Electromechanics of charge shuttling in dissipative nanostructures

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We investigate the current-voltage (*I-V*) characteristics of a model single-electron transistor where mechanical motion, subject to strong dissipation, of a small metallic grain in tunneling contact with two electrodes is possible. The system is studied both by using Monte Carlo simulations and by using an analytical approach. We show that electromechanical coupling results in a highly nonlinear *I-V* curve. For voltages above the Coulomb blockade threshold, two distinct regimes of charge transfer occur: At low voltages the system behaves as a static, asymmetric double junction and tunneling is the dominating charge transfer mechanism. At higher voltages an abrupt transition to a new ''shuttle'' regime appears, where the grain performs an oscillatory motion back and forth between the electrodes. In this regime the current is mainly mediated by charges that are carried on the grain as it moves from one electrode to the other.

I. INTRODUCTION

The mechanical properties of mesoscopic conductors and their influence on charge transport are very much in the focus of recent solid-state physics research. Certain anomalous behavior of nanowires[1,2] and the electrostatically controlled deformation of carbon nanotubes[3] are examples of an interplay between electrical and mechanical degrees of freedom that appear on the nanometer-length scale. Other examples where the heteroelastic nature of a material crucially affects single-electron tunneling have been found in studies of self-assembled metal-organic composite structures.

The relevant scenario associated with a strong electromechanical coupling is that significant deformations occur as a result of large Coulomb forces acting on charge accumulated in some small region: for instance, in a metallic cluster. Recently, a model system containing such a coupling was considered by Gorelik *et al.*,[4] who proposed a single-electron tunneling device containing a movable metallic cluster in tunneling contact with bulk metallic electrodes. In this device mechanically soft organic links serve both as elastic springs, keeping the cluster in place, and as tunnel barriers with resistances that are exponentially sensitive to the deformation of the springs. An important consequence of the interplay between single-electron tunneling and the mechanical vibration of the cluster in this model is the electromechanical instability predicted in Ref. 5: If a large enough bias voltage is applied between the electrodes, the equilibrium position of the grain loses its stability and cluster vibrations develop. Such vibrations give rise to a new mechanism of charge transfer, where electrons are transported through the system by the metallic cluster which performs shuttle motion between the electrodes. The electric current $I = 2Nef$ associated with this mechanism does not depend on the tunnel transparencies and is only determined by the frequency $f = \omega/2\pi$ of the elastic vibrations of the cluster and the number N of electrons carried by the cluster. Experimental evidence for a coupling between electron transfer and vibrational degrees of freedom has been found both for macroscopic[6] and microscopic[7–9] systems. Different aspects

of this phenomenon have also been theoretically investigated in several articles.[10–15]

In the work discussed above[4,5] it was shown that a large damping constant γ is detrimental for the development of the shuttle instability, and in the limit where $\gamma \gtrsim f$, elastic shuttling of the charge becomes impossible. The mechanical lability of the system, however, is still a dominating feature of the charge transport even in the limit of strong dissipation. What the consequences of such a lability would be is a question which needs to be answered. This is not only an academic question since coupling to intramolecular vibrations inside deformable organic molecules carrying current as well as friction in the medium through which a metallic cluster is moving may cause significant dissipation. The dissipative limit of electromechanical mesoscopic structures with movable parts is therefore important for understanding the functioning of realistic nanometer-size structures. Our objective in the present work is to study this limit.

We will consider the model system illustrated in Fig. 1. The current flow between the metallic electrodes is due to the tunneling of electrons between the electrodes and metallic cluster. This is assisted by the displacement of the cluster. An electrostatic force acts on the charged grain if a finite bias voltage is applied between the electrodes. The one-dimensional (1D) dynamics of the cluster is also governed by an elastic restoring force and a friction force. In contrast to
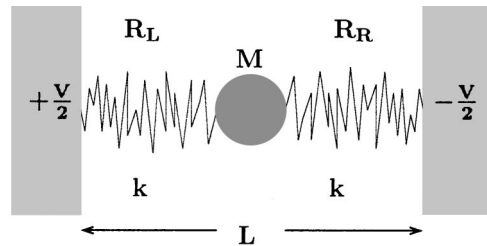

FIG. 1. Schematic picture of the model system, which consists of a metallic grain of mass M coupled by weak elastic links to two electrodes separated by a distance L. The elastic links act as springs with spring constant k. The tunneling resistances of the right and left junctions are R_R and R_L. A bias voltage V is applied across the system.

the approach developed in Ref. 5 we will consider the limit where the electric force dominates over the elastic force, which means that the dynamics of the charged cluster is determined by the interplay between Coulomb forces and friction. This, however, does not mean that the elastic forces can be totally neglected. For bias voltages slightly above the Coulomb blockade threshold when the cluster is in the center of the system, the dynamics of the cluster is actually very sensitive to the value of the elastic force. The low-temperature nonlinear charge transport through the system is affected both by the Coulomb blockade phenomenon and the mechanical motion of the cluster. These two phenomena are coupled since the threshold voltage for electron tunneling depends on the junction capacitances which in turn depend on the cluster position with respect to the electrodes. A general property is that the threshold voltage increases when the distance between the cluster and an electrode decreases.

In order to understand qualitatively the electromechanical charge transport scenario, let us consider a neutral cluster situated in its equilibrium position between the electrodes where the voltage threshold for electron tunneling has a minimum value, V_0. At zero temperature no tunneling is possible for voltages $V < V_0$, where V is the bias voltage applied between the electrodes. For $V > V_0$ tunneling onto the cluster becomes possible and the cluster can be charged. It is easy to understand that the direction of motion of the charged cluster, due to the Coulomb forces, will be away from the electrode which has supplied the extra charge to the cluster. After some time the extra charge will disappear, usually to the nearest electrode, which makes the cluster charge zero again. An important question at this stage is whether one more tunneling event to the nearest electrode is possible or not. The answer is not evident since the electrostatic threshold is different from the one at the initial point in the middle of the system. As we will see, depending on the applied bias voltage, we can have one of two possible situations. For voltages $V_0 < V < V_t$, where V_t is a threshold voltage which will be treated in more detail in Sec. IV C, the extra tunneling event is not possible. In this case the cluster is almost trapped near the electrode. Small oscillations in the vicinity of the trapping point are possible due to the action of the weak elastic force, but the cluster will not be pushed back by Coulomb forces. In this case the conductance is not assisted by significant cluster displacements between the electrodes. We call this regime the *tunneling regime* since the charge transfer is very similar to the conventional single-electron transport in a static system.

