Self-excitation in nanoelectromechanical charge shuttles below the field emission regime

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Abstract. The behaviour of a nanomechanical electron shuttle for applied dc-bias is investigated below the field emission regime. Simulations of the distribution of the electrical potential between the shuttling island and the leads show that field emission, which has recently been observed in a driven electron shuttle, can also play a role in the self-oscillating shuttle. For realistic experimental parameters of a silicon-based shuttle below the field emission regime, it is shown numerically that only one Coulomb step might be observable.

Single-electron tunnelling has been investigated for the past 30 years. In particular, metallic single-electron transistors (SETs) and semiconductor quantum dots (usually based on GaAs/AlGaAs heterostructures) have produced a large number of interesting experiments (for reviews see [1] and [2]). With the advent of nanoelectromechanical systems (NEMS), the realization of a SET which is shuttling charge between the two contacts by mechanical motion became possible (for a schematic view of such an arrangement see figure 1). A first theoretical proposal was given by Gorelik et al [3]. It was shown that an electrically isolated island, which is mechanically coupled to the two leads via molecules, will transport charge in periodical oscillations at the resonance frequency of the structure if a bias voltage $V_{sd}$ is applied across the island. As soon as $V_{sd}$ exceeds a certain critical voltage $V_C$, a Coulomb blockade (CB) staircase develops. In order to prove this, the current through the structure was calculated using an adapted version of the well-known Master equation (for more detail see below) numerically. The authors used a similar approach to calculate the electromechanical response of a superconducting island as well [4]. If spin-polarized electrons are shuttled between magnetic leads, giant magnetotransmittance effects are predicted [5].

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Figure 1. Schematic sketch of the shuttle. If self-excitation occurs, the shuttle starts to oscillate between the two electrodes (source and drain) at frequency $f_0$. The capacitance and the resistance between island and leads depend on the position of the island.

One of the most interesting opportunities for future application of a nanoelectromechanical electron shuttle seems to be the possibility of defining an extremely accurate current source. Conventional charge pumps based on SETs (so-called single-electron turnstiles [6]) suffer from effects of co-tunnelling, which drastically reduces their current accuracy. These effects are suppressed exponentially in the case of the single-electron shuttle. This fact is explained by the positions of the island, at which tunnelling can occur. In order to allow tunnelling onto the island, the distance between the island and the lead has to be on the order of the tunnelling length, which is of about 0.5 nm (field emission effects, as will be discussed later, are not taken into account at this point). The distance to the opposite electrode at this point of the shuttle’s motion is maximal, normally at least 50 nm. This, however, closes the tunnelling barrier exponentially and co-tunnelling is suppressed. Therefore, the accuracy of the single-electron shuttle is only limited by charge fluctuations. This fact has been shown by solving the Master equation for this set-up numerically and analytically and computing the related accuracy per oscillation period [7]. In an experiment, the current integrated over many oscillation periods would be measured. If the accuracy of a shuttle is low, this leads to considerably different results [8]. Another source of noise in the system is the mechanical motion of the island; even without stochastic forces the onset of the motion is accompanied by an increase in noise power [9].

An experimental situation very similar to the one proposed by Gorelik et al was realized using electromigrated gold contacts to a single C$_{60}$ molecule [10, 11]. In this set-up, however, charge was transferred even if the C$_{60}$ was at rest. The mechanical degree of freedom merely led to a change in the transmission probabilities for excited states. Thus, CB was obtained for the resting C$_{60}$ with additional ‘vibration (phonon) assisted’ tunnelling states. The extremely small size of such an arrangement makes it impossible to control details of the set-up. Therefore, arrangements in which the molecule is situated in the right places to allow charge shuttling are extremely difficult to prepare. In order to do this, self-assembly techniques are needed on top of the fabrication techniques for the electrodes.

