The charge shuttle as a nanomechanical ratchet

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We consider the charge shuttle proposed by Gorelik et al. driven by a time-dependent voltage bias. In the case of asymmetric setup, the system behaves as a ratchet. For pure AC drive, the rectified current shows a complex frequency dependent response characterized by frequency locking at fractional values of the external frequency. Due to the non-linear dynamics of the shuttle, the ratchet effect is present also for very low frequencies.

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The great burst in the study of Nano-Electro-Mechanical (NEMS) devices is unveiling several new perspectives in the realization of nanostructures where the charge transport is assisted by the mechanical degrees of freedom of the device itself. This is the case, for example, when nanomechanics $^1$ has been combined with single electron tunneling. Important experiments in this area are the use of a Single Electron Transistor (SET) as displacement sensor $^2$ or quantum transport through suspended nanotubes $^3$, oscillating molecules $^4, 5, 6, 7$ and islands $^8$. On the theoretical side, several works $^9, 10, 11, 12, 13, 14, 15, 16, 17, 18$ have already highlighted various aspects of the role of mechanical motion on single electron tunneling.

An exciting prototype example of mechanical assisted SET device has been proposed by Gorelik et al. $^2$ and named Single Electron Shuttle. The authors of Ref. $^2$ predicted that a SET with an oscillating central island can shuttle electrons between the electrodes leading to low noise transport $^9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20$. Although the realization of the charge shuttle is difficult experimentally, promising systems are $C^{60}$ molecules in break junctions $^4, 5$, or silicon structures $^8, 21$.

One of the advantage of this self-oscillating structure is the fact that one can generate very high frequency mechanical oscillation with static voltages. The fact that the system has an intrinsic and stable oscillating mode as the result of a static voltage suggests that the application of an oscillating voltage may lead to new interesting effects, related to the interplay between the external AC drive and the internal frequency of the device. Moreover, as the non-linearities of the dynamics have an important role, this interplay should emerge in a wide interval of the ratio of the two frequencies. Aim of this Letter is to study a shuttle driven by a time-dependent applied bias.

We in some details the case in which the external bias is AC and report a quite rich behaviour as a function of applied frequency. We find clear indications of frequency locking. The resulting DC current may have both signs, depending on the value of the frequency. The response to an AC field can give strong indications on the motion of the central island, even when the system is very far from the shuttling instability. A sizeable ratchet effect is present down to frequencies much smaller than the mechanical resonating frequency, due to the adiabatic change of the equilibrium position of the grain. In a very recent experiment, Scheible and Blick $^{21}$, already observed similar results to those presented in our work.

The single electron shuttle, shown in Fig. 1 is a SET where the central island can oscillate between the two leads $^4$. The central island is subjected to an elastic recoil force, a damping force due to the dissipative medium, and an electric force due to the applied bias. The island is connected to the left and right leads through tunnel junctions with resistances $R_L(x) = R_L(0)e^{x/\lambda}$ and $R_R(x) = R_R(0)e^{-x/\lambda}$ ($\lambda$ is the tunnelling length and $x$ is the displacement from the equilibrium position in absence of any external drive). The capacitances $C_g$ and $C$ couple the island to the gate and to the two leads, respectively. We neglect small variations of the capacitances due to the motion of the island as this dependence is weak when compared with the exponential dependence...
of the tunneling resistances on $x$. The system is biased
symmetrically at a voltage $V(t) = V_R = -V_L = V/2$, the
corresponding charging energy is $E_C = e^2/2C_S$ where $e$
is the electron charge, $C_S = C_g + 2C_I$, and the gate charge
$Q_g = C_g V_g$. For simplicity, we consider the case of low
substrates ($T < E_C$), charge degeneracy $(Q_g = e/2)$, and voltages
$|V| < E_C/e$. In this regime the grain can accommodate
only $n = 0$ or $1$ additional electrons (see right panel of
Fig. 1). All the properties of the nanomechanical ratchet
are captured already at this level.