If $V > V_t$, there is a possibility for another tunneling event between the grain and nearest lead to happen after the extra charge has tunneled off the cluster. This event changes the sign of the net charge on the grain. In this case the cluster can be pushed by the Coulomb force towards the more distant electrode where the above-described process repeats itself. The conductance is now assisted by significant displacements of the grain and this scenario is qualitatively similar to the shuttle vibrations in fully elastic electromechanical structures.[4] We call this regime the *shuttle regime* of charge transport. A sharp transition, corresponding to a current

jump, occurs in a small voltage interval between the two regimes.

II. MODEL SYSTEM

We will consider a model based on the picture in Fig. 1. This is a simplified model which, however, retains many of the interesting features of a "real" system. The system consists of a metallic grain of mass M placed in the gap between two bulk leads separated by a distance L. The displacement of the grain from the center of the system is measured by the coordinate X. (Our approach is based on a classical description of the grain displacement and is different from approaches where quantum cluster vibration assisted tunneling to the grain is considered.[11]) We consider only 1D motion of the grain between the leads. A bias voltage V is applied between the leads. In this simplified case we take into account only three different forces acting on the grain: a linear elastic restoring force $F_{el} = -kX$, a dissipative damping force $F_{diss} = -\gamma_d \dot{X}$, and an electrostatic force F_q. The electrostatic force is a function of the bias voltage V and the charge Q on the grain:

$$F_q = \frac{QV}{L} + \frac{X}{C_0 L^2} Q^2. \tag{1}$$

Here C_0 is a capacitance constant determined by the geometry of the system. To get this expression we assume that the capacitances C_L between the left lead and the grain and C_R between the grain and right lead can be approximated as parallel-plate capacitors and that all other capacitances can be neglected. The first term in Eq. (1) can be understood as the force from an effective electrostatic field V/L in the junction, which couples to the extra charge on the grain. The second term can be thought of as the interaction of the charge on the grain with image charges in the two leads. Note that the last term in Eq. (1) always results in an attraction of the charged grain towards the nearest lead. If we take these forces into account, we can write the equation of motion for the grain as

$$M\ddot{X} + \gamma_d \dot{X} + kX = \frac{QV}{L} + \frac{X}{C_0 L^2} Q^2. \tag{2}$$

We can now consider the Coulomb blockade regime where the Coulomb charging energy $E_c = e^2 / 2C$ is larger than both quantum and thermal fluctuations, $E_c \gg \hbar / RC, \beta^{-1}$, where R is the smallest tunneling resistance possible in the system and β is the inverse temperature. We thus assume that

$$R(X) \gg R_Q \equiv \frac{\pi \hbar}{2e^2} \approx 6.5 \ \text{k}\Omega$$

for all positions X available for the grain. (Note that soft matter springs always have some finite thickness even when compressed. Coating layers on the leads could also restrict the space available for the grain.) If the criteria for the Cou-

lomb blockade regime are met, we can consider electrons on the grain to be fully localized and express the charge on the grain as

$$Q(t) = en(t),$$

where $n(t)$ takes on only integer values. (e is the electron charge.) Let (n,Q_α) be the state of the system with n extra charges on the grain and the charge Q_α on the lead α ($\alpha = L,R$). It then follows from the "orthodox" Coulomb blockade theory[16,17] that the tunneling probabilities for the tunneling event $(n,Q_{L,R}) \rightarrow (n\pm 1, Q_{L,R} \mp e)$ to occur during the time Δt are

$$P_{L,R}^{\pm}(n,X,V,\Delta t) = \Delta t \, \frac{\Delta G_{L,R}^{\pm}(n,V,X)}{e^2 R_{L,R}(X)}$$

$$\times \left[1 - \exp\left(-\frac{\Delta G_{L,R}^{\pm}(n,V,X)}{k_B T} \right) \right]^{-1}, \quad (3)$$

where $\Delta G_{L,R}^{\pm}(n,V,X)$ is the decrease of free energy in the system as an electron tunnels to the right $(+)$ or to the left $(-)$ through the left (L) or right (R) tunnel junction, k_B is the Boltzmann constant, and $R_{L,(R)}$ is the resistance of the left (right) tunnel junction. This resistance depends exponentially on the displacement of the grain from the center of the system and can be written

$$R_L(X) = R_R(-X) = R_0 \exp(X/\lambda),$$

where R_0 is a constant prefactor and λ is referred to as the tunneling length. The tunneling length depends on the materials used in the system and for our system we estimate λ to be of the order of 1 Å.