First experimental realizations of charge shuttling in NEMS devices were demonstrated on silicon on insulator (SOI) substrates [12]. In these structures, however, the mechanical stiffness of the beam supporting the shuttling island was too large to allow self-excitation of the island as
Figure 2. Distribution of the electrostatic potential $\Phi$ close to one of the electrodes. The values of $\Phi$ were calculated with an electromagnetic finite element solver. It can be clearly seen that the potential drop is maximized close to the sharp corner of the island. This has to be taken into account if limits for the field emission regime are considered.

proposed in [3]. Therefore, an oscillating driving voltage ($V_{ac}$) was applied in addition to $V_{sd}$ to excite the mechanical motion. If the attenuation of such a shuttle is decreased by reducing the motion of the centre of mass, the phase behaviour between the ac-drive and the nanomechanical motion is resolved [13]. This phase relation leads to an effective bias $V_{eff}$ across the junction. The magnitude of this bias is large enough to destroy CB effects in the charge transport. These CB effects are visible, if the charging energy $E_C = e^2/2C$ fulfils the conditions $E_C \gg k_B T$ and $E_C \simeq V_{eff}$. If the bias becomes much larger than the charging energy the CB steps are no longer resolvable. Thus, an unknown number of electrons are transported during each cycle of the motion of the shuttle. The average value of this number can be concluded from the integrated value of the current $I_{sd}$ and the oscillating frequency of the resonator $f$ ($I_{sd} = nef$). This number $n$ is usually approximately 0.1 electrons per cycle of motion, meaning that during most cycles of the motion no electrons are transported.

This low number of transported electrons is greatly enhanced in some mechanical modes of motion due to field emission effects [14]. Microscopic details of the shape of the oscillating island and the deflection of the beam can alter the field between the electrodes and the island. The field can be increased to values above the field emission threshold. Typical values for this threshold are for metallic wires $E_{em} > 10^7$ V cm$^{-1}$. In the case of the nanomechanical pendulum presented in [14], the critical voltage for field emission was 500 mV.

The occurrence of field emission is easily seen in the dramatic increase of the current through the island in certain mechanical modes. It can be assumed that the island faces the electrode with a sharp corner instead of the flat edge in these modes. This leads to an increase of the field close to the sharp corners. Figure 2 shows a finite element calculation of the electrostatic potential $\Phi$ between the electrodes and the island in such a situation. The size of the island in this simulation

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is taken from recent experiments [14]. Due to the mechanical coupling to a silicon rod, the motion of the island between the electrodes can be more complicated than assumed in [3]. Therefore, the island can be slightly rotated compared to its position in the relaxed state. This rotation has a strong effect on the field between the island and the lead. It can be seen that the equipotential lines are much denser in the space between the island and the electrode than in the surrounding space. This leads to field emission already at lower voltages than in modes where the island faces the electrode with the flat edge.

The increase of current in the field emission regime can be a desirable effect. One of the problems of a NEMS-based shuttle are the low currents, which can be driven accurately through the structure. One possibility to increase the current level is to increase the oscillation frequency. It has been shown that above a certain frequency, the accuracy will decrease due to the influence of charge fluctuations. Controlled field emission can allow one to increase the current even at low frequencies of the shuttle.

Experiments [14] and the discussion presented here have shown that field emission can play a major role in nanomechanical charge shuttling. Other effects, which can be seen in experiments and therefore have to be included in realistic descriptions of the semiconductor-based shuttle are resulting from the fact that the tunnelling length is much shorter than the oscillation amplitude of the shuttle, which is a noticeable difference to the situation considered by Gorelik et al [3]. For the description of these effects, we turn to a system in which field emission does not occur. This is justified, because systems with, e.g., much smaller island size will not show field emission even at larger voltages than the ones applied in [14] to observe field emission.

In order to resolve single-charge transport, self-excitation of the mechanical oscillation upon an applied dc-voltage has to occur. In this paper, we present a model system based on realistic parameters for a silicon-based shuttle, in which this self-excitation is present. Motivated by usual experimental set-ups [12–14], we assume that one electrode is grounded instead of the symmetrically applied voltage used, e.g., in [3].

In figure 1, the experimental situation is sketched. A nanoscale island is situated in between two leads. The radius of the metallic island is 5 nm, the distance between the electrodes 100 nm. The silicon rod, which supports the island, is assumed to have the dimensions 75 nm × 75 nm × 530 nm. Using these parameters, we calculate a capacitance between the leads and the island of 0.5 aF. This capacitance corresponds to a charging energy $e^2/(2C)$ of 160 meV, which is well above $k_B T$ at room temperature. We therefore can assume that CB will dominate the transport behaviour of the oscillating island. The voltage corresponding to the CB energy ($e/C$) is then 320 mV.

