limit),[26–32] and that of very high frequencies, $\Omega\tau_d \gg 1$ (sudden or diabatic limit).[33–35] Nonadiabatic pumping is mainly studied as a side effect of photon-assisted tunneling,[36–38] where $\Omega\tau_d \gg 1$.

Unfortunately, it is quite cumbersome to calculate corrections to these limit cases. For instance, the analysis of higher-order corrections to the adiabatic approximation for the current gives neither simple nor insightful expressions.[32] In addition to the theoretical interest, a comprehensive approach bridging the limits of $\Omega\tau_d \gg 1$ and $\Omega\tau_d \ll 1$ also has a strong experimental motivation: Most current experimental realizations of quantum pumping deal with QDs in the Coulomb blockade regime and $\Omega\tau_d \sim 1$. This regime was recently approached (from below) by means of a diagrammatic real-time transport theory with a summation to all orders in Ω.[39] However, the derivation implied the weak tunnel coupling limit, whereas experiments[40–44] typically rely on tunnel coupling variations, which include both weak and strong coupling.

To address the above-mentioned issues and to account for the different time scales involved, it is natural to use a propagation method in the *time domain*.[45–49] In this work we express the current operator in terms of density matrices in the Heisenberg representation. We obtain the pumped current by truncating the resulting equations of motion for the many-body problem. This approximation is valid for temperatures T higher than the Kondo temperature T_K.[50] For

lower temperatures the Kondo effect starts to manifest, which requires a nonperturbative description.[27,28,31] Since we study pumping in the Coulomb-blockade regime where $T \gg T_K$, the truncation scheme we employ is expected to be an accurate approximation. The time dependence is treated exactly by means of an auxiliary-mode expansion.[47,51] This approach provides a quite amenable path to circumvent the usual difficulties of dealing with two-time Green's functions.[51] Moreover, it has been successfully applied to systems coupled to bosonic reservoirs[52] and to the description of time-dependent electron transport using generalized quantum master equations for the reduced density matrix.[47,53,54] Since the auxiliary-mode expansion is well controlled,[55] the accuracy of our method is determined solely by the level of approximation used to treat the many-body problem.

The formalism we put forward is illustrated by the study of the charge pumped through a QD in the Coulomb-blockade regime by varying its resonance energy and couplings to the leads. The external drive is parametrized by a single pulse, whose duration and amplitude can be arbitrarily varied. When this is done, the formalism is capable of reproducing all known results of the adiabatic limit and exploring transient effects beyond this simple limit.

The paper is organized as follows. In Sec. II we present the resonant-level model, as well as the theoretical framework employed in our analysis. In Sec. III we introduce the general propagation scheme, suitable for calculation of the pumping current at the adiabatic regime and beyond it. Next, in Sec. IV, we discuss a few applications of the method. Finally, in Sec. V we present our conclusions.

II. TIME-DEPENDENT INTERACTING RESONANT-LEVEL MODEL

The standard model for addressing electron transport through QDs is the Anderson interacting single-resonance model coupled to two reservoirs, one acting as a source and the other as a drain. Despite its simplicity, the model provides a good description for Coulomb-blockade QDs and for QDs in the Kondo regime, where the electrons are strongly correlated. In this paper we address the Coulomb-blockade regime, for QDs whose typical line width Γ is much smaller than the QD mean level spacing δ, justifying the use of the Anderson single-resonance model. In addition, in the Coulomb-blockade regime, Γ is much lower than the resonance charging energy U.

A. Setup

The total Hamiltonian is given by the usual threefold decomposition into a QD Hamiltonian $H_{\rm dot}$, a Hamiltonian $H_{\rm leads}$ representing the leads, and a coupling term $H_{\rm coup}$, namely,

$$H = H_{\rm dot} + H_{\rm leads} + H_{\rm coup}. \tag{1a}$$

The QD is modeled by a single level of energy $\varepsilon_{\rm d}(t)$, which can be occupied by spin-up and spin-down electrons, which interact through a contact interaction of strength U. The QD Hamiltonian reads

$$H_{\rm dot} = \sum_{s=\uparrow,\downarrow} \varepsilon_{\rm d}(t)\hat{n}_s + U\hat{n}_\uparrow\hat{n}_\downarrow, \tag{1b}$$

where $\hat{n}_s = \hat{c}_s^\dagger\hat{c}_s$, $\hat{c}_s^\dagger$, and $\hat{c}_s$ are the electron number, the creation, and the annihilation operators for the respective spin state $s = \uparrow, \downarrow$ in the dot.

The two reservoirs, labeled L (left) and R (right), are populated by noninteracting electrons, whose Hamiltonian reads

$$H_{\rm leads} = \sum_{\alpha\in{\rm L,R}} \sum_{ks} \varepsilon_{\alpha k}(t)\hat{b}_{\alpha ks}^\dagger\hat{b}_{\alpha ks}, \tag{1c}$$

where $\{\hat{b}_{\alpha ks}^\dagger\}$ and $\{\hat{b}_{\alpha ks}\}$ stand for the electron creation and annihilation operators for the α-reservoir state ks, respectively. The reservoir single-particle energies have the general form $\varepsilon_{\alpha k}(t) = \varepsilon_{\alpha k}^0 + \Delta\varepsilon_\alpha(t)$, with the $\Delta\varepsilon_\alpha$ accounting for a time-dependent bias. The stationary current due to a time-dependent bias was addressed several years ago.[56] For pumping, we take $\Delta\varepsilon_\alpha(t) = 0$, as usual. Finally, the coupling Hamiltonian is given by

$$H_{\rm coup} = \sum_{\alpha k} \sum_{s} T_{\alpha k}(t)\,\hat{b}_{\alpha ks}^\dagger\hat{c}_s + {\rm H.c.}, \tag{1d}$$

with $\{T_{\alpha k}\}$ denoting the coupling matrix element between the QD and reservoir α.

B. Equation-of-motion approach

We are interested in the electronic current from reservoir α to QD state s, which can be obtained from the current operator

$$\hat{J}_{\alpha s}(t) \equiv {\rm i}\sum_k [T_{\alpha k}(t)\hat{b}_{\alpha ks}^\dagger(t)\hat{c}_s(t) - T_{\alpha k}^*(t)\hat{c}_s^\dagger(t)\hat{b}_{\alpha ks}(t)]. \tag{2}$$

Here and in the following we use units where the elementary charge $e = 1$ and the reduced Planck constant $\hbar = 1$, unless otherwise indicated. To calculate $\hat{J}_{\alpha s}(t)$ we use the following equations of motion, which are obtained from the Hamiltonian [Eqs. (1)] by means of the Heisenberg equation,

$$\begin{aligned}
{\rm i}\partial_t\hat{b}_{\alpha ks}(t) &= \varepsilon_{\alpha k}(t)\hat{b}_{\alpha ks}(t) + T_{\alpha k}(t)\hat{c}_s(t), && \text{(3a)}\\
{\rm i}\partial_t\hat{c}_s(t) &= \varepsilon_s(t)\hat{c}_s(t) + U\hat{c}_s(t)\hat{n}_{\bar{s}}(t) \\
&\quad + \sum_{\alpha k} T_{\alpha k}^*(t)\hat{b}_{\alpha ks}(t), && \text{(3b)}\\
{\rm i}\partial_t\hat{n}_{\bar{s}}(t) &= \sum_{\alpha k}[-T_{\alpha k}(t)\hat{b}_{\alpha k\bar{s}}^\dagger(t)\hat{c}_{\bar{s}}(t) \\
&\quad + T_{\alpha k}^*(t)\hat{c}_{\bar{s}}^\dagger(t)\hat{b}_{\alpha k\bar{s}}(t)]. && \text{(3c)}
\end{aligned}$$

Analogous equations hold for $\hat{b}_{\alpha ks}^\dagger$ and $\hat{c}_s^\dagger$.