III. CURRENT-VOLTAGE CHARACTERISTICS

To make the treatment of the model easier we rewrite the equations in a dimensionless form. If we introduce the dimensionless time $\tau = t/t_0$ where $t_0 = \gamma_d L^2/eV_0$ is a time scale on which the grain crosses the distance L between the leads due to the electrostatic forces, the dimensionless length $x = X/L$, the dimensionless elastic vibration frequency $\omega = \sqrt{kL^2/eV_0}$, the dimensionless bias voltage $v = V/V_0$ where $V_0 = e/4C_0$ is the Coulomb blockade threshold in the center of the system, and the dimensionless constant $\alpha = MeV_0/L^2 \gamma_d^2$ which signifies the ratio between the electrostatic force and a typical dissipative damping force in the system, we can rewrite the equation of motion for the grain as

$$\alpha \ddot{x} + \dot{x} + \omega^2 x = nv + 4n^2 x. \quad (4)$$

We will focus on the case when the dissipative force dominates the electrostatic force while the latter dominates the elastic forces, $\omega^2 \ll \alpha \ll 1$. The free energy terms $\Delta G_{L,R}^{\pm}$ to be used in Eq. (3) are
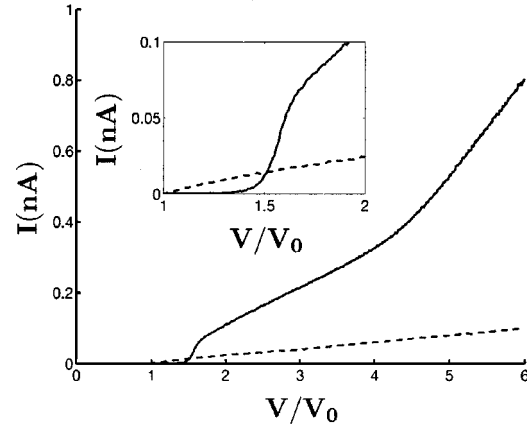

FIG. 2. The solid line shows the current-voltage characteristics obtained by a Monte Carlo simulation of the charge transport through the system sketched in Fig. 1. The calculated current, which was averaged over 20 μs, is plotted as a function of the bias voltage V scaled by the Coulomb blockade theshold voltage V_0, which applies if the movable grain is equally far from both electrodes. The dashed line displays the current through a static symmetric double junction for the same parameters. The parameters used in the simulation are $\alpha = 6.4 \times 10^{-4}$ and $\omega^2 = 4.27 \times 10^{-3}$. It is clear that for voltages between approximately V_0 and $1.5V_0$ (see the inset which shows a magnification of the voltage interval $1 < V/V_0 < 2$) the current through the model system is smaller than the current through the static symmetric double junction, whereas for higher voltages it is the other way around.

$$\Delta G_L^{\pm}(n,v,x) = \frac{eV_0}{2}(1 - 4x^2)\left(-1 \mp 2n \pm \frac{v}{1-2x} \right), \quad (5)$$

$$\Delta G_R^{\pm}(n,v,x) = \frac{eV_0}{2}(1 - 4x^2)\left(-1 \pm 2n \pm \frac{v}{1+2x} \right). \quad (6)$$

Note that the position dependence of $\Delta G_{L,R}^{\pm}$ given by Eqs. (5) and (6) results in a position-dependent Coulomb blockade threshold voltage. This means that whether tunneling in a junction is blocked or not at a certain voltage depends on where the grain is located at the moment.

Numerical approach

In a numerical approach we have peformed Monte Carlo simulations of the model system described. A fourth-order Runge-Kutta method was used to solve the equation of motion for the grain for small enough time steps for the charge on the grain to be considered constant during each step. After each time step the charge on the grain was updated by "rolling dice" and deciding whether to carry out a tunneling event using the tunneling probabilities of Eq. (3). The current was calculated as the average of the number of transferred electrons over a certain time interval. For our choice of parameters the average number of electrons transferred through the system stabilizes over a time period of approximately $64t_0$. In our calculations of the current-voltage characteristics we
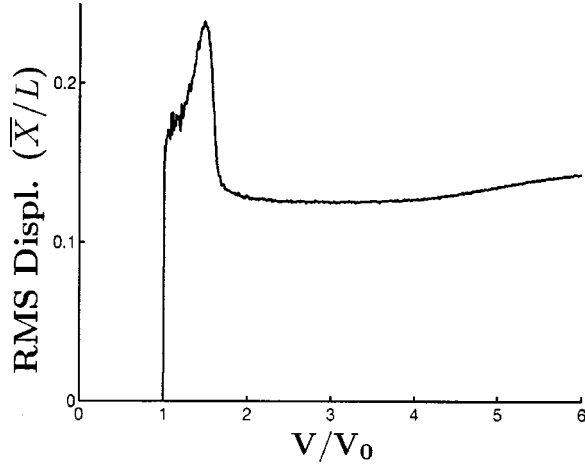
FIG. 3. The root-mean-square displacement of the grain from the symmetric position between the leads as a function of the bias voltage scaled by V_0, the Coulomb blockade threshold voltage in the center of the system. The parameters used in the simulation are $\alpha = 6.4 \times 10^{-4}$ and $\omega^2 = 4.27 \times 10^{-3}$. The distinction between the two different regimes of charge transfer is very clear. In the tunneling regime, the average displacement increases with the voltage and is larger than in the shuttle regime. In the shuttle regime, the average displacement is a slowly varying function of the voltage.

have averaged over $6.4 \times 10^3 t_0 = 20$ μs to reduce the numerical noise. The result of the calculation is plotted in Fig. 2.

If we now compare the current through the studied system with that through a static symmetric double junction as in Fig. 2 (see inset), it becomes very clear that there are two distinct parts of the current-voltage curve. For voltages V approximately between V_0 and $1.5V_0$ the current through the static symmetric double junction is larger than that through the system under consideration here. Since, as will be shown in the next section, charge transport in this regime is dominated by tunneling, we label this regime the *tunneling regime*. For voltages above approximately $1.5V_0$, on the other hand, the current through the present system is the larger one, and since, as will be shown below, charge transport in this regime is mechanically mediated by the grain, we label this regime the *shuttle regime*.

The distinction between the two regimes also becomes very clear if we consider the root-mean square of the displacement of the grain from the center of the system, $\bar{x}$, as a function of the bias voltage. This is plotted in Fig. 3. It is clear that the average displacement is much larger for the tunneling regime than for the shuttle regime. The average displacement is also increasing with the bias voltage for the tunneling regime, whereas for the shuttle regime it is a slowly varying function.

