Adiabatic charge pumping through quantum dots in the Coulomb blockade regime

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We investigate the influence of the Coulomb interaction on the adiabatic pumping current through a quantum dot. Using nonequilibrium Green’s functions techniques, we derive a general expression for the current based on the instantaneous Green’s function of the dot. We apply this formula to study the dependence of the charge pumped per cycle on the time-dependent pumping potentials. Motivated by recent experiments, the possibility of charge quantization in the presence of a finite Coulomb repulsion energy is investigated.

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I. INTRODUCTION

The basic idea of electron pumping, put forward in the pioneer work of Thouless, 1 is to generate a dc current through a conductor in the absence of an applied bias voltage. This may be accomplished by applying time-dependent perturbations to the conductor. In electronic transport through mesoscopic conductors, the typical experimental time scale over which these external perturbations vary is large compared to the lifetime of the electron inside the conductor (dwell time). In that case, the pumping mechanism is called adiabatic.

Adiabatic quantum pumping in mesoscopic noninteracting open quantum dots was investigated theoretically by Brouwer 2 by means of a scattering approach. Applying the emissivity theory introduced by Büttiker et al., 3 he demonstrated that the pumping current is proportional to the driving frequency and shows large mesoscopic fluctuations accounted by random matrix theory. This scattering approach has been employed to investigate several aspects of adiabatic quantum pumping in noninteracting systems such as the role of discrete symmetries on the pumped charge, 4 the effects of inelastic scattering and decoherence, 5,6 the role of noise and dissipation, 7 Andreev interference effects in the presence of superconducting leads, 8,9 as well as spin pumping. 10–13 Pumping phenomena in noninteracting systems have also been investigated using alternative theoretical approaches such as the formalism based on iterative solutions of time-dependent states 14 and the Keldysh formulation. 15 Both approaches can be used beyond the adiabatic approximation.

Experimentally, the first implementation of an electron pump was due to Pothier et al. 16 when charge was quantized due to Coulomb blockade (CB) effects. 16 Adiabatic phase-coherent charge pumping, though not quantized, was observed in open semiconductor quantum dots 17 and in carbon nanotube quantum dots. 18,19 Quantized charge pumping was recently observed in AlGaAs/GaAs nanowires using a single-parameter modulation, 20 a result with potential applications to metrology. An experimental realization of a quantum spin pump has also been implemented. 21

Pumping through interacting systems, where the scattering approach does not apply, has been much less studied so far. Using the slave-boson mean-field approximation, Aono investigated the spin-charge separation of adiabatic currents in the Kondo regime. 22 The behavior of the pumping current through a quantum dot in the Kondo regime was studied both for adiabatic 23 and nonadiabatic systems 24 using the Keldysh formalism. Quantum pumping was investigated both in the CB regime 25,26 as well as for almost open quantum dots. 27 The nonequilibrium Green’s functions technique has been employed to investigate adiabatic pumping through interacting quantum dots in infinite U systems. 28,29 The role of the Coulomb interaction in the adiabatic pumping current has also been investigated in the limit of weak tunneling and infinite-U using diagrammatic techniques. 30 The presence of electron-electron interactions was shown to improve charge quantization in onedimensional disordered wires under certain circumstances. 31 The effects of the coupling of the quantum dot to bosonic environments and its implications to charge quantization were analyzed in Ref. 32. The interplay of nonadiabaticity and interaction effects on the pumping current were also recently reported. 33,34

In the present paper we investigate adiabatic charge pumping through interacting quantum dots in the CB regime for temperatures much higher than the Kondo temperature. We consider quantum dots with a single level subjected to a finite Coulomb repulsion U in the case of double occupancy. We investigate the time dependence of the pumping current by keeping U finite, a scenario out of the domain of validity of the theory developed in Refs. 28 and 29. This allows us to identify the relevant time scales controlling the current amplitude in realistic situations. We develop a general formal-
ism, based on nonequilibrium Green’s functions, to investi-
gate the influence of the Coulomb interaction on the
adiabatic pumping current. We discuss some applications
and consequences of this formulation and evaluate several quan-
tities of interest numerically for a range of parameters. Fi-
nally, the possibility of charge quantization in the presence of
a finite Coulomb repulsion is investigated. The study of
charge quantization in the adiabatic regime is interesting by
its own, and is also a necessary step towards the understand-
ing of recent experiments\textsuperscript{[30]} dealing with nonadiabatic pump-
ing.

This paper is organized as follows. In Sec. II we present
the model used to calculate the time-dependent current flow-
ing through the quantum dot. Section III is devoted to the
explicit calculation of the relevant Green’s functions. In Sec.
IV, we apply this calculation to derive an expression for the
pumping current in the adiabatic approximation for systems
with finite \( U \). The numerical evaluation of the current as well
as a discussion of its consequences and implications is pre-
sented in Sec. V. Finally, Sec. VI is devoted to a brief sum-
mary of our findings and concluding remarks.