In the spirit of the scheme introduced by Caroli and coworkers,[57] we assume an initially uncorrelated density operator of the combined system, i.e., we set $T_{\alpha k}(t_0) \to 0$ for $t_0 \to -\infty$. Further, we apply the so-called wide-band limit,[58] which assumes that the density of states ρ_α and tunnel matrix elements $T_{\alpha k}$ are constant in the energy window relevant for transport. By means of the lead Green's function[58]

$$g_{\alpha k}(t,t') = \exp\left[-{\rm i}\int_{t'}^{t} dt''\varepsilon_{\alpha k}(t'')\right], \tag{4}$$

we can define the decay rate

$$\Gamma_\alpha(t,t') \equiv \sum_k T_{\alpha k}(t) g_{\alpha k}(t,t') T^*_{\alpha k}(t'), \tag{5a}$$

which becomes local in time in the wide-band limit, namely,

$$\begin{aligned}\Gamma_\alpha(t,t') &= \int d\varepsilon_k \rho_\alpha(\varepsilon_k) T_{\alpha k}(t) g_{\alpha k}(t,t') T^*_{\alpha k}(t') \\ &= \Gamma_\alpha(t)\delta(t-t').\end{aligned} \tag{5b}$$

In the following we replace the sum in Eq. (5a) with the expression involving the δ function in Eq. (5b).

The equation of motion for the reservoir operators $\hat{b}_{\alpha ks}$, Eq. (3a), is now readily integrated, yielding

$$\hat{b}_{\alpha ks}(t) = \hat{B}_{\alpha ks}(t) - \mathrm{i}\int_{t_0}^{t} dt' g_{\alpha k}(t,t') T_{\alpha k}(t') \hat{c}_s(t'), \tag{6a}$$

where we have used the lead Green's functions, Eq. (4), and introduced

$$\hat{B}_{\alpha ks}(t) \equiv g_{\alpha k}(t,t_0)\hat{b}_{\alpha ks}(t_0). \tag{6b}$$

Equations (6) are used to rewrite Eq. (3b) as

$$\begin{aligned}\mathrm{i}\partial_t \hat{c}_s(t) = &\left[\varepsilon_s(t) + U\hat{n}_{\bar{s}}(t) - \mathrm{i}\frac{\Gamma(t)}{2}\right]\hat{c}_s(t) \\ &+ \sum_{\alpha k} T^*_{\alpha k}(t)\hat{B}_{\alpha ks}(t).\end{aligned} \tag{7}$$

Here the wide-band limit, Eq. (5), is employed to obtain the decay term, proportional to $\Gamma(t) = \sum_\alpha \Gamma_\alpha(t)$. Similarly, we can rewrite Eq. (3c) as

$$\begin{aligned}\mathrm{i}\partial_t \hat{n}_{\bar{s}}(t) = \sum_{\alpha k}[&-T_{\alpha k}(t)\hat{B}^\dagger_{\alpha k\bar{s}}(t)\hat{c}_{\bar{s}}(t) \\ &+ T^*_{\alpha k}(t)c^\dagger_{\bar{s}}(t)\hat{B}_{\alpha k\bar{s}}(t)] - \mathrm{i}\Gamma(t)\hat{n}_{\bar{s}}(t).\end{aligned} \tag{8}$$

Here again the time integral of $\hat{b}_{\alpha ks}(t)$ is reduced to a decay width due to the wide-band limit, Eq. (5).

C. Expectation values and truncation schemes

The expression for the time-dependent current is given by the expectation value of the current operator $\hat{J}_{\alpha s}$ defined in Eq. (2). As will become clear later, it is useful to write this expectation value as

$$J_\alpha(t) = \frac{e}{\hbar}\sum_s \langle \hat{J}_{\alpha s}(t)\rangle = \frac{2e}{\hbar}\,\mathrm{Re}\sum_s \Pi_{\alpha s}(t), \tag{9}$$

with the *current matrices of the first order*

$$\Pi_{\alpha s}(t) \equiv \mathrm{i}\sum_k T_{\alpha k}(t)\langle \hat{b}^\dagger_{\alpha ks}(t)\hat{c}_s(t)\rangle. \tag{10}$$

These current matrices are an essential ingredient of our propagation scheme, which is based on finding equations of motion for $\Pi_{\alpha s}$. Such equations have been derived starting from a nonequilibrium Green's function formalism for noninteracting electrons.[51]

Exactly as for the operator equations above, we can use $\hat{b}_{\alpha ks}$ from Eq. (6) and employ the wide-band limit, Eq. (5), for the current matrices defined in Eq. (10). This leads to the following decomposition:

$$\Pi_{\alpha s}(t) = \Pi'_{\alpha s}(t) + \sum_k T_{\alpha k}(t)\Pi''_{\alpha ks}(t), \tag{11a}$$

$$\Pi'_{\alpha s}(t) = -\frac{\Gamma_\alpha(t)}{2}\langle \hat{n}_s(t)\rangle, \tag{11b}$$

$$\Pi''_{\alpha ks}(t) = \mathrm{i}\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{c}_s(t)\rangle. \tag{11c}$$

Having derived all relevant equations of motion for the operators, we can specify the respective equations for the two contributions Π' and Π''. The term Π' is the simplest and is basically given by the equation of motion for $\hat{n}_s$; cf. Eq. (8). The corresponding equation for the occupation $n_s(t) \equiv \langle \hat{n}_s(t)\rangle$ reads

$$\partial_t n_s(t) = 2\mathrm{Re}\sum_{\alpha k} T_{\alpha k}(t)\Pi''_{\alpha ks}(t) - \Gamma(t)n_s(t). \tag{12}$$

The above relation can be viewed as the charge conservation equation for the QD. The rate by which the charge in the QD changes is equal to the total electronic currents. The first term on the right-hand side (r.h.s.) of the equation can be interpreted as the current flowing into the QD, whereas the second term gives the current flowing out.

Since we do not consider spin-dependent driving or spin-polarized initial states, $n_s(t) = n_{\bar{s}}(t)$. This relation is not explicitly used in the derivation but is employed as a consistency check throughout the analysis.

The evaluation of Π'' requires the solutions for both the lead operator $\hat{b}_{\alpha ks}$ and the dot operator $\hat{c}_s$. Using these, we write

$$\begin{aligned}\partial_t \Pi''_{\alpha ks}(t) = &\,\mathrm{i}\Delta_{\alpha ks}(t)\,\Pi''_{\alpha ks}(t) \\ &+ T^*_{\alpha k}(t) f_{\alpha k} - \mathrm{i}U\Phi_{\alpha ks}(t).\end{aligned} \tag{13}$$

Here we have introduced the abbreviation

$$\Delta_{\alpha ks}(t) \equiv \varepsilon^0_{\alpha k} - \left[\varepsilon_s(t) - \mathrm{i}\frac{\Gamma(t)}{2}\right] \tag{14}$$

and used that

$$\begin{aligned}\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{B}_{\alpha ks}(t)\rangle &= \langle \hat{b}^\dagger_{\alpha ks}(t_0)\hat{b}_{\alpha ks}(t_0)\rangle \\ &= f_\alpha(\varepsilon_k) \equiv f_{\alpha k},\end{aligned} \tag{15}$$

with $f_\alpha(\varepsilon)$ the Fermi function describing the equilibrium occupation of lead α. The last term in Eq. (13) uses the *auxiliary current matrices of the second order*

$$\Phi_{\alpha ks} \equiv \mathrm{i}\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{c}_s(t)\hat{n}_{\bar{s}}(t)\rangle, \tag{16}$$

which will be subject to further approximations in the following.

Before we turn to the approximations, we would like to briefly discuss the physical meaning of $\Phi_{\alpha ks}$. The equation of motion for the two-electron density matrix $\langle \hat{n}_s(t)\hat{n}_{\bar{s}}(t)\rangle$ reads

$$\begin{aligned}\partial_t\langle \hat{n}_s(t)\hat{n}_{\bar{s}}(t)\rangle = &-2\Gamma(t)\langle \hat{n}_s(t)\hat{n}_{\bar{s}}(t)\rangle \\ &+ 2\mathrm{Re}\sum_{\alpha ks} T_{\alpha ks}(t)\Phi_{\alpha ks}(t),\end{aligned} \tag{17}$$

which follows from Eq. (8). The two-electron density matrix may be interpreted as the occupation of one QD level under the condition that the other one is occupied. The rate of

change of this conditional occupation is consequently given by tunneling into and out of the respective dot state under the same condition. The latter process is described by the first term on the r.h.s. of Eq. (17). The former process is governed by the auxiliary current matrices $\Phi_{\alpha ks}$, which can be rewritten in the suggestive form

$$2\mathrm{Re}\sum_k T_{\alpha k}(t)\Phi_{\alpha ks}(t) = \left\langle \hat{J}^{(\mathrm{in})}_{\alpha s}(t)\hat{n}_{\bar{s}}(t)\right\rangle. \tag{18}$$

Consequently, the current matrices $\Phi_{\alpha ks}$ describe the *conditional current* from reservoir α into the QD level with spin s.