IV. DISCUSSION

A. Tunneling regime

From Fig. 2 (inset) we see that for bias voltages just above the Coulomb blockade threshold V_0 (for the grain in the center position) the current is smaller than it is through a
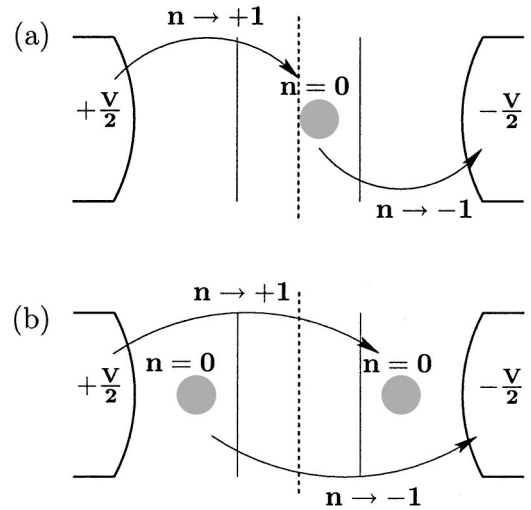

FIG. 4. Illustration of the concept of the open region which, in the pictures above, correspond to the space between the vertical solid lines. (a) If the grain is uncharged and located inside the open region, it is in tunneling contact with both leads at the same time. (b) When the grain is situated outside the open region, energy considerations show that tunneling to the near lead is blocked. Tunneling from the far lead is still possible; however, this process is strongly suppressed due to the exponential dependence of the tunneling resistance on the grain-lead separation.

static symmetric double junction. To understand this we should consider the x dependence of the tunneling rates. Assume that the grain starts out sitting uncharged in the center of the system and that the bias voltage is just above V_0. At this point two things are possible. One unit of charge can either tunnel onto the grain or off the grain. Since the system is symmetric, we consider only the first of these cases. The criterion for tunneling from the left lead to the grain is that the free energy is lowered after a tunneling event, $\Delta G_L^+ > 0$. Using Eq. (5) we find the corresponding inequality

$$ x > \frac{1}{2} - \frac{v}{2}. \tag{7} $$

Note that x is the normalized coordinate so that $-1/2 < x < 1/2$. We see that the Coulomb blockade threshold when the grain is at the center of the system is ($x=0$) is indeed V_0 ($v=1$). For lower voltages tunneling onto the grain from the *left* lead is still possible as long as the grain is to the *right* of the center position. However, this process is exponentially suppressed due to the increase of resistance with tunneling distance. If one considers tunneling from a neutral grain to the right lead, the same picture (with $x \rightarrow -x$) emerges. When the bias voltage is increased above V_0, tunneling onto the grain becomes possible if it is to the left of the center. We see here that if the bias voltage is not much higher than the Coulomb blockade threshold V_0, the *open region*, where both tunneling onto a neutral grain from the left lead or off a neutral grain to the right lead is allowed at the same time, is much smaller than the distance between the leads. The concept of the open region is illustrated with two examples in Fig. 4.

1: The grain is charged from the far lead.

2: Being charged, the grain is pushed to-

wards the near lead until a tunnel event

to that lead occurs.

3: The grain is slowly pulled back by the

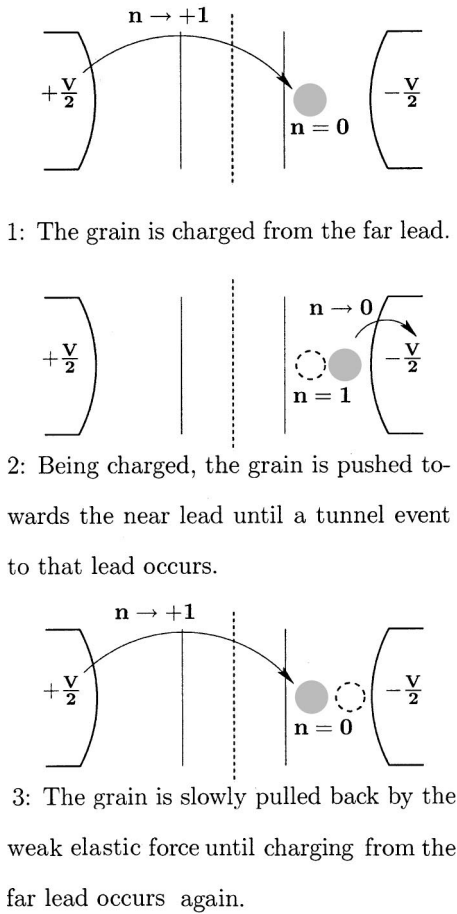weak elastic force until charging from the

far lead occurs again.

FIG. 5. Schematic illustration of the charge transfer mechanism in the tunneling regime. The grain performs small oscillations around an average position, located between the the open region border and the lead. In the figures above, the open region is bounded by the vertical solid lines in the center of each junction.

For a grain that has the charge $n=0$ and is located inside the open region, both processes $n \rightarrow +1$ and $n \rightarrow -1$ are allowed at the same time. If the grain is located outside the open region, it can only be charged from the far lead.