II. MODEL FOR TRANSPORT IN QUANTUM DOTS

We consider a quantum dot (QD) with a single isolated
resonance in the Coulomb blockade regime, as schematically
depicted in Fig. 1. The potential in the dot is controlled by a
time-dependent gate voltage \( V_g(t) \) such that the QD Hamil-
tonian reads

\[
H_{\text{dot}} = \sum_{s=\uparrow,\downarrow} n_s(t) d_s^\dagger d_s + U n_\uparrow n_\downarrow ,
\]

where \( n_s = d_s^\dagger d_s \) is the number operator and \( d_s^\dagger(d_s) \) is the cre-
ation (annihilation) operator for an electron with energy \( e_s(t) = \epsilon_0 + \eta V_g(t) \) and spin \( s \) in the QD. Here, \( e \) denotes
the electron charge and \( \eta \) is a lever arm factor for the gate
tVoltage. Two single-channel leads are attached to the QD. It is
assumed that electrons in the leads are noninteracting and
obey the Hamiltonian

\[
H_{\text{lead}} = \sum_k \sum_{a=L,R} \sum_{s=\uparrow,\downarrow} e_{k\alpha s} c_{k\alpha s}^\dagger c_{k\alpha s},
\]

where \( c_{k\alpha s}^\dagger \) and \( c_{k\alpha s} \) are, respectively, the creation and annih-
lilation operators for electrons with momentum \( k \) and spin \( s \)
in the lead \( \alpha \). The QD is separated from the leads by tun-
nealing barriers controlled by the lateral gates \( V_1 \) and \( V_2 \) (see Fig.
1). The coupling Hamiltonian reads

\[
H_{\text{lead-dot}} = \sum_{k,\alpha,s} [V_{ka}(t) c_{ka\uparrow}^\dagger d_s + \text{H.c.}].
\]

The tunneling matrix elements \( V_{ka} \) connect states in the leads
to the resonant state in the dot and are assumed to be spin
independent. The total Hamiltonian of our model is the sum
of these three contributions,

\[
\mathcal{H} = H_{\text{lead}} + H_{\text{dot}} + H_{\text{lead-dot}}.
\]

The coupling between the states in the leads and those in
the dot, combined with the dot charging energy, turns the
time evolution of the system into a nontrivial many-body
problem. As a result, we cannot apply a single-particle for-
malism to describe the transport through the system and the
usual scattering-matrix formulation for pumping currents\textsuperscript{[30]}
is inappropriate. To circumvent these difficulties, we employ
the Schwinger-Keldysh formalism and the equation-of-
motion method\textsuperscript{[35]} to calculate the current through an interact-
ing quantum dot in the CB regime.

Our starting point is the general expression for the time-
dependent current in terms of the quantum dot Green’s func-
tion \( G_{s\gamma}(t,t') \):\textsuperscript{[36,37]}

\[
J_a(t) = -\frac{2e}{\hbar} \text{Im} \left\{ \sum_{k,s} \int_{-\infty}^{t} dt' V_{ka}(t') e^{i\epsilon_{ka\alpha}(t-t')/\hbar} V_{ka}(t) \times[f_a(\epsilon_{ka\alpha}) G_{s\gamma}^{\alpha}(t,t') + G_{s\gamma}^{\alpha\dagger}(t,t')] \right\},
\]

where \( f_a(E) = [e^{(E-\mu_a)/k_B T} + 1]^{-1} \) is the Fermi function for
the lead \( \alpha \) maintained at a chemical potential \( \mu_a \) and tempera-
ture \( T \) and \( k_B \) is the Boltzmann constant. Throughout the text
we consider pumping in the absence of an external bias, that
is, \( \mu_B = \mu_L = \epsilon_F \). For convenience, we set \( \epsilon_F = 0 \). The lesser,
retarded, and advanced dot Green’s functions are defined as\textsuperscript{[35]}

\[
G_{s\gamma}^{\alpha}(t,t') = \frac{i}{\hbar} \langle d_s(t')d_s(t) \rangle,
\]

\[
G_{s\gamma}^{\alpha\dagger}(t,t') = -\frac{i}{\hbar} \theta(t-t') \langle d_s(t),d_s(t') \rangle,
\]

\[
G_{s\gamma}^{\alpha\dagger\dagger}(t,t') = \frac{i}{\hbar} \theta(t'-t) \langle d_s(t),d_s(t') \rangle.
\]

Now it remains to compute the Green’s function \( G_{s\gamma}(t,t') \)
which involves the quantum dot states. This is where the
many-body aspects of the problem make their way into the
pumping current. Section III is devoted to this issue.