1. Hartree-Fock approximation

The simplest approximation to $\Phi_{\alpha ks}$ consists in using the following factorization:

$$\begin{aligned}\Phi^{\mathrm{HF}}_{\alpha ks}(t) &\equiv \mathrm{i}\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{c}_s(t)\rangle\langle\hat{n}_{\bar{s}}(t)\rangle \\ &= n_{\bar{s}}(t)\;\Pi''_{\alpha ks}(t).\end{aligned} \tag{19}$$

Inserting this expression into Eq. (13) results in the following equation of motion:

$$\partial_t \Pi''_{\alpha ks}(t) = \mathrm{i}[\Delta_{\alpha ks}(t) - U n_{\bar{s}}(t)]\Pi''_{\alpha ks}(t) + T^*_{\alpha k}(t) f_{\alpha k}. \tag{20}$$

This result is equivalent to the Hartree-Fock approximation applied to the Anderson model standard two-electron Green's function.[58] Like any mean-field approach, it does not lead to a double-resonance Green's function, which is required to properly account for charging effects. Hence, as is well known, a good description of the Coulomb-blockade regime requires going beyond this level of truncation in the equations of motion.

2. Hubbard I approximation

Instead of factorizing $\Phi_{\alpha ks}$ directly, we proceed by deriving its equation of motion. By means of Eqs. (3) we get

$$\begin{aligned}\partial_t \Phi_{\alpha ks}(t) = {}& \mathrm{i}[\Delta_{\alpha ks} - U - \mathrm{i}\Gamma(t)]\Phi_{\alpha ks}(t) \\ &+ \sum_{\alpha',k'} T^*_{\alpha' k'}(t)\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{B}_{\alpha' k' s}(t)\hat{n}_{\bar{s}}(t)\rangle \\ &+ \sum_{\alpha',k'} [T_{\alpha' k'}(t)\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{c}_s(t)\hat{B}^\dagger_{\alpha' k'\bar{s}}(t)\hat{c}_{\bar{s}}(t)\rangle \\ &- T^*_{\alpha' k'}(t)\langle \hat{B}^\dagger_{\alpha ks}(t)\hat{c}_s(t)c^\dagger_{\bar{s}}(t)\hat{B}_{\alpha' k'\bar{s}}(t)\rangle].\end{aligned} \tag{21}$$

Note that the term proportional to U has only four operators in the expectation values because $\hat{n}_{\bar{s}}\hat{n}_{\bar{s}} = \hat{n}_{\bar{s}}$.

The approximation consists in neglecting matrix elements involving opposite spins, which renders the following factorizations:

$$\begin{aligned}\langle b^\dagger_{\alpha ks}(t_0)\hat{b}_{\alpha' k' s}(t_0)\hat{n}_{\bar{s}}(t)\rangle &\approx f_{\alpha k}\delta_{\alpha\alpha'}\delta_{kk'} n_{\bar{s}}(t), \\ \langle \hat{b}^\dagger_{\alpha ks}(t_0)\hat{c}_s(t)\hat{b}^\dagger_{\alpha' k'\bar{s}}(t_0)\hat{c}_{\bar{s}}(t)\rangle &\approx 0, \\ \langle \hat{b}^\dagger_{\alpha ks}(t_0)\hat{c}_s(t)\hat{c}^\dagger_{\bar{s}}(t)\hat{b}_{\alpha' k'\bar{s}}(t_0)\rangle &\approx 0.\end{aligned} \tag{22}$$

This approximation for the density matrices is equivalent to the truncation scheme employed in the nonequilibrium Green's function approach,[50,58] which yields the high-temperature limit of the Anderson model.

As a result of the factorization, we obtain the following compact equation of motion for the approximated second-order current matrices:

$$\begin{aligned}\partial_t \tilde{\Phi}_{\alpha ks}(t) = {}& \mathrm{i}[\Delta_{\alpha ks} - U - \mathrm{i}\Gamma(t)]\tilde{\Phi}_{\alpha ks}(t) \\ &+ T^*_{\alpha k}(t)\, f_{\alpha k}\, n_{\bar{s}}(t).\end{aligned} \tag{23}$$

The equations of motion for $n_s(t)$ [Eq. (12)], $\Pi''_{\alpha ks}(t)$ [Eq. (13) with $\Phi_{\alpha ks}$ replaced by $\tilde{\Phi}_{\alpha ks}$], and $\tilde{\Phi}_{\alpha ks}(t)$ [Eq. (23)] form a closed set of equations, which can be solved by means of the auxiliary-mode expansion discussed below.

III. AUXILIARY-MODE PROPAGATION SCHEME

The general idea of the auxiliary-mode expansion consists in making use of a contour integration and the residue theorem to perform the energy integration, for instance, in Eq. (11). To this end the Fermi function is expanded in a sum over simple poles (or auxiliary modes) and the respective integrals are given as finite sums (cf. Appendix A).

The transition to auxiliary modes (denoted by the index p) is facilitated by the following set of rules:

$$\varepsilon_{\alpha k}(t) \longrightarrow \chi^+_{\alpha p}(t), \tag{24a}$$

$$T^*_{\alpha k}(t) f_{\alpha k} \longrightarrow T_\alpha(t)\left(\frac{-\mathrm{i}}{\beta}\right), \tag{24b}$$

$$\sum_k T_{\alpha k}(t)\Pi''_{\alpha ks}(t) \longrightarrow \frac{1}{4}\Gamma_\alpha(t) + T_\alpha(t)\sum_p \Pi''_{\alpha sp}(t), \tag{24c}$$

which are derived in Appendix A. The first rule replaces the reservoir energy $\varepsilon_{\alpha k}$ with the (complex) pole $\chi^+_{\alpha p}$ of the expansion [cf. Eq. (A5)]. The second rule replaces the Fermi function with the respective weight, which is the same for all auxiliary modes. Finally, the third rule provides the actual expansion for the current matrices.

Applying these rules, the current matrices become

$$\Pi_{\alpha s} = \Pi'_{\alpha s}(t) + \Pi''_{\alpha s}(t), \tag{25a}$$

$$\Pi'_{\alpha s}(t) = -\frac{\Gamma_\alpha(t)}{2} n_s(t), \tag{25b}$$

$$\Pi''_{\alpha s}(t) = \frac{\Gamma_\alpha(t)}{4} + T_\alpha(t)\sum_p \Pi''_{\alpha sp}(t). \tag{25c}$$

The equation of motion for the auxiliary matrix $\Pi''_{\alpha sp}$ is obtained from Eq. (13). One arrives at

$$\begin{aligned}\mathrm{i}\partial_t \Pi''_{\alpha sp}(t) = {}& [\varepsilon_s(t) - \mathrm{i}\Gamma(t)/2 - \chi^+_{\alpha,p}(t)]\Pi''_{\alpha sp}(t) \\ &+ \frac{1}{\beta}T_\alpha(t) + U\;\Phi_{\alpha sp}(t)\,.\end{aligned} \tag{26}$$

The equations of motion for the auxiliary matrices $\Phi_{\alpha sp}$ are quite similar to those of Eq. (25c), namely,

$$\begin{aligned}\mathrm{i}\partial_t \tilde{\Phi}_{\alpha sp}(t) = {}& \left[\varepsilon_s(t) + U - \chi^+_{\alpha,p}(t) - \mathrm{i}\frac{3\Gamma(t)}{2}\right]\tilde{\Phi}_{\alpha sp}(t) \\ &+ \frac{1}{\beta}T_\alpha(t)\, n_{\bar{s}}(t).\end{aligned} \tag{27}$$

The solution of the above equations still requires a complete description of the population dynamics given by $n_s(t)$. The

latter can be directly obtained from Eq. (12) in terms of the current matrices

$$\partial_t n_s(t) = -\Gamma(t)\, n_s(t) + 2\mathrm{Re} \sum_\alpha \Pi''_{\alpha s}(t). \tag{28}$$

This concludes the derivation of the auxiliary mode propagation scheme. The set of Eqs. (26) to (28), with initial conditions $n_s(t_0) = 0$, $\Pi''_{\alpha s p}(t_0) = 0$, and $\tilde{\Phi}_{\alpha s p}(t_0) = 0$, can be solved numerically using standard algorithms. Before the desired time dependence of the parameters $\varepsilon_s(t)$ and $\Gamma(t)$ sets in, the system has to be propagated until a steady state is reached. In this way, transient effects arising from the choice of the initial state are avoided. For convenience we derive in Appendix B the expressions for the stationary occupations, which may also be used as initial values for n_s.