Let us now consider the case when the bias voltage is not much higher than the Coulomb blockade threshold V_0, which applies if the grain is in the center position. In this case the open region is much smaller than the distance between the leads. If a unit charge tunnels onto the grain from the left, the grain becomes positively charged and is thus affected by a force towards the negative (right) lead. It will start to accelerate towards that lead, but if the mass of the grain is very small and the dissipation large, the grain will reach a maximum velocity very quickly. As the grain comes close to the negative lead, the discharging process through the right junction becomes very probable. If the relaxation of the charge on the grain to the negative lead takes place outside the open region, the grain cannot be recharged by a negative unit charge from the negative lead. If dissipation is strong, the grain will stop very quickly and the very small elastic restoring force will start to move the grain very slowly towards the center of the system. At this time the grain is only in tunneling contact with the far lead and it will continue to move
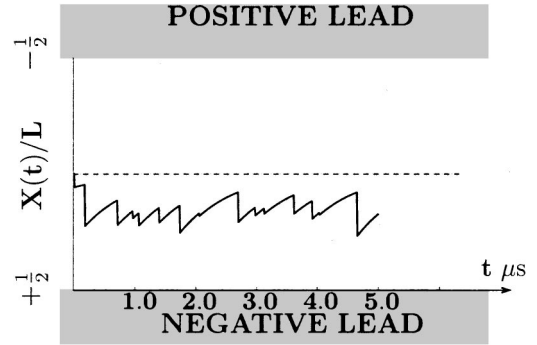

FIG. 6. Plot of the position of the grain as a function of time for the bias voltage $V=1.1V_0$ and the parameters $\alpha=6.4\times10^{-4}$ and $\omega^2=4.27\times10^{-3}$. For this voltage the behavior of the system is on average very much like a static symmetric double junction. The jaggedness of the curve comes from the very different velocities of charged and uncharged grains.

slowly towards the center, either until it reaches the open region and can be charged from either lead or until a tunneling event from the positive lead on the far side of the system occurs again. If the last of these two processes occurs, the charge on the grain becomes positive and the grain is accelerated towards the negative lead again, repeating the above described process. The resulting motion is thus an oscillation around an average position, which is located between the open region border and the lead. One cycle of such an oscillation is schematically illustrated in Fig. 5.

Tunneling from the far lead to the grain as the grain moves under the influence of the weak restoring force is possible but very unlikely, as can be seen from Eq. (7). This is due to the exponential dependence of the tunneling resistance on the separation between grain and lead. If the grain moves very slowly, however, there may be enough time for the grain to be charged from the far lead before it reaches the open region. As the bias voltage is increased, the size of the open region increases, thereby affecting the probability that the grain will reach the open region before getting charged from the far lead. This leads to a transition to the shuttle regime discussed in the next section.

We can thus conclude that the current through the system is smaller than that through a static symmetric double junction because the charge transfer mechanism is limited by tunneling through the more resistive tunnel barrier, just as is the case for a static asymmetric double junction. That this is actually the case is also confirmed by studying plots of the grain position as a function of time, obtained from Monte Carlo simulations of the system. Such a plot for $V=1.1V_0$ is shown in Fig. 6. For clarity the picture is embedded in a model system with the positions of the leads marked on the x axis. The plotted line traces out the position of the grain as a function of time. The sharpness in the curve depends on the two very different time scales in the system. The time scale for grain motion due to the electrostatic force when the grain is charged is much smaller than the time scale of grain motion caused by the weak elastic force when the grain is uncharged. From the plot we can conclude that, on average, the

charge transfer through the system looks like that through a static asymmetric double junction.

If we consider Eq. (7) and its counterpart

$$\Delta G_R^+(n=0,x)>0,$$

we see that for $V=1.1V_0$, the borders of the open region are located at $x=\pm 0.05$. When we compare this value to the average displacement of the grain at this voltage, it becomes clear that the average displacement is 3–4 times bigger. The grain thus performs an oscillatory motion around an average displacement, and these oscillations are possible because the average displacement is located quite far away from the border of the open region.

We can now compare the current for this regime (see Fig. 2) with the current through a static asymmetric double junction. The current through the latter type of double junction can be approximated by saying that the charge transfer to the far lead limits the current. Since the inverse of the tunneling rate is the average time between tunneling events, we can write the current I_{adj} through the asymmetric double junction as

$$I_{adj}=e\Gamma_{far\text{-}lead},\tag{8}$$

where $\Gamma_{far\text{-}lead}$ is the rate for tunneling events between the grain and far lead. Using Eq. (3) (Ref. 18) under, for instance, the assumptions $x>0$ and $T=0$, the current from the far lead would be

$$I_{adj}=\frac{e}{8R_0C_0}\frac{(1-4x^2)\left(-1+\dfrac{v}{1-2x}\right)}{\exp\left(\dfrac{L}{\lambda}x\right)}.\tag{9}$$

If we use the average displacement from Fig. 3, the current, as calculated by Eq. (9) and in the voltage interval $1<V/V_0<1.25$, turns out to be of the order 20% lower than the actual current through the our system. This is understandable since the small grain oscillations around the average displacement decrease the effective tunneling resistances seen by the charges transferred through the system.
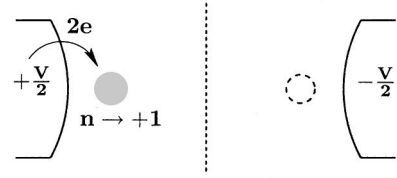
B. Shuttle regime

The statements made in the previous section mean that we can expect the current through our device to be very small on the scale of the current through a symmetric static double junction. On this scale, we can also expect that the current only increases slowly as the bias voltage is raised to slightly above the Coulomb blockade threshold in the center of the system. The current will continue to increase very slowly with the voltage. As the size of the open region increases it becomes more and more probable that an empty grain will reach the open region before it is recharged from the far lead. If the grain reaches the open region, charge transfer from the near lead suddenly becomes the dominating charge transfer mechanism. If we consider Eq. (7), we see that as the bias voltage V reaches $2V_0$, the open region has extended all the way to the leads. The grain will thus always move inside the
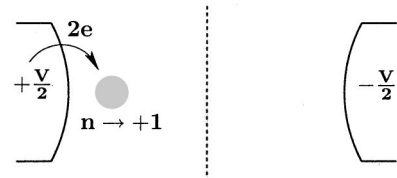
1: The grain is charged from the near lead.
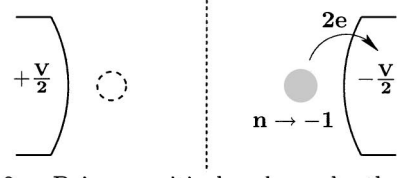
2: Being positively charged, the grain is pushed towards the other lead, where two charges tunnel off the grain.