In the simplest approximation the dynamics of the cen-
tral island is described by Newton’s law
\begin{equation}
\dot{x}(t) = -\omega_o^2 x(t) - \gamma \dot{x}(t) + \frac{eV(t)}{mL} n(t).
\end{equation}

Here $m$ is the mass of the grain, $\omega_o$ is the oscil-
lator eigenfrequency, $\gamma$ is a damping coefficient and
$L$ is the distance between the two leads. In the
regime of incoherent transport the (stochastic) evolu-
tion of the charge $-en(t)$ is governed by the follow-
ing four rates [23]:
\begin{equation}
\Gamma_{FL} = |eV(t)/4E_C| \Gamma_L(x) \Theta(V) \\
\Gamma_{FR} = |eV(t)/4E_C| \Gamma_R(x) \Theta(-V) \\
\Gamma_{TL} = |eV(t)/4E_C| \Gamma_L(x) \Theta(-V) \\
\Gamma_{TR} = |eV(t)/4E_C| \Gamma_R(x) \Theta(V)
\end{equation}
for $n = 0 \rightarrow 1$ transitions, $\Gamma_{TL} = |eV(t)/4E_C| \Gamma_L(x) \Theta(-V)$ and $\Gamma_{TR} = |eV(t)/4E_C| \Gamma_R(x) \Theta(V)$ for $n = 1 \rightarrow 0$ transitions. Here $FL$, $FR$, $TL$, and $TR$ stands for From/To and
Left/Right, indicating the direction for the electron
tunneling associated to the corresponding, $\Gamma_{L/R}(x) = [R_{L/R}(x)]^{-1}$ and $\Theta(t)$ is the Heaviside function.
The current $I$ is then determined by counting the net number of
electrons that have passed through the system in a given time $t$.

In most of the paper we consider the case of an oscil-
lating voltage bias $V(t) = V_o \sin(\omega t)$, where the
interplay of the two frequencies $\omega$ and $\omega_o$ is crucial.
If the system is perfectly symmetric no direct current can
be generated, since this would break the left/right
symmetry. We then concentrate on the asymmetric case
$R_{L}(0)/R_{L}(0) \neq 1$. We performed simulation of the
stochastic process governed by the four rates defined
above and by Eq. [4]. The results presented are ob-
tained by simulating $10^6$ events of tunneling for each
plotted point. After a transient time the system reaches a
stationary behavior. In Fig. 2 we show the station-
ary DC current as a function of the frequency of the
external bias. The rich structure shown in the figure is
generic, we observed a qualitatively identical behaviour
in a wide range of parameters. The existence of a
direct current as a result of an applied periodic modulation
shows that the charge shuttle, whose stochastic dynamics
has been defined above, behaves as a ratchet [22]. Since
our system is non linear, the external driving will affect
the dynamics also for values of $\omega$ very different from the
natural frequency $\omega_o$. Note that in this model the non-
linearities are intrinsic to the shuttle mechanism. They
are not due to a non-linear mechanical force, but they
stem from the time dependence of $n(t)$. As it is evident

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{
Current as a function of the frequency for $\epsilon = 0.5$, $\gamma/\omega_o = 0.05$, $\Gamma/\omega_o = 1$, and $R_R/R_L = 10$. The result of the simulation of the stochastic dynamics (points) is compared with the approximate $I_o$ (full line). In the small frequency region, enlarged in the inset, several resonances at fractional
values of $\omega_o$ appear. We also show (dotted) the analytical result from Eq. [4] in the adiabatic limit. The triangular dot indicates the numerical solution of the adiabatic equations. Lower inset: current noise from the simulation (points) and analytic result (dashed) for the static SET.
}\end{figure}

from Fig. 2 the ratchet behaviour is present also in the
adiabatic limit $\omega/\omega_o \ll 1$. In addition a series of reso-
nances, due to frequency locking [23] when $\omega \approx \omega_o q/p$, with $q$ and $p$ integers. In this case the motion of the
shuttle and the oscillating source become synchronized
in such a way that every $q$ periods of the oscillating
field the shuttle performs $p$ oscillations. In Fig. 2 we
also report the low frequency current noise (lower inset).
The net DC current results from large cancellations be-
tween positive and negative contributions. But the cur-
rent noise is always positive, thus it does not cancel. We
find that the noise remains very close to the value for a
SET $S = e^2 \Gamma_L \Gamma_R (\Gamma_L^2 + \Gamma_R^2)/\Gamma_L + \Gamma_R^3$ shown with a
dashed line in Fig. 2. At resonance, more ordered trans-
port is realized and current becomes less noisy.

