Spontaneously Symmetry-Broken Current in Coupled Nanomechanical Shuttles

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We investigate the transport and the dynamical properties of tunnel-coupled double charge shuttles. The oscillation frequencies of two shuttles are mode-locked to integer multiples of the applied voltage frequency $\omega$. We show that left/right-symmetric double shuttles may generate direct net current due to bistable motions caused by parametric instability. The symmetry-broken direct current appears near $\omega = \Omega_0/(2j - 1)$, $(j = 1, 2, \ldots)$, where $\Omega_0$ is the dressed resonance frequency of the relative motion of the two shuttles.

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Recently, nanoelectromechanical systems (NEMS) have attracted great attention due to fundamental aspects in new electrical transport properties as well as new technology complementary to conventional MEMS engineering [1]. A prototype of NEMS, single electron shuttle, was suggested by Gorelik et al. [2] which is a single electron transistor combined with its mechanical degree of freedom. The charge shuttles can be realized in two different ways in experiments. In a top-down approach, the charge shuttles can be realized by miniaturization of silicon structure [3, 4]. The other way is a bottom-up approach, where the charge shuttle is produced from molecules such as $C_{60}$ [5]. In this Letter, we report a theoretical study on the transport properties and the dynamics when two charge shuttles are coupled through electron tunneling. The nonlinearity involved in this system shows an interesting bistable regime, where the electric current characteristics are of potentially great importance in NEMS applications. An interesting situation arises when the two shuttles are totally symmetric. In this case, through a dynamical symmetry breaking the system produces a net direct electric current. Symmetry-broken electric current under time-periodic perturbation has been an interesting topic of many theories and experiments [6, 7] and classical dynamics which has been used for single shuttle [8].

We start with the formalism of single electron tunneling [9] and classical dynamics which has been used for single charge shuttle [8]. The drain lead is in the left side of the source lead where the ac voltage $V(t) = V_0 \sin (\omega t)$ is applied to the source compared to the drain, see Fig. 1. The capacitance is supposed to be not sensitive to the displacement while the resistance is a function of displacements $x_1$ and $x_2$:

$$R_1(x_1) = R_1(0)e^{x_1/\lambda},$$

$$R_2(x_2 - x_1) = R_2(0)e^{(x_2 - x_1)/\lambda},$$

$$R_3(x_2) = R_3(0)e^{-x_2/\lambda}.\tag{1}$$

Here, $\lambda$ is a phenomenological tunneling length. When the mutual capacitance of the $j$-th junction is $c_j$, the capacitance matrix is constructed as $C_{kl} = c_k + c_{k+1} - \epsilon c_k + c_{k+1}$, $-\epsilon$, for $l = k; k = l + 1, l = k - 1$, otherwise, respectively. The internal charging energy is given by $\epsilon(Q_1, Q_2) = 1/2 \sum_{k,l} (C^{-1})_{kl}Q_kQ_l$. The energy loss $E_j$ of the $j$-th junction is $E_1 = \frac{4\pi\epsilon_0}{c_1}eV + \epsilon(Q_1, Q_2) - \epsilon(Q_1 + e, Q_2)$, $E_2 = \frac{4\pi\epsilon_0}{c_2}eV + \epsilon(Q_1, Q_2) - \epsilon(Q_1 + e, Q_2 - e)$, and $E_3 = \frac{4\pi\epsilon_0}{c_3}eV + \epsilon(Q_1, Q_2) - \epsilon(Q_1, Q_2 + e)$ with the total capacitance $c_{tot}$. The rate of the tunneling from left to the right at the $j$-th junction at low temperature and environmental impedance is

$$\Gamma_{n_1,n_2}^{(j)} = \frac{1}{e^2R_j}E_j(V, Q_1, Q_2)\Theta[E_j(V, Q_1, Q_2)],\tag{2}$$

where the island charges $Q_1, Q_2$ are integer of $-e$: $Q_i = -n_ie$. By replacing $V, Q_1, Q_2$ with $-V, -Q_1, -Q_2$ in the right-hand side of the above equation, one can get $\Gamma_{n_1,n_2}^{(j)}$.