III. CALCULATION OF \( G_{s\gamma} \)

The current in Eq. (5) is given in terms of the quantum
dot Green’s functions \( G_{s\gamma}^{\alpha\dagger}(t,t') \) and \( G_{s\gamma}^{\alpha\dagger\dagger}(t,t') \). To write
expressions for them, we start by calculating the time-ordered
Green’s function \( G_{s\gamma}(t,t') \) defined as\textsuperscript{[35]}

\[
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\]
\[ G_{s,s}(t,t') = -i \frac{\delta}{\hbar} \langle \mathcal{T} [d_s(t) d_s^\dagger(t')] \rangle, \]

where \( \mathcal{T} \) is the time-ordering operator. The equation of motion for \( G_{s,s} \) is

\[ \left[ i\hbar \frac{\partial}{\partial t} - e_s(t) \right] G_{s,s}(t,t') = \delta(t-t') + U G_{s,s}^{(2)}(t,t') + \sum_{k,a} V_{ks}(t) G_{kas,kas}(t,t'). \]  

(8)

In Eq. (8) we have introduced the “contact” time-ordered Green’s function

\[ G_{s,kas}(t,t') = -i \frac{\delta}{\hbar} \langle \mathcal{T} [d_s(t) n_s(t) d^\dagger_{kas}(t')] \rangle, \]

(9)

which obeys the equation of motion

\[ \left( \frac{i\hbar}{\partial t} - e_{kas} \right) G_{s,kas}(t,t') = V_{ks}(t) G_{kas,kas}(t,t'), \]

(10)

as well as the second-order correlation function

\[ G_{s,s}^{(2)}(t,t') = -i \frac{\delta}{\hbar} \langle \mathcal{T} [d_s(t) n_s(t) d^\dagger_s(t')] \rangle, \]

(11)

which involves four fermionic operators and is generated by the interaction term \( U n_s n_{s\dagger} \). The same interaction term leads to the appearance of even higher-order correlation functions in the equation of motion for \( G^{(2)} \), namely,

\[ \left[ i\hbar \frac{\partial}{\partial t} - e_s(t) - U \right] G_{s,s}^{(2)}(t,t') = \delta(t-t')(n_s(t)) + \sum_{ka} \left[ V_{ka}^{*} \Gamma_{1,sas}^{(2)}(t,t') \right] \]

\[ + \sum_{ka} \left[ V_{ks}(t) \Gamma_{2,sas}^{(2)}(t,t') - V_{kt}^{*} \Gamma_{3,sas}^{(2)}(t,t') \right], \]

(12)

where the occupation number is defined as

\[ \langle n_s(t) \rangle = \langle d^\dagger_s(t) d_s(t) \rangle = i\hbar G_{s,s}^{-1}(t,t) \]

(13)

and we have introduced three lead-dot correlation functions,

\[ \Gamma_{1,sas}(t,t') = -i \frac{\delta}{\hbar} \langle \mathcal{T} [c_{kas}(t) n_s(t) d^\dagger_{s\dagger}(t')] \rangle, \]

(14)

\[ \Gamma_{2,sas}(t,t') = -i \frac{\delta}{\hbar} \langle \mathcal{T} [c_{kas}^\dagger(t) d^\dagger_{s\dagger}(t) d_s(t)] \rangle, \]

(15)

and

\[ \Gamma_{3,sas}(t,t') = -i \frac{\delta}{\hbar} \langle \mathcal{T} [c_{kas}(t) d^\dagger_{s\dagger}(t) d^\dagger_{s\dagger}(t')] \rangle. \]

(16)

At this level, one can verify that the equations of motion do not close. Going to the next level, one obtains new (higher-order) correlation functions and even more complicated expressions. To solve this problem, we shall recur to an approximate scheme, namely, the mean-field approximation.

**Formal solution of the equations of motion within the Hartree approximation**

We now focus on the Coulomb blockade regime and neglect spin correlations in the leads. That is, we assume that the Kondo temperature, \( T_K \sim U/\Gamma \), is very low, \( T_K \ll T \). As usual, \( \Gamma \) stands for the quantum dot’s linewidth which will be precisely defined in Sec. IV. Hence, with respect to Kondo correlations, we are in the high-temperature regime and the mean-field approximation is expected to be valid. Within this approximation, one can write the \( \Gamma^{(2)} \)'s as

\[ \Gamma_{1,sas}^{(2)}(t,t') = \langle n_s(t) \rangle G_{kas,kas}(t,t'), \]

(17)

and

\[ \Gamma_{2,sas}^{(2)}(t,t') = \Gamma_{3,sas}^{(2)}(t,t') = 0. \]

(18)

It has been shown that Kondo correlations are still absent in the next order of the equations-of-motion hierarchical truncation.\(^{36,39}\) The latter dresses the Green’s functions self-energies with higher-order terms in \( V \) that include, for instance, cotunneling processes. As long as \( e_s \) is of the order of \( k_B T \), we have verified that these contributions give only small corrections to the Hartree mean-field approximation.\(^{36}\) Thus, we write

\[ \left[ i\hbar \frac{\partial}{\partial t} - e_s(t) - U \right] G_{s,s}^{(2)}(t,t') = \langle n_s(t) \rangle \left[ \delta(t-t') + \sum_{ka} V_{ks}(t) G_{kas,kas}(t,t') \right], \]