IV. NONADIABATIC PUMPING

In this section we present two applications of the formalism developed above. As shown below, one of the interesting features of nonadiabatic pumping is the increasing delay in the current response to the external drive with growing driving speed. Hence, in distinction to the adiabatic limit, the current caused by a train of pulses can show interesting transient effects, whenever the pulse period is shorter than the system response time. To better understand nonadiabatic driving effects, we focus our analysis on single pulses and vary the speed by which their shape is changed.

It is worth stressing that our propagation method does not possess restrictions on the time dependence of the system driving parameters. In other words, the external time-dependent drive can be just a single pulse or a train of pulses; it can also be either fast or slow compared with the system internal time scales.

A. Symmetric monoparametric pumping

Let us begin by discussing the current generated by a single Gaussian voltage pulse changing the resonance energy as

$$\varepsilon_\mathrm{d}(t) = \varepsilon_0 + \varepsilon_1 \exp[-(t/t_\mathrm{p})^2]. \tag{29}$$

Here t_p sets the pumping time scale. We take $\Gamma_\alpha(t)$ to be time independent and equal for both leads, $\Gamma_\mathrm{L}(t) = \Gamma_\mathrm{R}(t) = \Gamma_0/2$. Since thereby $J_\mathrm{L} = J_\mathrm{R}$, we consider only J_L in the following.

Figure 1(a) shows the time dependence of the resonance energy according to Eq. (29). The parameters are taken as $\varepsilon_0 = \Gamma_0$, $\varepsilon_1 = -2\Gamma_0$, $k_\mathrm{B}T = 0.1\Gamma_0$. Left and right chemical potentials are equal, namely, $\mu_{\mathrm{L(R)}} = 0$, and the number of auxiliary modes is $N_\mathrm{F} = 160$. The two bottom panels show the instantaneous current J_L as a function of time for both the noninteracting ($U = 0$) and the interacting ($U \neq 0$) case. In the limit of large t_p, we use as a check for our results an analytical expression for the pumped current J_L, obtained for $U = 0$ within the adiabatic approximation.[12,28]

Here, due to the L/R symmetry, there is no net charge flowing through the QD. At any given time, both leads pump the same amount of charge in or out. In the driving scheme defined by Eq. (29), the QD is initially nearly empty. At $t = 0$, the resonance energy favors an almost-full occupation. For very slow pumping, large $t_\mathrm{p}\Gamma_0$, the current J_L depends only on the resonance energy $\varepsilon_\mathrm{d}(t)$: As the resonance dives into the Fermi sea, the QD is loaded with charge and the process is reversed as $\varepsilon_\mathrm{d}(t)$ starts increasing. This is no longer true when the drive is faster and $t_\mathrm{p}\Gamma_0$ decreases: Now one observes a retardation effect, namely, the J_L depends not only on the resonance position, but also on the driving speed. For fast driving one needs to integrate J_L over times much longer than t_p to observe a vanishing net charge per pulse.

In concluding this part, we would like to point to the possibility of the delay times depending on other pumping parameters, in particular, on the resonance energy. For example,

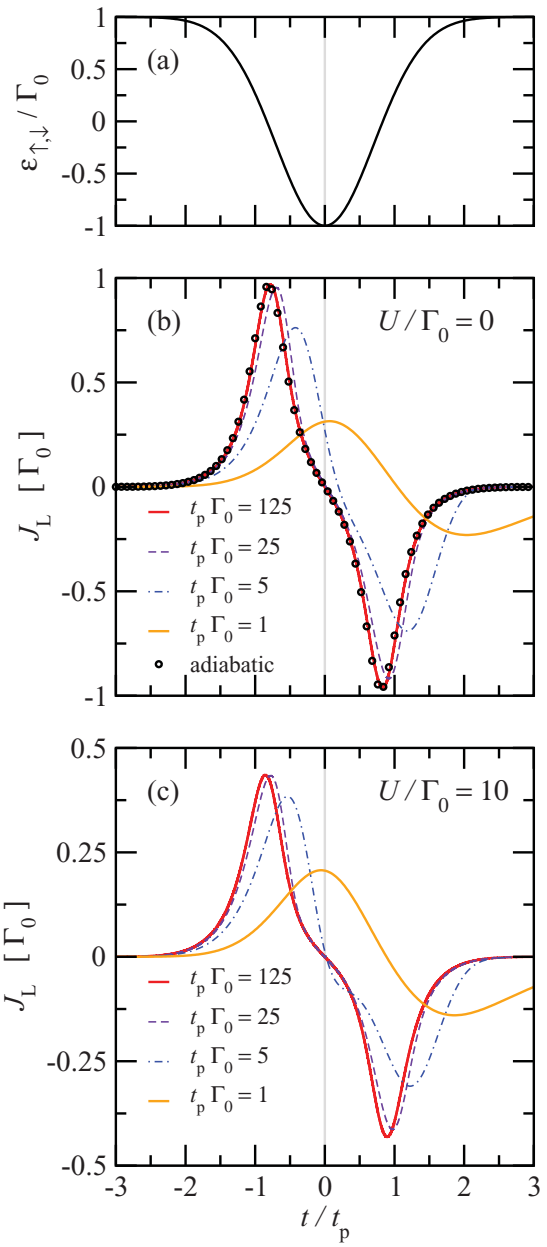

FIG. 1. (Color online) (a) Time dependence of the resonance energy according to Eq. (29). (b, c) Time-resolved current J_L for different pulse lengths t_p and $U = 0$ and $U/\Gamma_0 = 10$. Parameters used: $\varepsilon_0 = \Gamma_0$, $\varepsilon_1 = -2\Gamma_0$, $\mu_\alpha = 0$, $k_\mathrm{B}T = 0.1\Gamma_0$, and $N_\mathrm{F} = 160$ (number of auxiliary modes). Circles denote the adiabatic limit.[28]

in a recent study,[59] it was found that the charge-relaxation time of an *interacting* QD coupled to a single-reservoir depends strongly on the resonance energy. The implications of this behavior for pumping driven by single pulses or pulse trains will be the subject of future work.

B. Constrained two-parameter pumping

The pumped currents $J_{L,R}(t)$ characterize the time-dependent electron response to the external drive. However, in most applications one is only interested in the charge pumped per cycle Q_c or per pulse Q_p. In the latter case, Q_p is given as the time integral over the current, which we write in a symmetric way:

$$Q_p = \frac{1}{2}\int_{-\infty}^{+\infty} dt[J_L(t) - J_R(t)]. \tag{30}$$

One of the beautiful lessons learned from the investigation of adiabatic pumping establishes a proportionality relation between Q_p and the area swept by the time-dependent driving forces in parameter space.[12] In other words, the total charge flowing through a QD per cycle (or per pulse) in a *single-parameter adiabatic pump* vanishes. Due to the constraints of single-parameter pumps, in most applications at least two parameters are used.[2–5,8–11,40–44] On the other hand, by using a single-gate modulation one can realize a constrained two-parameter pump,[43] which implies that the time dependence of the parameters is ultimately coupled due to the modulation of only a single gate voltage. In the following we investigate the implications of this scenario for nonadiabatic pumping.