The behaviour of the shuttle is simulated numerically using the Master equation approach. Here, we assume that the current through the island is given by the probabilities to have $n$ electrons on the island $P_n$ and the transition rates from one charge state to another $\Gamma(n_i, n_j)$, $n_i,j$ being different numbers of electrons on the island. We can approximate the motion of the pendulum with the equation of motion for a damped harmonic oscillator around its equilibrium position $x = 0$ (at larger amplitudes the electrodes impose mechanical boundary conditions, the influence of these effects will be discussed later)

$$m\ddot{x} = -kx + \gamma\dot{x} + aVq, \quad |x| \leqslant x_{\max},$$  \hspace{1cm} (1)

where $q$ is the charge of the island. The direction of motion of the island changes sign at the positions $|x| = x_{\max}$. In between these two extremal points, the motion of the island can be
described as a weakly damped harmonic oscillator. For small amplitudes of motion, the oscillation is not affected by the boundary conditions imposed by the presence of the two electrodes. At larger amplitudes, the island bounces into the electrodes at \( |x| = x_{\text{max}} \) and reverses the direction of motion. The effective period of the resonator is given by the time the resonator needs to move between the two turning points. The value of the effective period can be directly taken from the numerical simulations. The mechanical damping is given by a quality factor \( Q = 10^4 \). Stochastic forces are neglected in the treatment of the mechanical properties of the oscillator. This can be justified because the mass of the resonator is large, which means that influences of temperature are comparably small. The resonators can also be operated at low temperatures, as has been shown in [12]. If the voltage \( V \) is large enough, the island starts to move towards the source electrode and electrons can tunnel onto the island. The number of electrons tunnelling at this point is determined by the Master equation

\[
\frac{2}{\nu} \dot{P}_n = e^{-x/\lambda} \Gamma(n - 1, n) P_{n-1} + e^{x/\lambda} \Gamma(n + 1, n) P_{n+1} - e^{-x/\lambda} \Gamma(n, n + 1) P_{n} - e^{x/\lambda} \Gamma(n, n - 1) P_{n}. \tag{2}
\]

The frequency \( \nu \) determining the rate at which the electrons can tunnel on and off the island is given by \( \nu = RC \), with \( R \) and \( C \) the resistance and capacitance of the junction at the point of smallest distance between the island and leads. The transition rates for the case that the bias is applied asymmetrically (i.e. the voltage is applied to one electrode, while the other electrode is grounded) are calculated according to [15]. Experimentally observable is the charge carried by the island averaged over many (of the order of \( 10^7 \)) cycles of motion. The goal of this project is to predict Coulomb steps observable in such a system. As charge noise usually is suppressed on a flat step (see e.g. [7]), we concentrate on the average current here. We solve the Master equation and the equation of motion of the shuttle for tunnelling lengths of \( \lambda = 3 \text{ nm} \) and \( \lambda = 0.5 \text{ nm} \). The important parameter is the ratio between \( \lambda \) and the largest distance between the electrodes and the island \( x_{\text{max}} \). In the regime of the current paper, \( x_{\text{max}} \gg \lambda \), therefore the actual tunnelling takes place at a much smaller portion of the shuttle’s motion compared to results shown in [3], where \( x_{\text{max}} > \lambda \), but on the same order of magnitude. The results are shown in figure 3. In all our calculations, transient processes are not taken into account (in order to set the shuttle into motion larger voltages are necessary). Below a critical voltage \( V_C \), the shuttle is not moving and thus no current transport can be observed. While the smaller tunnelling length is motivated by experiments, the larger tunnelling length \( (\lambda = 3 \text{ nm}) \) is used here to compare the results with the situation given in [3]. At this value of \( \lambda \), charge transport sets in at a comparably low voltage. At this voltage, the shuttle can perform harmonic oscillations between the two electrodes at the resonance frequency \( f_0 \) of the pendulum (island plus supporting silicon rod). In our simulations, we use \( \omega_0 = 2\pi f_0 \approx 1 \text{ GHz} \). Since we need a net charge of the island in order to apply large enough forces on the pendulum, the shuttle does not move if the net charge of the island is too small. If the charge exceeds a certain number of electrons \( n_{\text{min}} \) (for \( \lambda = 3 \text{ nm} \), we obtain \( n_{\text{min}} \approx 5 \)) the force can set the shuttle into motion. Increasing \( V_{\text{sd}} \) further leads to a larger number of electrons taking part in the transport process. In this regime, the current obeys the relation \( I = nef_0 \), where \( n \) is the number of electrons, which is transferred during each revolution of the pendulum. Due to the rather large value of \( \lambda \), the tunnelling takes place before the island can touch the leads. Therefore, the harmonic oscillator is a good approximation for the motion of the pendulum. The results described so far are very similar to the results presented by Gorelik et al [3] for a much smaller system.