(19)

where the occupation number \( \langle n_s(t) \rangle \) has to be determined self-consistently for all times. Equations (8), (10), and (19) form a closed set of equations of motion that determines the time-ordered Green’s function \( G_{s,s} \). Using analytical continuation and the Langreth rules\(^{36,40}\) we can then find the Green’s functions \( G_{s,s}^{R} \) and \( G_{s,s}^{A} \) that appear in the expressions for the current, Eq. (5). For convenience, let us define two auxiliary time-ordered Green’s functions \( g_s \) and \( g_s^U \) that obey the equations of motions

\[ \left[ i\hbar \frac{\partial}{\partial t} - e_s(t) - U \right] g_s(t,t') = \delta(t-t'), \]

(20)

and

\[ \left[ i\hbar \frac{\partial}{\partial t} - e_s(t) - U \right] g_s^U(t,t') = \delta(t-t'), \]

(21)

respectively. By analytical continuation into the complex plane, we can rewrite Eq. (19) as

\[ G_{s,s}^{(2)mf}(t,t') = g_s^U(t,t')(n_s(t')) + \sum_{ka} \int d\tau g_s^U(t,\tau) \times \langle n_s(\tau) \rangle V_{ks}(\tau) G_{kas,kas}(\tau', t'). \]

(22)

The equation for \( G_{kas,kas}(t,\tau) \) can also be obtained in a similar manner. Using Eq. (10), the equation of motion for the time-ordered Green’s function for free electrons in the leads, namely,
and the rules of analytical continuation, we conclude that the contour-ordered Green’s function \( G_{s,k} (\tau, \tau') \) obeys the equation

\[
\left( -i\hbar \frac{\partial}{\partial \tau} - \epsilon_{k\alpha} \right) G_{k\alpha}(\tau, \tau') = \delta(\tau - \tau'),
\]

(23)

and the pumping frequency \( \tau_{\text{pump}} \) lies in the range between \( 10^{-8} \) to \( 10^{-2} \) ns. The mean dwell time is given by the inverse of the resonance width \( \Gamma \). To estimate it, let us first recall that the dot single-particle mean level spacing is \( \Delta = \frac{2 \pi \hbar^2}{(\lambda m')^2} \), where \( \lambda \) is the dot effective area and \( m' = 0.067m_e \) for GaAs. We obtain \( \Delta = 7.6 \mu eV(\mu m)^2/\lambda \), where \( \lambda \) is given in square microns. For the Coulomb blockade regime, typical resonance widths are \( \Gamma = 0.01 - 0.1 \Delta \). As a result, \( \tau_{\text{pump}} = \gamma / \Gamma \approx 0.8 - 8 \) ns \((\mu m)^2/\lambda \) for most devices. For \( \lambda \) much smaller than \( 1 \) \((\mu m)^2 \), we find that \( \tau_{\text{pump}} \gg \tau_D \). In this case we can safely employ the so-called adiabatic approximation, which precisely relies on the fact that the time scale over which the system parameters vary is large compared to the lifetime of the electron in the dot.

**A. Adiabatic approximation for the Green’s functions**

A convenient way to separate slow and fast time scales is to reparametrize the Green’s functions as

\[
G(t, t') \rightarrow G(t-t', \frac{t+t'}{2}),
\]

(29)

that is, the time variables are replaced by a (fast) time difference \( \delta t = t-t' \) and a slow mean time \( \bar{t} = (t+t')/2 \). We implement the adiabatic approximation to lowest order by expanding the Green’s functions up to linear order in the slow variables, namely,

\[
G(t-t', \frac{t+t'}{2}) = G(t-t', \bar{t} + \frac{t-t'}{2}) \frac{\partial G}{\partial \bar{t}} |_{\bar{t} = \bar{t}}.
\]

(30)

In what follows we formally write

\[
G(t-t', \bar{t}) = G^{(0)}(t-t', \bar{t}) + G^{(1)}(t-t', \bar{t}),
\]

(31)

where the zeroth order refers to equilibrium quantities, while the adiabatic contributions, linear in the slow time variable (and in our case proportional to the pumping frequency), are collected in the first-order correction. The accuracy of our approximation can be tested by inspecting higher-order terms. We will return to this issue in Sec. V, when we present our results.

Let us now describe how the approximate scheme works. Using the mean-time parametrization, we write Eq. (26) as

\[
\bar{g}_s(t-t', \bar{t}) = g_s(t-t', \bar{t}) + U(n_s(\bar{t})) \times \int_{-\infty}^{\infty} dt_1 \bar{g}_s(t-t_1, \frac{t_1+\bar{t}}{2}) \bar{g}_s^{(0)}(t_1-t_1', \frac{t_1+t'_1}{2}) \bar{g}_s(t_1-t_1', \frac{t_1+t'_1}{2}).
\]

(32)

Expanding \( \bar{g}_s \) in the slow variables as in Eq. (30) and taking the Fourier transform with respect to the fast variable, namely, \( \hat{g}(\omega, \bar{t}) = \int_{-\infty}^{\infty} dt(d(t-t')) g(t-t', \bar{t}) \exp[i\omega(t-t')] \), we obtain

\[
\hat{g}_s(\omega, \bar{t}) = \hat{g}_s^{(0)}(\omega, \bar{t}) + \hat{g}_s^{(1)}(\omega, \bar{t}),
\]