1. Pulse scheme

Specifically, let us consider voltage pulses of the form

$$S(t,\delta) = 1 - 2\exp[-(2\sqrt{\ln 2}\, t/t_p - \delta)^2]. \tag{31}$$

Here t_p measures the characteristic pulse time, whereas δ governs the time the pulse sets in. The numerical factor $2\sqrt{\ln 2}$ ensures that t_p is the full width at half-maximum of the pulse, which simplifies the following discussion. By tuning the delay, one can conveniently switch between a single parameter ($\delta = 0$) and a two-parameter setup ($\delta \neq 0$). Further, the time dependence of the resonance energy and the coupling strengths (decay widths) are chosen as

$$\varepsilon_d(t) = \varepsilon_0 + \varepsilon_1 S(t,0), \tag{32a}$$

$$\Gamma_R(t) = \frac{\Gamma_0}{2}[1 - S(t,0)], \tag{32b}$$

$$\Gamma_L(t) = \frac{\Gamma_0}{2}[1 + S(t,\delta_L)]. \tag{32c}$$

This choice takes into account that the coupling strengths depend exponentially on the gate voltage.[43] The constraint is imposed by setting $\delta_R = 0$ and the specific value of δ_L. For this driving parametrization, the resonance and the decay widths are ε_0 and Γ_0, respectively, for both asymptotic limits of $|t| \gg t_p$. In the following, the parameters are taken as $\varepsilon_0 = 0$, $\varepsilon_1/\Gamma_0 = 4$, $k_BT/\Gamma_0 = 1/10$, and interaction energy either $U = 0$ or $U/\Gamma_0 = 10$. In Fig. 2 the time dependence of ε_d and $\Gamma_{L/R}$ is illustrated for three cases: $\delta_L = 0$ and $\delta_L = \pm 1$. As mentioned above, in each case the coupling to the right reservoir Γ_R follows the time dependence of the resonance energy. When the latter attains its minimal value at $t = 0$, which brings the energy well below the chemical potential of the reservoirs, the coupling to the right reservoir is *minimal*. On the other hand, the behavior of the coupling to the left reservoir can be influenced by the value of δ_L. For $\delta_L = -1$ the *maximum* of Γ_L comes before $t = 0$, while for $\delta_L = +1$ it is attained after $t = 0$. In the case $\delta_L = 0$ the coupling to the left reservoir is maximal simultaneously with Γ_R being minimal at $t = 0$. In the following the response to these drivings is investigated.

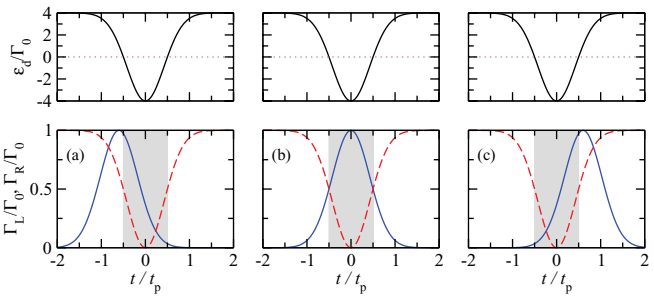

FIG. 2. (Color online) Time dependence of the resonance energy ε_d (upper row) and the decay widths Γ_L [lower row; solid (blue) line] and Γ_R [lower row; dashed (red) line] for three cases: (a) $\delta_L = -1$, (b) $\delta_L = 0$, and (c) $\delta_L = 1$. Dotted lines indicate the chemical potential in the reservoirs and the shaded area shows the times when the resonance energy is below the chemical potential.

2. Adiabatic pumping

Knowing the time dependence shown in Fig. 2, one can readily predict the behavior of Q_p in the adiabatic limit. In this case, electron flow occurs when the resonance energy matches the chemical potential of the reservoirs. In our pulse scheme, $\varepsilon_d(t)$ equals the chemical potential at $t = -t_p/2$ and $t = +t_p/2$, corresponding to the onset of charging and decharging of the QD, respectively. Further, the direction of the net current is determined by the difference in the couplings to the reservoirs at these very times. For example, for $\delta_L = -1$, one finds $\Gamma_L > \Gamma_R$ while charging and $\Gamma_L < \Gamma_R$ while decharging. Consequently, the net current is directed from left to right and Q_p is expected to be *positive*. For $\delta_L = +1$ the situation is opposite and Q_p should be *negative*. Finally, for $\delta_L = 0$ the couplings are equal at both instants of time and the net current is vanishing. These expectations are confirmed by our results for the adiabatic regime, $t_p\Gamma_0 \gg 1$, and different values of U/Γ_0, which are shown in Fig. 3(a). As already mentioned, one observes $Q_p = 0$ for $\delta_L = 0$ (monoparametric pumping). As $|\delta_L|$ begins to increase, $|Q_p|$ increases as well. In this scenario, when the resonance energy matches the chemical potential, electrons load the dot from the left (or right) and later they are unloaded to the right (or left, depending on the sign on δ). For larger values of $|\delta_L|$, the left reservoir participates less in the loading or unloading of the QD and the charge per pulse vanishes accordingly.

For interaction strengths $U \gg \varepsilon_1$ the double occupation of the QD is suppressed, and consequently, in the adiabatic regime, Q_p is half the value of Q_p for the noninteracting case. The numerical results indicate that within the Hubbard I

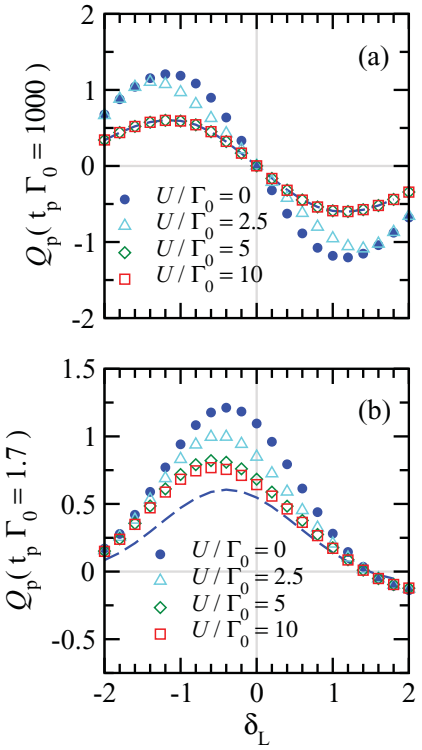

FIG. 3. (Color online) Charge per pulse Q_p vs pulse shift δ_L in the long-pulse limit (upper panel) and at $t_p = 1.7\,\Gamma_0^{-1}$ (lower panel). Dashed lines indicate half of the no-interacting result.

approximation, $U \neq 0$ does not introduce new time scales to the problem for $t_p\Gamma_0 \gg 1$, and its major effect is to correct the spin degeneracy factor in the equations for the $U = 0$ case.

3. *Nonadiabatic pumping*

None of the aforementioned features are observed in the nonadiabatic pumping regime. Figure 3(b) shows, for example, that, for short pulses there is no simple relation between Q_p for $U = 0$ and Q_p for $U \neq 0$. Moreover, compared to the adiabatic regime the charge per pulse can be substantially larger in this regime. Unfortunately, the behavior of Q_p in this regime is not as easily predicted in general, since the evolution of the parameters $\{\varepsilon_d, \Gamma_L, \Gamma_R\}$ after the onset of loading and unloading has to be taken into account. This is because in the nonadiabatic regime the QD charging and decharging, and consequently the current, are *delayed with respect to the external system changes*, as shown in Sec. IV A. The quantitative behavior depends on the precise magnitude of the delay, which is determined by the pulse length. Taking, for example, the case $\delta_L = 0$, one finds from Fig. 2(b) that $\Gamma_L > \Gamma_R$ while the resonance energy is below the chemical potential and charging occurs. During the de-charging, when $\varepsilon_d > \mu_{L,R}$, one finds $\Gamma_R > \Gamma_L$. Consequently, the current is expected to flow mainly from left to right, which leads to a positive charge per cycle. For a sufficiently long delay of the response, i.e., for sufficiently short pulses, one finds the relations of Γ_L and Γ_R presented above for all δ_L. Thus, Q_p has to become positive independent of δ_L in the limit of fast driving. This is confirmed by the results shown in Fig. 3(b). The interesting implications of this result are discussed at the end of this section.

