Time-dependent current of interacting quantum capacitors subjected to large amplitude pulses

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Abstract. We investigate the time-dependent response of an interacting mesoscopic capacitor using the Floquet-Green function formalism applied to a single-level Anderson model. We obtain closed expressions for the current and the occupation valid for arbitrary values of the applied ac potential in the limit of small frequencies. In the noninteracting case, we obtain nonsinusoidal responses when the ac amplitude allows crossings between the dot level and the Fermi energy of the attached reservoir. For interacting electrons treated within the Hartree approximation, we self-consistently calculate the capacitor current as a function of time and find a decrease of the peak amplitudes due to the on-site Coulomb repulsion.

1. Introduction

Electron dynamics in phase-coherent conductors yield a universal value of the charge relaxation resistance for single-channel capacitors and small ac amplitudes, independently of the transmission probability [1, 2]. When the ac amplitude applied to the capacitor is large such that the dot level crosses the reservoir Fermi energy, Fèvre et al. found [3] that during the first (second) half-cycle of the voltage pulse the capacitor emits (absorbs) one electron. The resulting quantized current in terms of the elementary charge $e$ has immediate applications for metrology and quantum computation and is crucial, in general, for the electronic manipulation of quantum conductors in real time.

Since quantum dots are small cavities, adding extra electrons causes electron-electron repulsion to become a major issue. The relation between electronic interactions and time-dependent transport in quantum capacitance-resistance circuits has been investigated in a number of works [4, 5, 6, 7, 8, 9]. However, most of these works assume that the pulse amplitude is small. Interestingly, Ref. [10] has formulated a scattering theory for arbitrary pulse strengths valid for noninteracting electrons and fast electron sources. It is the aim of this work to consider both electron-electron interactions and large amplitude voltages in order to investigate the role of interaction effects in the time-dependent current of quantum capacitors coupled to ac fields.

We propose an Anderson model for a single level in the vicinity of a gate that generates the oscillating ac voltage. The current is expressed in terms of the dot Green’s function. We first address the noninteracting case and then Coulomb interactions are treated within the Hartree approximation. We find that the dot occupation becomes a nonsinusoidal (but periodic) function of time for high ac amplitudes. Correspondingly, the current peaks increase as the ac amplitude
Theoretical Model

We consider a mesoscopic capacitor formed with an ac-gated quantum dot that can exchange carriers through a constriction with a coupled electron reservoir (see Fig. 1). In our case, the dot has a single energy level and we take into account the electron-electron interactions via the on-site charging energy $U$. Thus, our time-dependent Hamiltonian reads

$$
\mathcal{H} = \sum_{k\sigma} \varepsilon_{k\sigma} C_{k\sigma}^\dagger C_{k\sigma} + \sum_{k\sigma} \left( V_k^\dagger d_{\sigma}^\dagger C_{k\sigma} + V_k C_{k\sigma} d_{\sigma} \right) + \sum_{\sigma} \tilde{\varepsilon}_{\sigma}(t) d_{\sigma}^\dagger d_{\sigma} + U n_\uparrow n_\downarrow. \tag{1}
$$

The first term in the right-hand side describes noninteracting electrons in the reservoir and the second term represents the coupling between localized and conduction electrons with tunnel strength $V_k$. Here, $\sigma = \{\uparrow, \downarrow\}$ labels the spin state. In the third term of Eq. (1), $\tilde{\varepsilon}_{\sigma}(t) = \varepsilon_{\sigma} + \varepsilon_{ac}(t)$ is the energy level driven by the ac monochromatic potential $\varepsilon_{ac}(t) = \varepsilon_{ac} \cos \Omega t$ with $\varepsilon_{ac}$ the ac amplitude and $\Omega$ the frequency. In the following, we assume spin degeneration and $\varepsilon_{\uparrow} = \varepsilon_{\downarrow} \equiv \varepsilon_d$.

Finally, the fourth term takes into account the on-site Coulomb repulsion with $n_{\sigma} = d_{\sigma}^\dagger d_{\sigma}$ the number operator for dot electrons.

The time-dependent current is given by the rate of change in time for the occupation expected value, $I(t) = e \partial_t \sum_{\sigma} \langle n_{\sigma}(t) \rangle = e \partial_t \sum_{\sigma} \int d\varepsilon \frac{G^{<}_{\sigma,\sigma}(t,\varepsilon)}{(2\pi i)}$, where $G^{<}(t,\varepsilon)$ is the lesser Green’s function in the mixed energy-time representation [11], which is obtained from the definition $G^{<}(t,t') = i \langle d_{\sigma}^\dagger(t') d_{\sigma}(t) \rangle$ and the relation $G^{<}(t,t') = \int d\varepsilon e^{-i\varepsilon(t-t')} G^{<}(t,\varepsilon)/(2\pi)$. Then, our problem is reduced to finding the dot occupation. We are interested in an expansion up to leading order in $\Omega$:

$$
I(t) = I^{(1)}(t) + \ldots = e \partial_t \sum_{\sigma} \langle \langle n_{\sigma}^{f}(t) \rangle + \ldots \rangle \tag{2}
$$

where the indices $f$ (frozen) and $(1)$ indicate zero and first order in $\Omega$, respectively. The frozen term corresponds to a stationary problem with time-dependent parameters [12].