Now we come to the equations of motion. The time evolution of the probability $P_{n_1,n_2}$ for the island charges $Q_1 = -n_1e$, $Q_2 = -n_2e$ is given by the following rate equation

$$\frac{dP_{n_1,n_2}}{dt} = \Gamma_{n_1,n_2}^{(1)}P_{n_1,n_2} + \Gamma_{n_1+1,n_2}^{(1)}P_{n_1+1,n_2} + \Gamma_{n_1,n_2+1}^{(2)}P_{n_1,n_2+1} + \Gamma_{n_1+1,n_2+1}^{(2)}P_{n_1+1,n_2+1}$$

FIG. 1: A schematic figure of the double charge shuttle.

\begin{align*}
\Gamma_{n_1,n_2}^{(1)} & = \frac{1}{e^2R_j}E_j(V, Q_1, Q_2)\Theta[E_j(V, Q_1, Q_2)], \tag{2} \\
\Gamma_{n_1+1,n_2}^{(1)} & = \frac{1}{e^2R_j}E_j(V, Q_1, Q_2)\Theta[E_j(V, Q_1, Q_2)], \\
\Gamma_{n_1,n_2+1}^{(2)} & = \frac{1}{e^2R_j}E_j(V, Q_1, Q_2)\Theta[E_j(V, Q_1, Q_2)], \\
\Gamma_{n_1+1,n_2+1}^{(2)} & = \frac{1}{e^2R_j}E_j(V, Q_1, Q_2)\Theta[E_j(V, Q_1, Q_2)],
\end{align*}
FIG. 2: (a) The symmetry-broken DC current in units of $I_0 = V_0 / R$ vs. frequency of the applied AC voltage. The solid line refers to the result from the full calculations mentioned in the text and the dashed line refers to the result from the simplified calculation in the adiabatic limit. The parameters are fixed to $c = 100$ aF, $R = h / e^2$, $\lambda = 20$ nm, $L = 500$ nm, $\omega_0 = 50$ MHz, $\gamma = 0.025 \omega_0$, $m = 1.1 \times 10^{-21}$ Kg, and $V_0 = 10.8$ mV. (b) The corresponding stroboscopic plot of $x = x_1 - x_2$ obtained for a fixed phase of the oscillating voltage.

$$\hat{I}^{(2)}_{n_1+1,n_2-1} P_{n_1+1,n_2-1} + \hat{I}^{(3)}_{n_1,n_2-1} P_{n_1,n_2-1} + \hat{I}^{(3)}_{n_1,n_2+1} P_{n_1,n_2+1} - \sum_{j=1}^{3} \left( \hat{I}^{(i)}_{n_1,n_2} + \hat{I}^{(j)}_{n_1,n_2} \right) P_{n_1,n_2}.$$  

At low temperatures the fluctuation of the displacement $x,\bar{x}$ are negligible compared to the charge fluctuations. While the charge fluctuations are important to the noise properties, we suppose $1/T$ be much smaller than the typical time scale of displacement and investigate the mechanical motions using the mean island charge $\langle Q_i(t) \rangle = -e \langle n_i(t) \rangle = -e \sum_{n_1,n_2} n_i P(n_1,n_2,t)$. The island charges experience the force produced by the electric field $-V(t)/L$:

$$\dot{x}_i + \gamma_i \dot{x}_i + \omega_0^2 x_i = -\frac{V(t)}{m_i L} \langle Q_i(t) \rangle, \quad i = 1, 2 \quad (3)$$

where $L$ is the source-drain distance and $\gamma_i, \omega_0$ denote the friction constant and the natural angular frequency of $i$-th shuttle. Note that the resonators are modelled as linear oscillators. The nonlinearity of the full system comes from the coupling via tunneling. The electric current from the source in the right-hand side to the drain in the left-hand side is computed as

$$I(t) = e \sum_{n_1,n_2} \left( \hat{I}^{(1)}_{n_1,n_2} - \hat{I}^{(1)}_{n_1,n_2} P_{n_1,n_2}(t) \right). \quad (4)$$

In the following we will consider a symmetric configuration: $\omega_0 = \omega, \gamma_i = \gamma, m_i = m, R_1(0) = R_3(0) = 0.5 R_2(0) \equiv R$, and $c_1 = c_3 = 2 c_2 \equiv c$. In Fig. 2(a), we plot the time-averaged current $I_{DC} = \frac{2}{\pi} \int_0^{2\pi} I(t) dt$ from the configuration of the adiabatic limit. Therefore we may rely on the adiabatic approach for the analysis of the bistability.