Finally, in Fig. 4 we summarize and corroborate the discussion of nonadiabatic pumping. It shows the charge pumped due to the pulse as a function of pulse length $t_p\Gamma_0$ in the noninteracting ($U = 0$) and the Coulomb-blockade ($U = 10\Gamma_0$) regimes. In the latter case $Q_p \leqslant 1$ for all pulse lengths. As discussed above, the amount of pumped charge Q_p depends very strongly on the value of $t_p\Gamma_0$. In the limit of large pulse lengths, Q_p approaches the respective adiabatic value, while for $t_p\Gamma_0 \to 0$ the charge per pulse vanishes. Moreover, one finds that Q_p is indeed positive for small pulse lengths. This has the intriguing consequence that the charge per pulse can change its sign, sweeping from short to long pulses. This is shown in Fig. 4(c) for $\delta_L = 1$, where Q_p is negative in the adiabatic regime. A more general and quantitative analysis of this effect is certainly desirable but beyond the scope of this article. It may lead, however, to interesting new applications. It is also worth mentioning that, by changing the pumping parameters, it is possible to optimize the charge pumped per pulse and, in particular, to find situations where $Q_p = 1$, which may be very interesting for metrologic purposes.[60]

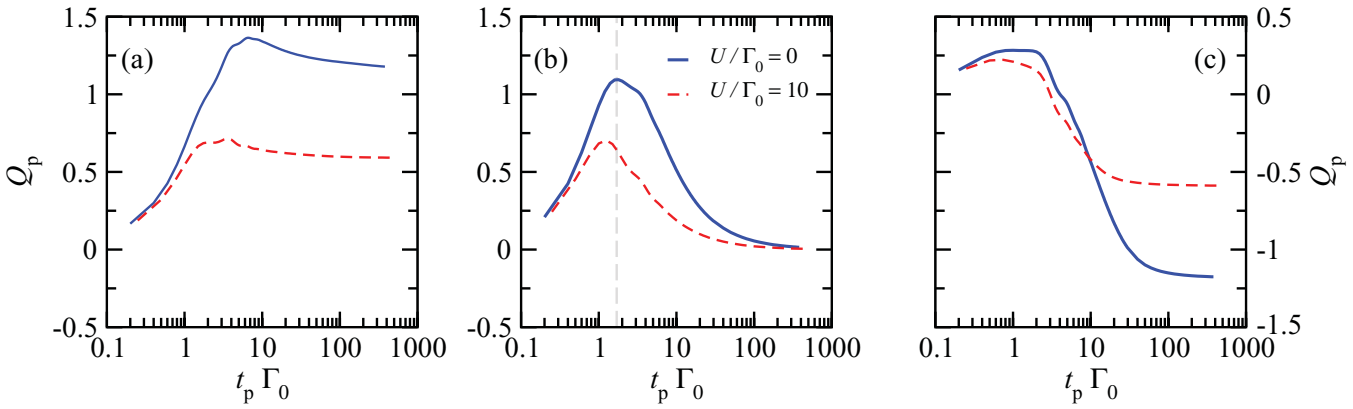

FIG. 4. (Color online) Charge pumped per pulse Q_p versus pulse length t_p for the pulse scheme given by Eq. (31). The solid (blue) line represents the noninteracting case, while the dashed (red) line represents $U/\Gamma_0 = 10$. We consider threecases: (a) $\delta_L = -1$, (b) $\delta_L = 0$, and (c) $\delta_L = 1$.

V. CONCLUSIONS

We have presented a new method for analyzing nonadiabatic charge pumping through single-level QDs that takes Coulomb interactions into account. The method is based on calculating the time evolution for single-electron density matrices. The many-body aspects of the problem are approximated by truncating the equations of motion one order beyond mean field. The novelty is the way in which the time evolution is treated: By means of an auxiliary-mode expansion, we obtain a propagation scheme that allows for dealing with arbitrary driving parameters, fast and slow. The method presented in this paper can be applied to a wide range of coupling parameters Γ_α, provided one avoids the Kondo regime. Hence, we are not restricted to the weak coupling limit where Q_p, the charge pumped per pulse, is rather small.

The results presented for single pulses are also valid for pulse trains, provided the time between the pulses is sufficiently long. One can expect to find qualitatively new and interesting effects by decreasing the time lag. The propagation scheme allows, in principle, for study of transient effects. In addition, by propagating over a periodic sequence of pulses it constitutes a complementary approach to the more familiar periodic driving. In this regard, our propagation scheme has the potential to be a valuable tool and provide deeper insights into nonadiabatic quantum pumps.

ACKNOWLEDGMENT

This work was supported in part by CNPq (Brazil).

APPENDIX A: AUXILIARY-MODE EXPANSION

Here we motivate the rules given in Sec. III. To begin with we introduce correlation functions, which can be approximated by finite sums. Then we write the current matrices in terms of these finite sums.

1. Correlation functions and mode expansion

As we will show later, in the present case we have to consider the following reservoir correlation function:

$$\begin{aligned} C_\alpha(t',t) &\equiv \sum_k T_{\alpha k}(t) g_{\alpha k}(t',t) T^*_{\alpha k}(t') f_\alpha(\varepsilon_k) \\ &= \int \frac{d\varepsilon}{2\pi}\, \Gamma_\alpha(\varepsilon,t',t)\, f_\alpha(\varepsilon) \\ &\quad \times \exp\left\{ \mathrm{i} \int_{t'}^{t} dt''[\varepsilon + \Delta\varepsilon_\alpha(t'')] \right\}, \end{aligned} \tag{A1}$$

where the line-width function Γ_α is defined as usual:[58]

$$\begin{aligned} \Gamma_\alpha(\varepsilon,t',t) &\equiv 2\pi \sum_k T_{\alpha k}(t) T^*_{\alpha k}(t') \delta(\varepsilon - \varepsilon_{\alpha k}) \\ &= 2\pi\, T_\alpha(t) T^*_\alpha(t') \rho_\alpha. \end{aligned} \tag{A2}$$

In the second line we have used the wide-band limit.

In order to perform the energy integration in Eq. (A1), we expand the Fermi function $f(\varepsilon)$ as a finite sum over simple poles,

$$f(\varepsilon) \approx \frac{1}{2} - \frac{1}{\beta} \sum_{p=1}^{N_\mathrm{F}} \left(\frac{1}{\varepsilon - \chi_p^+} + \frac{1}{\varepsilon - \chi_p^-} \right), \tag{A3}$$

with $\chi_p^\pm = \mu \pm x_p/\beta$ and $\mathrm{Im}\, x_p > 0$. Instead of using the Matsubara expansion,[61] with poles $x_p = \mathrm{i}\pi(2p-1)$, we use a partial fraction decomposition of the Fermi function,[55] which converges much more rapidly than the standard Matsubara expansion. In this case the poles $x_p = \pm 2\sqrt{z_p}$ are given by the eigenvalues z_p of a $N_\mathrm{F} \times N_\mathrm{F}$ matrix.[55] The poles are arranged such that all poles χ_p^+ (χ_p^-) are in the upper (lower) complex plane. As in the Matsubara expansion, all poles have the same weight.

Employing the expansion given by Eq. (A3), one can evaluate the energy integrals by contour integration in the upper or lower complex plane depending on the sign of $t - t'$. Thereby, the integral in Eq. (A1) becomes a (finite) sum of the residues. For $t \geqslant t'$, one gets

$$C_\alpha(t',t) = \frac{1}{2}\Gamma_\alpha(t)\delta(t-t') + T_\alpha(t) \sum_p C_{\alpha p}(t,t_1), \tag{A4a}$$

$$C_{\alpha p}(t',t) \equiv \frac{-\mathrm{i}}{\beta} T_\alpha(t') e^{\mathrm{i}\int_{t'}^{t} dt'' \chi^+_{\alpha p}(t'')}, \tag{A4b}$$

with the auxiliary modes for reservoir α given by

$$\chi^+_{\alpha p}(t) = [\mu_\alpha + \Delta\varepsilon_\alpha(t)] + x_p/\beta. \tag{A5}$$

Here, μ_α is the chemical potential and $\Delta\varepsilon_\alpha(t)$ is due to the time-dependent single-particle energies $\varepsilon_{\alpha k}(t)$ of the reservoir Hamiltonian [Eq. (1c)].