In the following we provide a more detailed analysis by solv-
ing the problem analytically in some tractable limits and
by analyzing in more details the behaviour of the shuttle
in the frequency locked case.

If the electric force is much smaller than the mechanical
one, $\epsilon = eV_o/(\omega_o^2 m \lambda L) \ll 1$, one can take into account the
force generated by the stochastic variable $n(t)$ only on
average by substituting into Eq. [4] its mean: $\langle n(t) \rangle = P(t)$ where $P(t)$ is the probability to have occupation
$n = 1$ in the grain. The charge dynamics in the central
island is then described by a simple master equation
\begin{equation}
P(t) = -\Gamma_1(t) P(t) + \Gamma_2(t),
\end{equation}
with $
\Gamma_1(t) = |eV(t)/4E_C| (\Gamma_L [x(t)] + \Gamma_R [x(t)])$
and
\begin{equation}
\Gamma_2(t) = |eV(t)/4E_C| (\Gamma_L [x(t)] \Theta[v(t)] + \Gamma_R [x(t)] \Theta[v(t)])
\end{equation}
The rates depend on the time $t$ through the voltage $V(t)$ and the position of the grain $x(t)$. The instantaneous (average) current through the structure is

$$I_a(t)/e = (1 - P(t)) \Gamma_{FL} - P(t) \Gamma_{TL}(t),$$

(3)

where the subscript in the current indicates that the fluctuations of the force acting on the shuttle, due to the discrete nature of the charge tunneling, are neglected. As shown in Ref. [3] the shuttle instability, at constant bias, is controlled by the ratio $\epsilon \omega_o/\gamma$, we can thus assume both parameters small, but their ratio arbitrary.

In the adiabatic limit ($\omega \ll \omega_o$ and $\epsilon \omega_o/\gamma \ll 1$) it is possible to find an approximate solution of Eqs. [11] and [2]. In this case the position of the grain is given by the local stationary solution of Eq. [11] $x/\lambda = \epsilon \Gamma_2(x, V)/\Gamma_1(x, V)$. Solving this equation in lowest order in $\epsilon$ one obtains

$$I_a(\omega \ll \omega_o) = \epsilon \frac{V_o^2 e^3 \Gamma_L \Gamma_R (\Gamma_L - \Gamma_R)}{32 \Gamma_L \Gamma_R (\Gamma_R + \Gamma_L)^2}. \quad (4)$$

The corresponding value is shown in Fig. [2]. The (small) difference with the full numerics is due to the expansion in $\epsilon$. By solving numerically the equation for the local equilibrium position of the grain, one obtains the result indicated by the triangular dot at $\omega = 0$ in the inset of Fig. [2] [20]. If $\epsilon \gamma/\omega_o$ is larger than the critical value for shuttling, the behavior is completely different. The grain will oscillate at its natural frequency $\omega_o$ with the amplitude slowly modulated by $V(t)$. The modulation will be small, since for small $\epsilon$ the effect of a change in the value of $V$ affects the mechanical motion only after several oscillations. In this case the rectified current is much smaller than in the adiabatic limit.

We now discuss in more details the dependence of the current on the external frequency. The most prominent structure, observed also in the experiments of Ref. [21], is present in our simulations at $\omega \approx \omega_o$, and it corresponds to the main mechanical resonance. The current changes sign across the resonance. This behaviour is due to the phase relation between the driving voltage and the displacement of the grain. We verified this conjecture by solving Eq. [2] with $x(t) = A \sin(\omega t - \phi)$. By calculating the current as a function of $\phi$ and using the usual resonant dependence for $\phi(\omega) = \arctan[(\omega^2 - \omega_o^2)/\omega \eta]$ we could reproduce qualitatively the behavior of Fig. [2].