2.1. Noninteracting case

Let us first consider noninteracting electrons ($U = 0$). After lengthy but straightforward algebra, we find

$$
\langle n_{\sigma}^{f}(t) \rangle = \int d\varepsilon f(\varepsilon) D_\sigma(t,\varepsilon) \tag{3}
$$

$$
I^{(1)}(t) = -e \sum_{\sigma} \int d\varepsilon (\partial_\varepsilon f(\varepsilon)) (\partial_\varepsilon \varepsilon_{ac}(t)) D_\sigma(t,\varepsilon) \tag{4}
$$
where \( D_{\sigma}(t, \varepsilon) = \Gamma/\left[ \pi \left( (\varepsilon - \varepsilon_{\sigma} - \varepsilon_{ac}(t))^2 + \Gamma^2 \right) \right] \) is the instantaneous density of states for the coupled dot with \( \Gamma = 2\pi \sum_{k\sigma} |V_k|^2 \delta(\varepsilon - \varepsilon_{k\sigma}) \) the broadening due to hybridization. The Fermi distribution is \( f(\varepsilon) = (1 + \exp [(\varepsilon - E_F)/k_B T])^{-1} \), where the Fermi energy \( E_F = 0 \) is set as the reference energy and \( T \) is the temperature. Time is measured in units of \( 1/\Omega \) such that current is given in terms of \( e\Omega \).

We show in the inset of Fig. 2 the dot occupation per spin, \( \langle n^f \rangle = \langle n^f_\uparrow \rangle = \langle n^f_\downarrow \rangle \), as a function of \( \Omega t \) for different values of \( \varepsilon_{ac} \) and a fixed position of the energy level. In the frozen regime, the electronic potential is instantaneously adjusted to the variation of the ac field. As a consequence, \( \langle n^f \rangle \) attains its maximum value when \( \Omega t = \pi + 2\pi m \) (\( m = 0, 1, \ldots \)). For small ac amplitudes (black full line) the response is sinusoidal, as expected. For larger amplitudes, during the first half-cycle of the pulse the occupation increases (an electron is absorbed) whereas during the second half-cycle the occupation decreases (an electron is emitted). This effect is more visible for increasing values of \( \varepsilon_{ac} \), which allow \( \varepsilon_d \) to cross over \( E_F \). Interestingly, the modulation of \( \langle n^f \rangle(t) \) becomes nonsinusoidal for high values \( \varepsilon_{ac} \) (blue dot-dashed line). The main panel of Fig. 2 presents the current to first order in the ac frequency. For small pulses the current is nearly zero. Larger amplitudes generate current peaks (dips) during the absorption (emission) part of the process. As \( \varepsilon_{ac} \) increases, the current pulses become narrower and more separated. Between pulses the occupation remains roughly constant and the current is close to zero.

2.2. Interacting electrons

Now we take into account the Coulomb interaction \( (U \neq 0) \). For metallic dots with good screening properties, it is a valid approximation to consider the Hartree approach, which amounts to decoupling higher-order correlators in the following way: \( \ll d_\sigma, d_\sigma^\dagger n_\sigma \gg (t, t') \approx G_{\pi,\sigma}(t, t') \langle n_\sigma \rangle \langle t' \rangle \). Hence, the equation of motion for the Green’s function can be exactly solved. We find that both the frozen dot occupation and the current to first order in \( \Omega \) take the same form as in Eqs. (3) and (4) but replacing \( \varepsilon_{ac}(t) \) with \( \varepsilon_{ac}(t) + U <n^f_\sigma> (t) \). As a consequence, Eq. (3) becomes a self-consistency equation for \( \langle n^f \rangle \) and the dot occupation has to be solved iteratively.

The inset of Fig. 3 shows the results of our numerical evaluations for the frozen occupation in the Hartree approximation at a fixed value of the dot level varying the interaction strength. We keep the ac amplitude with a large value \( (\varepsilon_{ac} = 5\Gamma) \). We observe that the peak maxima decrease while the minima stay constant when \( U \) increases. We attribute this behavior to a repulsion effect that hampers the process of emission and absorption of electrons since an extra energy is to be paid in order to populate the dot. This implies that the current peaks are significantly lower than in the noninteracting case (see main panel of Fig. 3). Our results suggest that
mean-field interactions can be understood as an effective ac potential with a lowered amplitude. Elucidating this effect further will be subject of a future work.

3. Conclusions
We have investigated the dynamical response of a single-level quantum dot attached to a reservoir and in the presence of an external ac potential of arbitrary amplitude. We have described the current and occupation behavior in the adiabatic limit (small ac frequencies) using a mixed energy-time Green’s function formalism applied to an Anderson Hamiltonian model. We have found strong effects of the electron-electron interactions that lower the amplitude of the current peaks. This result is important in view of recent advances that propose mesoscopic capacitors as useful resources for metrology due to the quantization of the ac current. Further work is needed to study higher-order currents beyond the adiabatic limit [10], stronger electronic correlations (Kondo limit) [5, 8] or the role of temperature driven potentials in thermoelectric setups [13].

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