(33)

with
\[ g_{1s}(\omega, t) = g_{s1}^{(0)}(\omega, t) + iU(n_{s1}^{(0)}(t))g_{s1}^{(0)}(\omega, t)g_{s1}^{(0)}(\omega, t), \] (34)

and
\[ g_{1s}^{(1)}(\omega, t) = g_{s1}^{(1)}(\omega, t) + U[n_{s1}^{(1)}(t)]g_{s1}^{(0)}(\omega, t) + \langle n_{s1}^{(1)}(t) \rangle g_{s1}^{(0)}(\omega, t), \] (35)

where
\[ \langle n_{s1}(t) \rangle = \langle n_{s1}^{(0)}(t) \rangle + \langle n_{s1}^{(1)}(t) \rangle \] (36)

is introduced following the same principle as the one described after Eq. (30).

Equation (35) is further simplified by the fact that the lowest order corrections to terms involving \( g_{1s}^{(1)} \) and \( g_{s1}^{(1)} \) vanish for the retarded component. To demonstrate this, let us consider the retarded component
\[ g_{1s}^{(1)}(t-t') = -\frac{i}{\hbar} \Theta(t-t') \exp \left[ -\frac{i}{\hbar} \int_{t'}^{t} dt_1 \epsilon_j(t_1) \right]. \] (37)

Expanding \( \epsilon_j(t_1) \) around the mean time \( \overline{t} = (t+t')/2 \), namely, \( \epsilon_j(t_1) = \epsilon_j(\overline{t}) + \epsilon_j(\overline{t})(t_1-\overline{t}) \) we obtain
\[ g_{1s}^{(1)}(\omega, t) = f(\omega)\left[ g_{s1}^{(0)}(\omega, t) - g_{s1}^{(0)}(\omega, t) \right] \] (42)

Here \( f(\omega) = [\exp(\hbar \omega/k_B T) + 1]^{-1} \).

We proceed in the same way to obtain an expression for \( G_{s1,s} \). The result is
\[ G_{s1,s}(\omega, t) = G_{s1,s}^{(0)}(\omega, t) + G_{s1,s}^{(1)}(\omega, t), \] (43)

with
\[ G_{s1,s}^{(0)}(\omega, t) = g_{s1}^{(0)}(\omega, t) + g_{s1}^{(0)}(\omega, t) \Sigma_{s1,s}(\omega, t)G_{s1,s}^{(0)}(\omega, t) \] (44)

and
\[ G_{s1,s}^{(1)}(\omega, t) = \frac{i\hbar}{2} \frac{\partial g_{s1}^{(0)}(\omega, t)}{\partial \omega} \frac{\partial G_{s1,s}^{(0)}}{\partial \omega}(\omega, t) + \frac{i\hbar}{2} \frac{\partial g_{s1}^{(0)}(\omega, t)}{\partial \omega} \frac{\partial G_{s1,s}^{(0)}}{\partial \omega}(\omega, t) - \frac{i\hbar}{2} g_{s1}^{(0)}(\omega, t) \frac{\partial G_{s1,s}^{(0)}}{\partial \omega}(\omega, t) \] (45)
In Eq. (45) we have introduced
\[ S_{\omega}^{(1)}(\omega, \tau) = \sum_{k \omega} \left[ \hat{V}_{\omega}(\tau) \hat{V}_{\omega}(\tau) - \text{H.c.} \right] \frac{\partial G_{\omega}(\omega, \tau)}{\partial \omega}. \] (46)

In what follows we use the wide-band approximation, where \( \Sigma(\omega, \tau) \rightarrow \Sigma(\tau) \), in which case the above equations are simplified further.

From Eqs. (44) and (45), we obtain \( G^r \) and \( G^< \), which are needed to calculate \( J_{\alpha} \), Eq. (5), in the adiabatic approximation for the Coulomb blockade regime. Since the zeroth order terms are essentially equilibrium quantities, we are allowed to use the fluctuation-dissipation theorem to compute \( G^{(0)<} \) without much effort: \( G^{(0)<}(\omega, \tau) = -2i f(\omega) \text{Im} \left[ G^{(0)}(\omega, \tau) \right] \). For \( G^{(1)<} \) this is no longer possible and we have to use the Langreth rules. The resulting expressions are rather long and will be omitted here.

The occupation numbers \( \langle n_{\alpha}^{(0)} \rangle \) and \( \langle n_{\alpha}^{(1)} \rangle \) that appear in Eqs. (44) and (45) are calculated self-consistently using
\[ \langle n_{\alpha}^{(i)} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\alpha, \omega}^{(i)<}(\omega, \tau), \] (47)
where \( i = 0 \) or \( 1 \). In the absence of an external magnetic field, which is the case considered here, \( \langle n_{\alpha}^{(0)} \rangle = \langle n_{\alpha}^{(1)} \rangle \).