3: Being negatively charged, the grain is pushed back to the first lead, where the process starts over.

FIG. 7. Schematic illustration of the charge transfer mechanism in the shuttle regime. The grain performs oscillations back and forth between the leads, loading and unloading two charges at each turning point.

open region. In this case, the charge transfer cycle looks quite different from the picture in the previous section. When the grain gets positively charged, it will move towards the negative lead. As the grain gets closer to the lead, the tunnel resistance decreases exponentially and finally the charge on the grain will tunnel from the grain to the lead. When the grain loses its charge, it will stop very quickly due to the high dissipation. The grain now starts to move very slowly towards the center of the system, but since the time scale of charge exchange with the near lead is much shorter than that of movement due to the elastic force, another tunnel event can occur and the grain can get negatively charged. This means that the grain will be accelerated towards the positive lead, where a similar procedure will occur. The grain will now continue to move back and forth in this fashion, shuttling charge across the junction. Figure 7 shows a schematic illustration of this charge transfer mechanism.

The exponentially large tunnel resistances limiting the current in the tunneling regime are now gone, since all tunneling events occur when the grain is close to the leads. The oscillations of the grain thus effectively lower the tunnel barriers seen by the transferred charges, which leads to a large increase in the current.
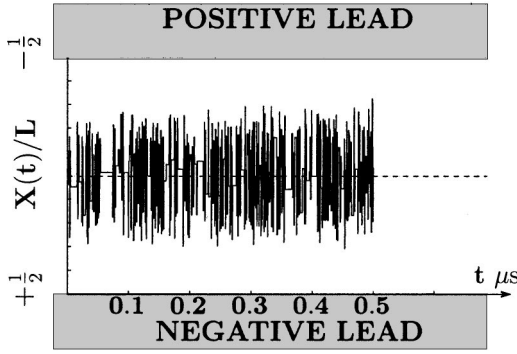
FIG. 8. Plot of the position of the grain as a function of time for the bias voltage $V=2.0V_0$ and the parameters $\alpha=6.4\times 10^{-4}$ and $\omega^2=4.27\times 10^{-3}$. For this voltage an uncharged grain is everywhere in tunneling contact with both leads so that the charge transfer cycle illustrated in Fig. 7 is possible.

We can now proceed as in the case of the tunneling regime and consider a plot of the grain position as a function of time for some bias voltage in this interval. In Fig. 8 we have made such a plot for the bias voltage $V=2.0V_0$. As in Fig. 6 the plot is shown together with the model system so that the positions of the leads are marked on the x axis. The plotted line traces out the position of the grain as a function of time. The grain performs a stochastic but still oscillatory motion back and forth through the system. For this voltage an uncharged grain is everywhere in tunneling contact with both leads so that the charge on the grain can change by $2e$ at each approach of a lead. This means that the grain will always be pushed by the electrostatic force, which explains the much shorter time scale for grain motion in Fig. 8 compared to Fig. 6. (Note also the factor of 10 difference in scale on the time axes in the two plots.)

Let us now go back and consider the I-V curve in Fig. 2 again. For a bias voltage of approximately $4.5V_0$, the I-V curve changes slope over a relatively short voltage interval. The reason for this is the transition to a regime where two extra charges are allowed on the grain; i.e., four charges can be transported across the system in each shuttle cycle. To get a better understanding of this, we should consider the case $\Delta G_L^+(n=1,x)>0$, i.e., the condition that the free energy decrease should be positive when one charge tunnels from the left lead onto an already charged grain. Using Eq. (5), we get the condition

$$x>\frac{1}{2}-\frac{v}{6}. \qquad (10)$$

We thus see that when $V=3V_0$ ($v=3$) a new open region develops, where electron tunneling is allowed from the left lead when the grain charge is $n=1$ and to the right lead when the grain charge is $n=-1$. If we remind ourselves of what went on in the tunneling regime, we cannot expect that the current will change much until the size of this region is of the same size as the amplitude of the grain oscillations. As can be seen from Fig. 2, nothing new happens to the I-V characteristics when $V=3V_0$. However, approximately when $V=4.5V_0$, there is a transition to the new regime. From Eq.
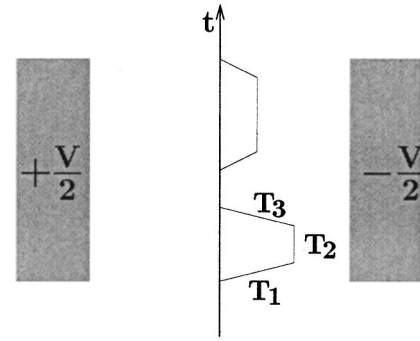

FIG. 9. Schematic illustration of the three parts of the average half-period for a shuttle cycle discussed in the text. Two different kinds of period times are illustrated. The further the grain moves towards the lead, the shorter the time T_2 can be expected to be.

(10) we get that, at $v=4.5$, the open region borders for $n=1$ have extended to approximately $x\in(-0.25,0.25)$. At this voltage, the grain oscillations should thus be inside the new region most of the time, allowing the transfer of four charges in each shuttle cycle.

It is important to note here that the transition in the I-V curve is not sharp. As the open region for $n=1$ grows wider, it will become more and more probable that, as the grain moves across the system, it will transport two charges instead of only one charge. As is normally the case for shuttle transport,[4] we can consider a current-frequency relationship

$$I=2\mathcal{N}ef,$$

where $\mathcal{N}$ is defined by this equation and represents an average number of extra electrons transported on the grain and where f is the vibrational frequency of the grain. Both $\mathcal{N}$ and f are functions of the bias voltage. Note also that $\mathcal{N}$ is not usually an integer.