From Fig. [2] it is clear that additional structures appear also for $\omega \approx \omega_o/q$ (magnified in the upper inset), with $q = 2, 3, \ldots$ (the numerical results indicate that, except for the fundamental frequency, even $q$ are favorite with respect to odd ones). As we already anticipated, the motion of the shuttle and the oscillating source become synchronized at commensurate frequencies whose ratio is $p/q$. This ratio, known also as the winding number, can be defined more precisely as

$$w = \lim_{t \to \infty} \theta(t)/\omega t$$

(5)

where $\theta(t)$ is the accumulated angle of rotation of the representative point $(\hat{x}, \hat{\phi})$ $[\theta(t)/2\pi$ gives the number of oscillations performed by the shuttle during the time $t]$. When the system is frequency locked at a winding number $w$, it is possible to define the phase shift $\phi(t) = [\theta(t) - w \omega t]$. After a transient time for perfect locking $\phi$ should not depend on $t$ (apart from a small fluctuation if the motion is not perfectly harmonical). An additional important quantity to analyze is thus the phase shift variance $\langle \Delta \phi \rangle^2 = \langle \phi^2 \rangle - \langle \phi \rangle^2$. This is calculated by sampling 20 points per cycle over $10^3$ cycles. For a given $w$ the smaller is the value of $\Delta \phi$, the better the system locks to that external frequency. The numerical results for $w, \phi$, and $\Delta \phi$ are shown in Fig. [3] and Fig. [4].

In Fig. [3] we show the dependence of the winding number as a function of the external frequency (top panel) together with the analysis of $\Delta \phi$ (lower panel) calculated from the stochastic simulation and from the average approximation (short dashed line). The locking at rational winding numbers is confirmed by the presence of plateaux of decreasing width. As expected the most stable plateau is at $w = 1$: the system locks very well at this frequency. We find that this holds up to very high frequency in the average approximation, where $w = 1$ seems the only possible winding number. The stochastic simulation would indicate instead that for $\omega/\omega_o \gtrsim 1.3$ the locking with $w = 1$, as defined from Eq. [3], is no more established. However, by studying $\Delta \phi$ for $w = 1$ in the whole frequency range, one actually obtains that a correlation is always present (i.e., $\Delta \phi < \pi/\sqrt{3} \approx 1.81$) even when Eq. [3] gives a value of $w$ different from one. The stochastic fluctuations thus unlock the shuttle glob-
FIG. 4: Phase shift $\phi$ (same parameters and same notation of Fig. 3). The phase shift is shown only when $\Delta \phi < 1.7$ (cfr. Fig. 3). When locking is achieved in presence of the stochastic fluctuations $\phi$ remains the same of the average simulation.

ally, but not locally. Looking at the presence of local locking at other winding numbers we find that for instance $w = 2$ is clearly present for $\omega > 1$ and reversely $w = 1$ is present around $\omega = 1/2$ (see long dashed lines in lower panel of Fig. 3). For global locking, only one phase variance is minimal. It corresponds to the “dominant” winding number. The presence of correlations of other winding numbers may indicate partial locking at these winding numbers (as in the region $0.6 \lesssim \omega \lesssim 0.9$ for $w = 1$ and 2) or the contribution of higher armonics of $x(t)$ (as in the region $\omega > 1$).

The dependence of the phase shift, see Fig. 4 around each resonance is also remarkable. It is very similar to the behavior of a forced harmonic oscillator, but instead of evolving from 0 to $\pi$ it goes from $\phi_o$ to $\phi_o + \pi$, where $\phi_o$ depends on the resonance. With the aim of understanding the behaviour of the current close to the resonance, we also considered the adiabatic limit, and looked for harmonic oscillations superimposed to the adiabatic solution given before. This can be verified numerically by searching a periodic solution of period $2\pi/\omega$ for $P(t)$. We find that in this case the direct current is non vanishing and that it depends strongly on $\phi$. Using the phase dependence given by the full numerical calculation we could reproduce the shapes of the resonances.

In this Letter we showed that the charge shuttle under time-dependent driving behaves as a ratchet. In the case of a AC bias the response of the shuttle is rather rich due to the non-linear dynamics of the grain. All the results obtained here can be tested experimentally, indeed the very recent paper by Scheible and Blick 21 already reports on some of the properties related to the main resonance.

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