2. Current matrices

The set of Eqs. (13) and (23) can be formally solved. In order to write down these solutions we define the following functions:

$$g_s(t,t') \equiv \mathrm{e}^{-\mathrm{i}\int_{t'}^{t} dt''[\varepsilon_s(t'') - \mathrm{i}\frac{\Gamma(t'')}{2}]}, \tag{A6a}$$

$$g^U_s(t,t') \equiv \mathrm{e}^{-\mathrm{i}\int_{t'}^{t} dt''[\varepsilon_s(t'') + U - \mathrm{i}\frac{\Gamma(t'')}{2}]}. \tag{A6b}$$

With these definitions the formal solution of Eq. (13) reads

$$\begin{aligned} \Pi''_{\alpha k s}(t) &= \int_{t_0}^{t} dt'\, g_s(t,t') g_{\alpha k}(t',t) \\ &\quad \times [T^*_{\alpha k}(t') f_\alpha(\varepsilon_k) - \mathrm{i}U\tilde{\Phi}_{\alpha k s}(t')], \end{aligned} \tag{A7}$$

where we have assumed $\Pi''_{\alpha k s}(t_0) = 0$, corresponding to our choice of an initially uncorrelated density matrix (see Sec. II A). An analogous equation holds for $\tilde{\Phi}_{\alpha k s}(t)$, again with $\tilde{\Phi}_{\alpha k s}(t_0) = 0$. We can combine these two expressions to

get, for the second part of the current matrix,

$$\Pi''_{\alpha s}(t) = \sum_k T_{\alpha k}(t)\Pi''_{\alpha k s}(t) = \int_{t_0}^{t} dt' C_\alpha(t',t) g_s(t,t') - \mathrm{i}U \int_{t_0}^{t} dt' g_s(t,t') \int_{t_0}^{t'} dt'' C_\alpha(t'',t) g_s^U(t',t'') n_{\bar{s}}(t''), \tag{A8}$$

where we have used the definition of the correlation function C_α given by Eq. (A1). Finally, by means of expansion (A4) of the correlation functions, we obtain an expansion of the current matrices,

$$\sum_k T_{\alpha k}(t)\Pi''_{\alpha k s}(t) = \frac{1}{4}\Gamma_\alpha(t) + T_\alpha(t) \sum_p \Pi''_{\alpha s p}(t), \tag{A9a}$$

$$\Pi''_{\alpha s p}(t) \equiv \int_{t_0}^{t} dt' C_{\alpha p}(t',t) g_s(t,t') - \mathrm{i}U \int_{t_0}^{t} dt' g_s(t,t') \times \int_{t_0}^{t'} dt'' C_{\alpha p}(t'',t) g_s^U(t',t'') n_{\bar{s}}(t''), \tag{A9b}$$

which resembles the last rule of Eqs. (24). Using the explicit expression for $\Pi''_{\alpha s p}$ and taking the time derivative, one can easily verify the first two rules given by Eqs. (24). Similarly, one also obtains an expression for $\tilde{\Phi}_{\alpha s p}$, which reads

$$\tilde{\Phi}_{\alpha s p}(t) \equiv \int_{t_0}^{t} dt'' C_{\alpha p}(t'',t) g_s^U(t,t'') n_{\bar{s}}(t''). \tag{A10}$$

The time derivative of this expression is given by Eq. (27).

APPENDIX B: STATIONARY OCCUPATIONS

If neither the couplings $T_{\alpha k}$ (and thus Γ) nor the levels ε_s or $\varepsilon_{\alpha k}$ depend on time, the level occupations n_s and the currents J_α converge to stationary values. These values can be obtained by setting all time derivatives in the respective equations of motion to 0. In order to simplify the notation we characterize the stationary values by omitting the time argument.

We specify below the level occupations for the two approximations discussed in Sec. II C. Therefore we use

$$n_s = \frac{1}{\Gamma} 2\mathrm{Re} \sum_{\alpha k} T_{\alpha k} \Pi''_{\alpha k s}, \tag{B1}$$

which follows directly from Eq. (11b).

1. Hartree-Fock

Within the Hartree-Fock approximation [Sec. II C 1], from Eq. (20) we get

$$\Pi''_{\alpha k s} = \mathrm{i} \frac{T^*_{\alpha k} f_{\alpha k}}{\Delta_{\alpha k s} - U n_{\bar{s}}}. \tag{B2}$$

Plugging this into Eq. (B1), changing the k summation into an integral over ε, and using definition (14), for the wide-band limit [Eq. (5)] we get

$$n_s = \sum_\alpha \Gamma_\alpha \int \frac{d\varepsilon}{2\pi} \frac{f_\alpha(\varepsilon)}{(\varepsilon - \varepsilon_s - U\, n_{\bar{s}})^2 + \left(\frac{\Gamma}{2}\right)^2}. \tag{B3}$$

Equation (B3) is a nonlinear equation for n_s and has to be solved numerically.

2. Hubbard I

We obtain the stationary conditional current $\tilde{\Phi}_{\alpha k s}$ for the Hubbard I approximation [Sec. II C 2] from Eq. (23) as

$$\tilde{\Phi}_{\alpha k s} = \mathrm{i} \frac{T^*_{\alpha k} f_{\alpha k} n_{\bar{s}}}{\Delta_{\alpha k s} - U + \mathrm{i}\Gamma}. \tag{B4}$$

This expression can be used for the stationary Π'' in Eq. (13):

$$\Pi''_{\alpha k s} = \mathrm{i} \frac{T^*_{\alpha k} f_{\alpha k}}{\Delta_{\alpha k s}} + \mathrm{i} \frac{T^*_{\alpha k} f_{\alpha k} U n_{\bar{s}}}{\Delta_{\alpha k s} [\Delta_{\alpha k s} - U + \mathrm{i}\Gamma]}. \tag{B5}$$

We use Eq. (B1) and definition (14) and, finally, get, for the occupation, the following integral:

$$n_s = \sum_\alpha \Gamma_\alpha \int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon)[A'(\varepsilon) + n_{\bar{s}} A''(\varepsilon)], \tag{B6a}$$

$$A'(\varepsilon) \equiv \frac{1}{(\varepsilon - \varepsilon_s)^2 + \left(\frac{\Gamma}{2}\right)^2}, \tag{B6b}$$

$$A''(\varepsilon) \equiv A'(\varepsilon) \frac{U[4(\varepsilon - \varepsilon_s) - U]}{(\varepsilon - \varepsilon_s - U)^2 + \left(\frac{3\Gamma}{2}\right)^2}. \tag{B6c}$$

This time the equation is linear in $n_{\bar{s}}$ and can be solved explicitly. In the limits $U \to 0$ and $U \to \infty$, it is $A''(\varepsilon) = 0$ and $A''(\varepsilon) = -A'(\varepsilon)$, respectively. The former limit corresponds to noninteracting electrons and Eq. (B6a) gives the correct expression for the occupation.[58] The latter case describes the situation with very strong interactions.