For later convenience, we assume the V\( \kappa_{\omega} \) to be energy independent and use the flat and wide-band approximation to define
\[ \Gamma_{\alpha}(\omega, \tau) = 2\pi|V_{\alpha}(\omega, \tau)|^2 \rho_{\alpha} \equiv 2\pi|V_{\alpha}(\tau)|^2 \rho_{\alpha} = \Gamma_{\alpha}(\tau), \] (48)
with \( \rho_{\alpha} \) denoting the density of states in the lead \( \alpha \). We also introduce
\[ \Gamma(\tau) = \sum_{\alpha} \Gamma_{\alpha}(\tau) \] (49)
as the total decay width. As we discuss next, the current in Eq. (5) is easily cast in terms of these quantities.

**B. Current in the adiabatic approximation**

To evaluate the time integral in the general expression for the current, we proceed as in Eq. (30) and expand all terms in the integrand to linear order in the slow variables. The resulting expression for the pumped current depends explicitly on \( G^r(\omega, \tau) \) and \( G^<(\omega, \tau) \). Since \( G^r \) is related to occupations (and hence to fluctuations) and \( G^< \) to dissipation, as shown by standard linear-response theory, it is natural to break the current into two parts,
\[ J_{\alpha}(\tau) = J_{\alpha}^{\text{fl}}(\tau) + J_{\alpha}^{\text{dis}}(\tau), \] (50)
where the fluctuation term is
\[ J_{\alpha}^{\text{fl}}(\tau) = -\frac{e}{\hbar} \sum_{\alpha} \text{Im} \left[ \frac{\Gamma_{\alpha}(\tau)}{2} \right. \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\alpha, \omega}^{(1)<}(\omega, \tau) \left. \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\alpha, \omega}^{(1)<}(\omega, \tau) \right], \] (51)
while the dissipation term is given by
\[ J_{\alpha}^{\text{dis}}(\tau) = -\frac{e}{\hbar} \sum_{\omega} \Gamma_{\alpha}(\omega, \tau) \langle n_{\alpha}(\omega, \tau) \rangle. \]

Now we are ready to use the adiabatic expansion for the Green’s function, \( G_{\alpha, \omega} = G_{\alpha, \omega}^{(0)} + G_{\alpha, \omega}^{(1)} \), and to identify the zeroth and the first-order contributions to the pumped current, \( J^{(0)} \) and \( J^{(1)} \), respectively. It can be shown that the zeroth order current vanishes, as expected by the fluctuation-dissipation theorem.

The first-order contribution to the current due to fluctuations is given by
\[ J_{\alpha}^{(1)f}(\tau) = -\frac{e}{\hbar} \Gamma_{\alpha}(\tau) \sum_{\omega} \langle n_{\omega}^{(1)}(\omega, \tau) \rangle, \] (53)
while the first-order dissipation term is given by
\[ J_{\alpha}^{(1)dis}(\tau) = J_{\alpha}^{(1)d}(\tau) + J_{\alpha}^{(1)b}(\tau), \] (54)
where
\[ J_{\alpha}^{(1)d}(\tau) = -\frac{e}{\hbar} \sum_{\omega} \text{Im} \left[ \Gamma_{\alpha}(\omega, \tau) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\alpha, \omega}^{(1)<}(\omega, \tau) \right], \] (55)
and
\[ J_{\alpha}^{(1)b}(\tau) = -\sum_{\omega} \text{Re} \left\{ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left( -\frac{\partial f}{\partial \omega} \right) \frac{d}{dt} \left[ \Gamma_{\alpha}(\omega, \tau) G_{\alpha, \omega}^{(0)}(\omega, \tau) \right] \right\}. \] (56)
The reason for breaking the dissipation term into two contributions is that \( J_{\alpha}^{(1)b}(\tau) \) is a total derivative in time. Integrated over a pumping period, this current term does not contribute to the pumped charge. This provides a good check for the numerical calculations presented in Sec. V. We also successfully verified that our analytical expressions yield the same results as other pumping formulations in the \( U \to 0 \) limit.

Equations (50), (53), and (55) constitute the principal results of this paper. In the following, we will use these expressions to investigate the role of interactions on the pumped current. Specifically, we will study how interactions affect the dependence of the pumped current on \( U \), temperature, and the phase difference between the pumping perturbations.

**V. RESULTS AND DISCUSSIONS**

In this section we compute numerically the pumping current, Eq. (50), and investigate the dependence of the magnitude of the leading contribution to the total charge pumped per cycle,
\[ Q = \int_0^{t_{\text{pump}}} dt J_{\alpha}^{(1)}(t), \] (57)
on several model parameters. In particular, we discuss in which conditions the pumped charge can be quantized to its
maximum value, $|e|$. To accomplish this goal, we consider the following parametrization for tunnel couplings:

$$\Gamma_a(t) = \Gamma_{0,a} + \Delta\Gamma_a \cos(\Omega t + \phi_a),$$

(58)

where $a=R,L$ and $\Gamma_{0,a}$ and $\Delta\Gamma_a$ are real constants. We also assume that the quantum dot resonance energy varies in time as

$$\epsilon(t) = \epsilon_0 + \epsilon_1 \cos(\Omega t).$$

(59)

Notice that since $\epsilon_0 = \epsilon_1$, we have dropped the spin index. In the following, all parameters are chosen to ensure that the system is clearly in Coulomb blockade regime, $\Gamma \ll U$. Typically, we take $\Gamma_{0,R}/U = \Gamma_{0,L}/U = 0.1$ and $\Delta\Gamma_R = \Delta\Gamma_L = 0.05U$ in our numerical calculations.