In the adiabatic limit the electronic relaxation is much faster than the mechanical motion, i.e.

$$\omega R \epsilon , \omega_0 R \epsilon \ll 1. \quad (5)$$

In this case, a classical circuit analysis of Fig. 1 on the charges $q_j$ accumulated in each capacitor $c_j$ gives

$$\frac{q_1}{R_1 c_1} - \frac{q_2}{R_2 c_2} = -\frac{q_2}{R_2 c_2} - \frac{q_3}{R_3 c_3} = 0 \quad (6)$$

From the solutions of the above linear equations, the net charges of each islands $Q_1 = q_1 - q_2, Q_2 = q_2 - q_3$ are simply given by

$$Q_1 = V c e^{x_1/\lambda} - e^{x_2-x_1}/\lambda, \quad Q_2 = V c e^{x_1/\lambda} + 2 e^{x_2-x_1}/\lambda + e^{-x_2/\lambda} \quad (7)$$

Plugging these into the equation of motion for the mechanical degree of freedom 8 gives the equation of motion for the center of mass coordinate

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \frac{e V(t)^2}{2 m L} \frac{e^{x_1/\lambda} - e^{-x_2/\lambda}}{e^{x_1/\lambda} + 2 e^{-x_2/2\lambda} + e^{-x_1/\lambda}} \quad (9)$$

where $x = x_1 - x_2$ is the relative coordinate. Clearly, $X = 0$ is a solution, in agreement with our numerical finding that the center of mass is not moving. Exploiting this fact, the equation of motion for the relative coordinate $x$ can be derived as

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \frac{e V(t)^2 \sin^2 \omega t}{m L} \tanh \frac{3x}{4\lambda} \quad (10)$$

negative or positive depending on the initial conditions. The initial conditions are specified by the initial position $x_1, x_2$ and the velocities $\dot{x}_1, \dot{x}_2$ at a given starting time. In the regime of zero current all initial conditions are attracted to an unique stable asymptotic solution (the so-called attractor). In the nonzero current case, two such attractors coexist and cause a dynamical symmetry breaking.

The global behaviour of the attractors can be conveniently represented on a stroboscopic section (a special case of a Poincaré section 9) defined by a fixed value of the phase of the driving voltage. Fig. 2(b) shows the stroboscopic section at a fixed phase of the applied voltage. We find the center of mass coordinate does not move; $X = (x_1 + x_2)/2 \approx 0$ for all frequencies $\omega$. Meanwhile in the regime of nonzero DC current we find two symmetry-related solutions for the relative coordinate $x = x_1 - x_2$.

We may get further insight by investigating the adiabatic limit of the system. In Fig. 2 we plot the DC current and relative coordinates computed from the adiabatic approach using dotted lines. One can notice that the full numerical results are quite close to those obtained in the adiabatic limit. Therefore we may rely on the adiabatic approach for the analysis of the bistability.
From the above equation one can see that \( x = 0 \) is a trivial solution. However, this solution can be unstable as we will prove in the following. Note that if a nontrivial solution of \( x(t) \) exists then \(-x(t)\) is also a solution. This is the pair of bistable solutions. Since the equation is invariant under the time-translation operation \( t \rightarrow t + \pi / \omega \), a periodic solution should satisfy \( x(t + \pi / \omega) = \pm x(t) \). As will be shown later, this parity is important for the nonzero DC current.

The electric current in the adiabatic limit can be expressed as \( I(t) = q_1(t)/[R_1(x) c_1] = V(t)/[R_1(x) + R_2(x_1, x_2) + R_3(x_2)] \). Therefore the time-averaged DC current reads

\[
I_{DC} = I_0 \frac{\omega}{4\pi} \int_{t_0}^{t_0+2\pi/\omega} \sin \omega t \frac{\sin \omega t}{e^{\pi t/2\lambda} + e^{-\pi t/2\lambda}} dt, \quad (11)
\]

where \( I_0 = V_0/R \). The dashed line in Fig. 2(a) was obtained using the above formula which also shows a clear bistability.