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Figure 3. Current through the shuttle as a function of applied source–drain bias. The current was calculated for different values of the tunnelling length $\lambda$. Dotted line: $\lambda = 3$ nm. This situation corresponds to a system with much smaller size cf [3]. At a critical value of $V_{sd}$ the shuttle starts to oscillate. Towards higher bias voltage the current rises in a CB staircase. Solid line: $\lambda = 0.5$ nm. This value of $\lambda$ is more realistic and thus effects of the large size of the silicon-based system become visible. Because the shuttle hits the electrodes during the oscillations, only one step of the CB staircase remains visible. Inset: current normalized to the number of electrons during each period of the oscillation. In this plot a second step can be seen for $\lambda = 0.5$ nm.

If we assume an experimentally more realistic value of the tunnelling length ($\lambda = 0.5$ nm) the behaviour of the system changes due to the much larger mechanical stiffness of the silicon rod compared to the molecules assumed in [3]. The number of electrons required to set the shuttle into motion is now $n_{\text{min}} = 10$. Due to the reduced value of $\lambda$ the shuttle touches the electrodes during the oscillation. This does not necessarily mean that the tunnelling contact is replaced by a purely metallic contact. Our previous measurements [16] have shown that even at very low distances, the contact between the metal on the shuttle and the metal on the electrodes is not metallic. Possible reasons for this behaviour are either small impurities on the metal layer or the fact that some of the underlying silicon is more protruding than the evaporated gold on top of it. If these imperfections are small, an almost perfect tunnelling contact can be formed without showing a metallic short.

Under these conditions, the oscillation of the pendulum deviates from the behaviour found for $\lambda = 3$ nm. The pendulum bounces back from the electrodes, very much like the metalized table tennis ball, which carries a macroscopic amount of charges in between two capacitor plates. This leads to an effective decrease of the oscillation period. The $I–V$ curve shown in figure 3 (solid line) shows only one step in the current, indicating that at only this number of electrons ($n = 10$), current transport takes place through the island. This surprising result can be explained by the anharmonic response of the pendulum to the applied $V_{sd}$. At lower voltages, the charge of the island $n$ is zero due to the small value of $\lambda$. Once the shuttle is set into motion, the large applied voltage causes a large $n$, which in turn causes a large electrostatic force on the island. This large force leads to a large amplitude of the pendulum. The motion of the island between the electrodes is still well described by the harmonic oscillator shown in equation (1), but it
starts touching the leads in the turning points. This reduces the effective period of the oscillation. Therefore, an increase in voltage leads to a deviation of the current $I$ from the simple $I = n e f_0$ relation, which was valid if the shuttle does not touch the leads. If the current is normalized to the number of electrons during each oscillation of the shuttle, a second step at $n = 11$ becomes visible, which is concealed in the not normalized $I–V$ curve by the described shortening of the effective period.

The response of a nanomechanical charge shuttle to applied dc-voltages has been calculated for a realistic silicon structure. The interesting effect is that the observed $I–V$ curves deviate substantially from the behaviour predicted for much smaller systems [3]. Due to the larger mechanical stiffness, the system has to be operated at voltages where the shuttle touches the electrodes. As a consequence of this fact, only one step in the $I–V$ curve is found, as opposed to the Coulomb staircase found in smaller systems. In past experimental realizations, the accuracy of the shuttle could not be tested, because the shuttle had to be driven by an oscillating gate voltage $V_G$. In this paper, we presented a realistic model for the electron shuttle driven by pure dc-voltages. A structure built with these parameters could show accurate charge transport.

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