As already stressed, the analysis is restricted to the first-order adiabatic correction. Hence, since the current is linear in $\Omega$, the charge pumped per cycle does not depend on the pumping rate. The accuracy of this approximation depends on the magnitude of the second-order corrections. Intuitively, the adiabatic approximation becomes more accurate as the ratio $\hbar\Omega/\Gamma_0$ becomes smaller. A closer analysis of the time derivatives of the Green’s functions induced by the adiabatic expansion reveals that the dimensionless parameter controlling the adiabaticity is rather $\xi = \max\{\hbar\Omega/\Gamma_0, \hbar\Omega\epsilon_1/\Gamma_0^2\}$. Although the fact that the results presented here are always valid for a sufficiently slow pumping, such that $\xi \ll 1$, there is no simple way to estimate the accuracy of the approximation for a given pumping rate $\Omega$. To be quantitative, one has to evaluate the second-order correction within the adiabatic approximation, which is a quite daunting task. Instead, we used a rough estimate of these higher-order contributions by studying a single representative term that appears in the second-order Green’s function. We found that it scaled with $\xi$ as predicted, up to a numerical factor of order 1.

Figure 2 displays the result of the self-consistent calculation of the zeroth order occupation $\langle n^{(0)}_\uparrow \rangle$, Eq. (47), as function of the position of the resonance $\epsilon$ for three values of the temperature: $k_B T/U = 0.01$ (black solid line), $k_B T/U = 0.05$ (blue dotted line), and $k_B T/U = 0.1$ (red dashed line). Here $\Gamma_0/0.1U$ and the Fermi energy is set to zero, $\epsilon_F = 0$.

transport. For low temperatures, this is the dominant mechanism of transport, whereas for higher temperatures thermal fluctuations can also induce charge transfer through the quantum dot. This explains why the features in the curve become sharper as temperature decreases.

The first-order correction to the quantum dot occupation number $\langle n^{(1)}_\uparrow \rangle$, also calculated self-consistently using Eq. (47), is shown in Fig. 3 as a function of time for several values of $\epsilon_0$. It is important to emphasize that $\langle n^{(1)}_\uparrow \rangle$ is intrinsically a time-dependent quantity and depends on the pumping parameters dynamics, in contrast to $\langle n^{(0)}_\uparrow \rangle$. Notice that the magnitude of $\langle n^{(1)}_\uparrow \rangle$ is typically much smaller than $\langle n^{(0)}_\uparrow \rangle$. We observe that the maximum values of $\langle n^{(1)}_\uparrow \rangle$ occur for $\epsilon_0 = \epsilon_F$. When the position of the level $\epsilon_0$ deviates significantly from $\epsilon_F$, charge pumping is attenuated and the magnitude of the current is smaller.

After computing $\langle n^{(1)}_\uparrow \rangle$, the next step is to calculate the first-order correction to the time-dependent current $J^{(1)}_\uparrow(t)$ given by the sum of the fluctuation term $J^{(1)\text{fl}}_\uparrow(t)$, Eq. (53), and the dissipation terms $J^{(1)\text{dis}}_\uparrow(t)$ and $J^{(1)\text{dis}}_\downarrow(t)$, Eqs. (55) and (56), respectively. A typical result is shown in Fig. 4 where we plot the frequency-independent quantity $J^{(1)}_\uparrow/\Omega$ as a function of time over a full pumping cycle. It is important to point out that the second dissipation term, $J^{(1)\text{dis}}_\downarrow(t)$, does not contribute to the total charge pumped per cycle since it is proportional to a total time derivative. Consequently, its time

$$J^{(1)}_\uparrow/\Omega = \int_0^t J^{(1)}_\uparrow(t) dt = \int_0^t J^{(1)\text{fl}}_\uparrow(t) dt + \int_0^t J^{(1)\text{dis}}_\uparrow(t) dt.$$

(57)

FIG. 3. (Color online) First-order correction to the quantum dot occupation number, $\langle n^{(1)}_\uparrow \rangle$, as a function of time over a complete pumping cycle for three values of $\epsilon_0$: $\epsilon_0/U = -0.075$ (blue dotted line), $\epsilon_0/U = 0$ (black solid line), and $\epsilon_0/U = 0.075$ (red dashed line). Temperature is $k_B T/U = 0.01$, $\phi_0 = -\phi_F = \pi/2$, $\epsilon_1/U = 0.05$, $\Gamma_0/0.1U = 0.1$, and $\Delta\Gamma/R = 0.05$.