C. Analytical description of the shuttle regime

In this section we present an analytical approach to modeling the current through the system for bias voltages in the range $2<V/V_0<3$. In this voltage interval, the grain can only shuttle one charge at a time in each direction. Since the motion of the grain is strongly influenced by the random tunneling events, we have to consider the period time in an averaged sense and write the current as

$$I=\frac{2e}{t_0\bar{T}}, \qquad (11)$$

where $\bar{T}$ is the dimensionless average oscillation period and $t_0=\gamma_d L^2/eV_0$ is the typical time scale in the system. We make the assumption that we can divide the average period into the three parts schematically illustrated in Fig. 9. Since the system is symmetric with respect to the center of the system, it is enough to consider half a cycle.

The first part of the average period, T_1, is the average time it takes a grain with one excess charge to move from the center of the system towards the negative lead to the position where, on average, the excess charge is relaxed to the nega-

tive lead. After the charge has relaxed to the negative lead, the grain stops very quickly and, on the average, sits still during the time T_2 before one more charge tunnels to the negative lead. As this happens, it takes the grain the time T_3 to get back to the center of the system, where it repeats a mirror version of this cycle towards the positive lead. Note also that the further the grain moves towards the lead, the shorter the time T_2 can be expected to be. As the grain passes the center of the system towards one lead, there is at each position a certain probability that the charge on the grain will tunnel to the lead. Wherever the tunneling event occurs, the two average times T_2 and T_3 are determined by the first time T_1, which is determined by the position at which the tunneling event occurred. We can therefore write the average period time as

$$\bar{T} = 2 \int_0^{x_{max}} \tau(x) P(x) dx, \tag{12}$$

where $\tau(x)$ is the half-period for a grain that reaches position x as it travels from the center of the system towards the lead. This half-period now consists of the sum of three partial times $\tau_1(x)$, $\tau_2(x)$, and $\tau_3(x)$, where the indexes refer to the same parts of the half-period as the time indexes illustrated in Fig. 9.

To find the probability density $P(x)$, we can consider an ensemble consisting of N grains. These grains all start out at the center of the system, have charge $n=1$, and move towards the negative lead. We can first find the relative number of grains $m(x)/N$ that still has a charge of $n=1$ at x by noting that

$$\frac{d\left(\dfrac{m(x)}{N}\right)}{dx} = -\frac{m(x)}{N} \frac{\Gamma_R^+(n=1,x)}{\dot{x}}. \tag{13}$$

This is an ordinary separable differential equation with the solution

$$\frac{m(x)}{N} = \frac{m(0)}{N} \exp\left(-\int_0^x \frac{t_0 \Gamma_R^+(n=1,x')}{\dot{x}(x')} dx' \right). \tag{14}$$

Since all grains in the ensemble have charge $n=1$ at $\tau=0$, we see that $m(0)/N=1$. We can now find the probability density $P(x)$ as the relative number of grains in the ensemble that stops at precisely x, i.e., minus the derivative of $m(x)/N$:

$$P(x) = \frac{t_0 \Gamma_R^+(n=1,x)}{\dot{x}(x)} \exp\left(-\int_0^x \frac{t_0 \Gamma_R^+(n=1,x')}{\dot{x}(x')} dx' \right). \tag{15}$$

The next step is to find the half-period $\tau(x)$. Since we are working in the high-dissipation limit $\alpha \ll 1$, acceleration times are very short compared to the time scales of movement of the grain and tunneling. This means that we can to a good approximation find the parts $\tau_1(x)$ and $\tau_3(x)$ by integrating the equation for the velocity of the grain,[19]

$$\dot{x} = nv + 4n^2 x, \tag{16}$$

from $\tau=0$ to $\tau=\tau'(x)$ and for $n=\pm 1$. The resulting traveling times are

$$\tau_1(x) = \frac{1}{4} \ln\left(1 + \frac{4x}{v} \right), \tag{17}$$

$$\tau_3(x) = -\frac{1}{4} \ln\left(1 - \frac{4x}{v} \right). \tag{18}$$

To find the time τ_2 we first assume that the grain will not move on the scale of the tunneling length during this time. This means that the tunneling rates are time independent and that we, if the grain sits with zero charge at x, can expect the average time before a tunneling event occurs to be

$$\tau_2(x) = \frac{1}{t_0 \Gamma_R^+(n=0,x)}. \tag{19}$$

At zero temperature we can expect the time to be

$$\tau_2(x) = \frac{8 R_0 C_0}{t_0} \frac{\exp\left(-\dfrac{L}{\lambda} x \right)}{(1 - 4x^2)\left(-1 + \dfrac{v}{1 + 2x} \right)}. \tag{20}$$

We have thus arrived at the following expression for the current through the system in the bias voltage interval $2 < V/V_0 < 3$:

$$I = \frac{e}{t_0 \int_0^{x_{max}} [\tau_1(x) + \tau_2(x) + \tau_3(x)] P(x) dx}, \tag{21}$$

where $\tau_1(x)$, $\tau_2(x)$, and $\tau_3(x)$ are given by Eqs. (17), (20), and (18) and $P(x)$ is given by Eq. (15).

We have, with the same parameters as used in our earlier Monte Carlo simulations, numerically calculated the current given by Eq. (21). The results are shown in Fig. 10. The solid line corresponds to the Monte Carlo simulations of the system and the circles correspond to the values obtained from Eq. (21). The agreement between the numerical studies and the analytical approach is very good, which is a strong indication that the charge shuttle mechanism description of the charge transfer is applicable also in highly dissipative systems.