*Current address: Department of Applied Physics, Chalmers University of Technology, S-41296 Göteborg, Sweden; alexander.croy@chalmers.se

[1] D. J. Thouless, Phys. Rev. B **27**, 6083 (1983).
[2] H. Pothier, P. Lafarge, C. Urbina, D. Esteve, and M. Devoret, Europhys. Lett. **17**, 249 (1992).
[3] J. M. Martinis, M. Nahum, and H. D. Jensen, Phys. Rev. Lett. **72**, 904 (1994).
[4] M. Switkes, C. M. Marcus, K. Campman, and A. C. Gossard, Science **283**, 1905 (1999).
[5] L. DiCarlo, C. M. Marcus, and J. S. Harris, Phys. Rev. Lett. **91**, 246804 (2003).
[6] P. J. Leek, M. R. Buitelaar, V. I. Talyanskii, C. G. Smith, D. Anderson, G. A. C. Jones, J. Wei, and D. H. Cobden, Phys. Rev. Lett. **95**, 256802 (2005).
[7] S. K. Watson, R. M. Potok, C. M. Marcus, and V. Umansky, Phys. Rev. Lett. **91**, 258301 (2003).
[8] Y.-S. Shin, W. Song, J. Kim, B.-C. Woo, N. Kim, M.-H. Jung, S.-H. Park, J.-G. Kim, K.-H. Ahn, and K. Hong, Phys. Rev. B **74**, 195415 (2006).

[9] A. Fuhrer, C. Fasth, and L. Samuelson, Appl. Phys. Lett. **91**, 052109 (2007).
[10] M. R. Buitelaar, V. Kashcheyevs, P. J. Leek, V. I. Talyanskii, C. G. Smith, D. Anderson, G. A. C. Jones, J. Wei, and D. H. Cobden, Phys. Rev. Lett. **101**, 126803 (2008).
[11] A. Fujiwara, K. Nishiguchi, and Y. Ono, Appl. Phys. Lett. **92**, 042102 (2008).
[12] P. W. Brouwer, Phys. Rev. B **58**, R10135 (1998).
[13] F. Zhou, B. Spivak, and B. Altshuler, Phys. Rev. Lett. **82**, 608 (1999).
[14] O. Entin-Wohlman, A. Aharony, and Y. Levinson, Phys. Rev. B **65**, 195411 (2002).
[15] I. L. Aleiner, P. W. Brouwer, and L. I. Glazman, Phys. Rep. **358**, 309 (2002).
[16] M. Moskalets and M. Büttiker, Phys. Rev. B **64**, 201305(R) (2001).
[17] Y. Makhlin and A. D. Mirlin, Phys. Rev. Lett. **87**, 276803 (2001).
[18] F. Romeo and R. Citro, Phys. Rev. B **82**, 085317 (2010).
[19] P. Sharma and C. Chamon, Phys. Rev. Lett. **87**, 096401 (2001).
[20] E. R. Mucciolo, C. Chamon, and C. M. Marcus, Phys. Rev. Lett. **89**, 146802 (2002).
[21] M. Martínez-Mares, C. H. Lewenkopf, and E. R. Mucciolo, Phys. Rev. B **69**, 085301 (2004).
[22] M. G. Vavilov, V. Ambegaokar, and I. L. Aleiner, Phys. Rev. B **63**, 195313 (2001).
[23] M. Moskalets and M. Büttiker, Phys. Rev. B **66**, 205320 (2002).
[24] L. Arrachea and M. Moskalets, Phys. Rev. B **74**, 245322 (2006).
[25] E. R. Mucciolo and C. H. Lewenkopf, Int. J. Nanotechnol. **4**, 482 (2007).
[26] R. Citro, N. Andrei, and Q. Niu, Phys. Rev. B **68**, 165312 (2003).
[27] T. Aono, Phys. Rev. Lett. **93**, 116601 (2004).
[28] J. Splettstoesser, M. Governale, J. König, and R. Fazio, Phys. Rev. Lett. **95**, 246803 (2005).
[29] E. Sela and Y. Oreg, Phys. Rev. Lett. **96**, 166802 (2006).
[30] D. Fioretto and A. Silva, Phys. Rev. Lett. **100**, 236803 (2008).
[31] L. Arrachea, A. Levy Yeyati, and A. Martin-Rodero, Phys. Rev. B **77**, 165326 (2008).
[32] A. R. Hernández, F. A. Pinheiro, C. H. Lewenkopf, and E. R. Mucciolo, Phys. Rev. B **80**, 115311 (2009).
[33] B. L. Hazelzet, M. R. Wegewijs, T. H. Stoof, and Y. V. Nazarov, Phys. Rev. B **63**, 165313 (2001).
[34] R. Sánchez, E. Cota, R. Aguado, and G. Platero, Phys. Rev. B **74**, 035326 (2006).
[35] M. Braun and G. Burkard, Phys. Rev. Lett. **101**, 036802 (2008).
[36] R. H. Blick, R. J. Haug, D. W. van der Weide, K. von Klitzing, and K. Eberl, Appl. Phys. Lett. **67**, 3924 (1995).
[37] T. H. Oosterkamp, L. P. Kouwenhoven, A. E. A. Koolen, N. C. van der Vaart, and C. J. P. M. Harmans, Phys. Rev. Lett. **78**, 1536 (1997).
[38] L. E. F. Foa Torres, Phys. Rev. B **72**, 245339 (2005).
[39] F. Cavaliere, M. Governale, and J. König, Phys. Rev. Lett. **103**, 136801 (2009).
[40] M. D. Blumenthal, B. Kaestner, L. Li, S. Giblin, T. J. B. M. Janssen, M. Pepper, D. Anderson, G. Jones, and D. A. Ritchie, Nature Phys. **3**, 343 (2007).
[41] S. J. Wright, M. D. Blumenthal, G. Gumbs, A. L. Thorn, M. Pepper, T. J. B. M. Janssen, S. N. Holmes, D. Anderson, G. A. C. Jones, C. A. Nicoll, and D. A. Ritchie, Phys. Rev. B **78**, 233311 (2008).
[42] B. Kaestner, V. Kashcheyevs, G. Hein, K. Pierz, U. Siegner, and H. W. Schumacher, Appl. Phys. Lett. **92**, 192106 (2008).
[43] B. Kaestner, V. Kashcheyevs, S. Amakawa, M. D. Blumenthal, L. Li, T. J. B. M. Janssen, G. Hein, K. Pierz, T. Weimann, U. Siegner, and H. W. Schumacher, Phys. Rev. B **77**, 153301 (2008).
[44] S. J. Wright, M. D. Blumenthal, M. Pepper, D. Anderson, G. A. C. Jones, C. A. Nicoll, and D. A. Ritchie, Phys. Rev. B **80**, 113303 (2009).
[45] Y. Zhu, J. Maciejko, T. Ji, H. Guo, and J. Wang, Phys. Rev. B **71**, 075317 (2005).
[46] S. Kurth, G. Stefanucci, C.-O. Almbladh, A. Rubio, and E. K. U. Gross, Phys. Rev. B **72**, 035308 (2005).
[47] S. Welack, M. Schreiber, and U. Kleinekathöfer, J. Chem. Phys. **124**, 044712 (2006).
[48] V. Moldoveanu, V. Gudmundsson, and A. Manolescu, Phys. Rev. B **76**, 085330 (2007).
[49] P. Myöhänen, A. Stan, G. Stefanucci, and R. van Leeuwen, Phys. Rev. B **80**, 115107 (2009).
[50] Y. Meir, N. S. Wingreen, and P. A. Lee, Phys. Rev. Lett. **66**, 3048 (1991).
[51] A. Croy and U. Saalmann, Phys. Rev. B **80**, 245311 (2009).
[52] C. Meier and D. J. Tannor, J. Chem. Phys. **111**, 3365 (1999).
[53] J. Jin, X. Zheng, and Y. Yan, J. Chem. Phys. **128**, 234703 (2008).
[54] A. Croy and U. Saalmann, New J. Phys. **13**, 043015 (2011).
[55] A. Croy and U. Saalmann, Phys. Rev. B **80**, 073102 (2009); **82**, 159904(E) (2010).
[56] A.-P. Jauho, N. S. Wingreen, and Y. Meir, Phys. Rev. B **50**, 5528 (1994).
[57] C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, J. Phys. C **4**, 916 (1971).
[58] H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, Berlin, 2007).
[59] J. Splettstoesser, M. Governale, J. König, and M. Büttiker, Phys. Rev. B **81**, 165318 (2010).
[60] M. W. Keller, Metrologia **45**, 102 (2008).
[61] G. D. Mahan, *Many Particle Physics*, 2nd ed. (Plenum, New York, 1990).