FIG. 4. (Color online) The three terms that contribute to the first-order correction to the pumping current as a function of time: $J^{(1)\text{fl}}_\uparrow(t)$ (blue dotted line), $J^{(1)\text{dis}}_\uparrow(t)$ (red dashed line), and $J^{(1)\text{dis}}_\downarrow(t)$ (black solid line). Here we set $\epsilon_0 = 0$ and take the other model parameters as in Fig. 3.
FIG. 5. (Color online) Three-dimensional graph of $Q$ as a function of $\phi_L$ and $\phi_R$. Temperature is $k_B T / U = 0.01$ while $\epsilon_0 = 0$, $\epsilon_1 / U = 0.05$, $\Gamma_0 / U = 0.1$, and $\Delta \Gamma / U = 0.05$.

integral over a complete pumping cycle must vanish, a result that has been confirmed numerically. The analysis of Fig. 4 reveals that these three current terms, as $\langle n(t) \rangle$, exhibit maxima precisely at the instants when the resonance energy level $\epsilon(t)$ crosses the Fermi energy. In the case of Fig. 4, where $\epsilon_0 = 0$, these maxima occur at $t = \pi / 2 \Omega$ and $t = 3 \pi / 2 \Omega$.

There is an intuitive interpretation for the role of the pumping parameters of our model, $\Gamma_R \phi_L (t)$ and $\phi_L$, that helps us to understand the time dependence observed above: in Eq. (59) we fixed the phase offset of $\epsilon(t)$ to zero. In this situation, for $0 \leq t \leq \tau_{\text{pump}} / 2$ the resonance energy $\epsilon$ decreases with time. As a consequence, during this half pumping period $\langle n \rangle$ increases with time, which corresponds to loading negative charge into the quantum dot. In this time interval, the sign of the pumping current depends on the phase difference between $\phi_R$ and $\phi_L$. The situation is reversed for $\tau_{\text{pump}} / 2 \leq t \leq \tau_{\text{pump}}$.

FIG. 6. Charge pumped per cycle as a function of the level position $\epsilon_0$ for $\epsilon_1 / U = 0.05$, $k_B T / U = 0.01$, $\phi_L = -\phi_R = \pi / 2$, $\Gamma_0 / U = 0.1$, and $\Delta \Gamma / U = 0.05$. The charge is measured in units of the electron charge $e$.

We are now ready to study the dependence of $Q$ on $V_g(t)$, related to $\epsilon_0$ and $\epsilon_1$, as well as on the dot-leads couplings, represented in our model by $\Gamma_0$ and $\Delta \Gamma$. In Fig. 6 we show the charge pumped per cycle $Q$ calculated as a function of $\epsilon_0$. Charge pumping is enhanced whenever a quantum dot resonance, $\epsilon_0$ or $\epsilon_0 + U$, crosses the Fermi level, resulting in the two peaks of Fig. 6.

FIG. 7. Charge pumped per cycle as a function of the resonance oscillation amplitude $\epsilon_1$ for $\epsilon_0 = 0$, $\Gamma_0 / U = 0.1$, $\Delta \Gamma / U = 0.05$, $k_B T / U = 0.01$, and $\phi_L = -\phi_R = \pi / 2$. The charge is measured in units of the electron charge $e$.

FIG. 8. (Color online) Charge pumped per cycle as a function of $\Gamma_0$ for different values of temperature: $k_B T / U = 0.05$ (black solid line), $k_B T / U = 0.1$ (blue dotted line), and $k_B T / U = 0.2$ (red dashed line). Here $\epsilon_0 = \Gamma$, $\epsilon_1 / U = 0.05$, $\Delta \Gamma / \Gamma_0 = 1$, and $\phi_L = -\phi_R = \pi / 2$.
VI. CONCLUSIONS

In conclusion, we have investigated adiabatic charge pumping through quantum dots in the Coulomb blockade regime. We specifically studied the impact of Coulomb interaction on the pumping current amplitude for the finite-U Anderson model, in contrast to previous works that treated the infinite-U case.28

We have derived a general expression for the adiabatic pumping current that is proportional to the instantaneous Green’s function of the dot. This formula was then applied to compute the time dependence of the total charge pumped per cycle through the dot. This allowed us to analyze several aspects of experimental relevance such as the dependence of the pumped charge on temperature and on the phase difference between time-dependent perturbations.

We find that, within the adiabatic regime, there is a large range of parameters that can be used to maximize the charge pumped per cycle. For this purpose, we find that it is advantageous to (i) tune the bias gate voltage to pump with the QD in resonance with the Fermi energy in the leads; (ii) maximize the pumping amplitude $\Delta \Gamma$ and, possibly, $\epsilon_1$ as well; (iii) minimize temperature.

We were not able to find a set of parameter values that gives one unit of charge $e$ per pumping cycle within the parameter ranges allowed by our approximations. We do not discard such interesting possibility, but our investigations hint that it may only be possible for very particular pulse formats, not necessarily sinusoidal, and within a narrow parameter interval. The possibility of spin pumping and the consideration of the double-dot case are under investigation and will be reported soon.

Note added. Recently, we became aware of Ref. 43 that deals with a similar problem using the diagrammatic real-time approach.

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42 Although this demonstration has been made for the retarded component, it also applies for the lesser and greater ones.