It is also of interest to know the threshold voltage V_t and the width ΔV of the transition from the tunneling regime to the shuttle regime. In order to estimate these we can consider small oscillations Δx of the grain around some average position x_0. Without loss of generality we can assume that $x_0 > 0$; i.e., the grain oscillates on the right-hand side of the system. If we assume that the oscillation amplitudes are not very big, we can estimate the velocity of the grain to be

$$v_{IN} \approx -\omega^2 x_0 \tag{22}$$

for grains moving towards the center of the system due to the elastic force. On average it moves during the time
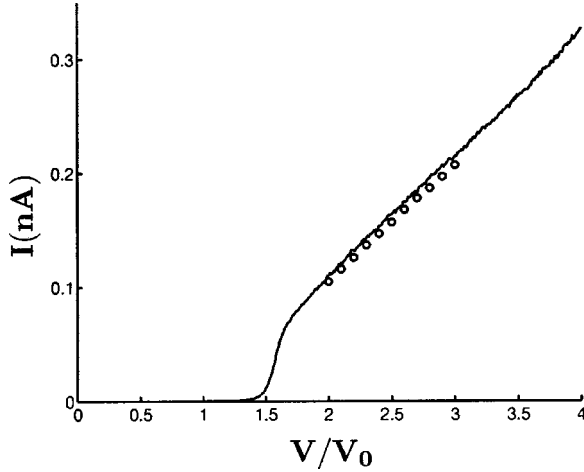
FIG. 10. Comparison between the current obtained by Monte Carlo simulations of the system shown in Fig. 1 (solid line) and the current as calculated by using the analytical expression in Eq. (21) (circles). The parameters used in the simulation are $\alpha = 6.4 \times 10^{-4}$ and $\omega^2 = 4.27 \times 10^{-3}$.

$$\tau_{IN} \approx \frac{1}{t_0 \Gamma_L^+(n=0,v,x_0)} \qquad (23)$$

before it is charged from the far lead. When the grain is moving towards the lead due to the electrostatic force acting on the extra charge on the grain, it approximately moves with the velocity

$$v_{OUT} \approx (v + 4x_0). \qquad (24)$$

The average time it will move before the extra charge tunnels to the right lead is

$$\tau_{OUT} \approx \frac{1}{t_0 \Gamma_R^+(n=1,v,x_0)}. \qquad (25)$$

For the position x_0 to be stable the average the distance the grain moves in each direction has to be equal to each other. We thus get the relation

$$\frac{\omega^2 x_0}{f_L} e^{(L/\lambda)x_0} = \frac{(v+4x_0)}{f_R} e^{-(L/\lambda)x_0}, \qquad (26)$$

where $f_L = -1/2 + C_R V/e$ and $f_R = 1/2 + C_L V/e$ are functions of the right and left capacitances and the bias voltage and that are of order unity as long as the grain is not close to the open region border. Rearranging the factors in Eq. (26) and taking the logarithm of both sides we get

$$2\frac{L}{\lambda} x_0 = \ln\frac{1}{\omega^2} + \ln\frac{v+4x_0}{x_0} + \ln\frac{f_R}{f_L}. \qquad (27)$$

Under the conditions that we are not close to the open region border and that the elastic force is very weak we can neglect the last two terms on the right-hand side of Eq. (27). In this case we get the average position for the grain as

$$x_0 \approx -\frac{\lambda}{2L} \ln\omega^2. \qquad (28)$$

If $\Delta x \ll x_0$, one can, by comparing the average position x_0 for the grain with the open region border $(v-1)/2$, estimate the threshold voltage

$$V_t = V_0\left(1 - \frac{\lambda}{L}\ln\frac{kL^2}{eV_0}\right), \qquad (29)$$

which corresponds to the transition from the tunneling regime to the shuttle regime.

We can now use the expression for x_0 to estimate the width of the oscillations as

$$\Delta x \sim 2\frac{\lambda}{L}\frac{R_0 C_0}{t_0}\sqrt{\omega^2}\ln\frac{1}{\omega^2}. \qquad (30)$$

From Eq. (7) we know that the open region expands linearly with the bias voltage. When the oscillations are completely outside the open region we can expect the system to be in the tunneling regime. When the open region has expanded to include the oscillations, the system should be in the shuttle regime. The open region border expands Δx if the voltage is increased with $\Delta V/V_0 = 2\Delta x$ and we thus get the relative transition width as

$$\frac{\Delta V}{V_t - V_0} = \frac{\Delta x}{x_0} \sim 4\frac{R_0 C_0}{t_0}\sqrt{\omega^2} = 4\frac{\omega_{sh}}{\omega_R}\eta^{-1/2}, \qquad (31)$$

where $\omega_{sh} = t_0^{-1} = eV_0/\gamma_d L^2$ is a typical grain oscillation frequency, $\omega_R = 1/R_0 C_0$ is a characteristic tunneling frequency, and $\eta = \omega^2 = kL^2/eV_0$ represents the strength of the electromechanical coupling. From Eq. (31) one can see that there are two cases when there is a very sharp transition between the two regimes. The first case is when the electromechanical coupling becomes very strong. The second case is when the shuttle frequency is low compared to the rate of tunneling. In our system these conditions are realized by the assumed weak elastic forces and the high rate of dissipation associated with the moving grain.

V. CONCLUSIONS

The main conclusion resulting from our analysis is that an electromechanical coupling in dissipative nanometer-sized Coulomb blockade structures cannot be viewed simply as an additional channel for absorbing the power associated with the current injected into the system. Instead a new mechanism of mechanically assisted charge transfer occurs, which increases the current exponentially and which to some extent is related to the shuttling of electrical charges, predicted for weakly dissipative electromechanical structures.[4,5] We have shown that the electromechanical coupling results in a highly nonlinear I-V curve with two distinct regimes of charge transport. More features of the charge transfer might be

available by studying the noise properties of the system. Since the noise is sensitive to the dynamical properties of the system, noise measurements can give additional information about the interplay between elasticity and dissipation in real nanoelectromechanical structures.

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[18] Note that $P_{L,R}^{\pm} = \Delta t \Gamma_{L,R}^{\pm}$.

[19] This equation is valid under the assumption that the acceleration time is much shorter than the time scale of the motion of the grain, which is the case due to the high dissipation in contrast to the weak elastic force.