Now we are going to show that the origin of the symmetry-broken current and the bistability is parameteric instability. By linearizing the term \( \tan h (3x/4\lambda) \) in the right hand side of Eq. (10), we get

\[
\ddot{x} + \gamma \dot{x} + \Omega_0^2 \left[ 1 - \frac{\mu^2}{1 + \mu^2} \cos(2\omega t) \right] x = 0, \quad (12)
\]

where \( \mu = \frac{V_0}{\omega_0} \sqrt{3} \frac{\lambda}{2\Omega_0} \) and \( \Omega_0 \) is the dressed harmonic frequency of the relative motion;

\[
\Omega_0 = \omega_0 \sqrt{1 + \mu^2} = \sqrt{\omega_0^2 + \frac{3\lambda V_0^2}{8\lambda m L}}. \quad (13)
\]

Equation (12) is called a damped Mathieu equation which is a paradigm for studying parametric resonance \[11\]. The stability analysis in Ref. [10] up to second order of \( M \) shows that the motion is unstable in the interval \( \omega_- < \omega < \omega_+ \) where

\[
\omega_\pm = \Omega_0 \left( 1 \pm \frac{1}{2} \sqrt{M^2 - \gamma^2/\Omega_0^2 + \frac{11}{16} M^2} \right), \quad (14)
\]

with \( M = \frac{\pi}{2(1 + \mu^2)} \). This interval is called principal instability interval. Obviously, the interval has finite width only if \( M > \gamma/\Omega_0 \), i.e. the strength of the driving, \( V_0 \), must be sufficiently large in order to get parametric instability.

From the above analysis and Fig. 2(b) we conclude that when entering the principal instability interval from the right hand side the unique attractor turns into an unstable solution (a repeller) thereby creating two new attractors. This scenario leading to bistability is termed a supercritical pitchfork bifurcation. The bifurcation occurring when entering the principal instability interval from the left hand side is different which can be seen from the abrupt change of the value of \( x \). Here we have three attractors and two repellers (not shown). The repellers and the central attractor (\( x = 0 \)) merge in a subcritical pitchfork bifurcation creating a repeller at \( x = 0 \).

In Fig. 3 we plot the phase diagram of \( \mu \) vs. \( \omega/\omega_0 \) which indicates the locations of the bistable regimes computed from Eq. (10). The dotted line denote the analytic results in Eq. (14) from the linearized equation (12). The reasonable agreement of the parameters showing the instability confirms that the parametric amplification causes the instability in the system. Beside the principal instability region there are higher-order regions in which the ratio of the frequency of the oscillators and the applied voltage is mode-locked to \( p = 2, 3, \ldots \). These regions, and also the principal instability region, are called Arnol’d tongues \[11\].

The second interval of instability denoted by \( p = 2 \) in Fig. 3 arise from second harmonics of the system. The analytic formula for this region from the stationary solutions in Ref. [11] gives

\[
\omega_\pm = \frac{1}{2} \Omega_0 \left( 1 + \frac{5}{12} M^2 \pm \frac{1}{8} \sqrt{M^4 - (4\gamma/\Omega_0)^2} \right). \quad (15)
\]

The higher order bistable regions are found in our numerical calculations. The center of the intervals in each bistable regions are located where

\[
\omega \approx \frac{\Omega_0}{p}; \quad p = 1, 2, 3, \ldots. \quad (16)
\]

The main characteristics of the each bistable region is that the (unharmonic) frequency of the relative motion is given by \( p \omega \) even though there is a mismatch between the natural harmonic frequency and the frequency of the voltage, which is called mode-locking in the field of nonlinear dynamics \[6\]. In Fig. 4 we plot the time series
of the relative coordinate \( x \) for various frequencies corresponding to different bistable regimes. One can clearly see the \( p \)-th order mode-locking. For instance, in spite of the large mismatch between \( \omega \) and \( \omega_0 \) when \( p = 1 \) (\( \omega = 1.45\omega_0 \)) the oscillation frequency is clearly given by \( \omega \).

It is important to note that the rectified DC current arises only when \( p \) is an odd number of integer. When \( p \) is even, the periodic solution \( x(t) \) has even parity i.e. \( x(t+\pi/\omega) = x(t) \). In this case the integration in Eq. (11) from \( t_0 \) to \( t_0 + \pi/\omega \) is cancelled by the integration from \( t_0 + \pi/\omega \) to \( t_0 + 2\pi/\omega \).

One may ask whether the parametric instability can cause symmetry breaking already in a single shuttle system. When we write the tunnel resistances as \( R_1(x) = R(0)e^{+x/\lambda} \) and \( R_2(x) = R(0)e^{-x/\lambda} \) where \( x \) is the coordinate of the shuttle, the equation of motion is given by \( \ddot{x} + \gamma \dot{x} + \omega_0^2 x = -\frac{eV_0^2}{m}\sin^2 \omega_0 t \tanh \frac{\pi}{\lambda} \) similar to Eq. (10). Therefore, in the sense of the mechanical motion, the parametric resonance gives rise to the bistability and the bifurcation diagram is quite similar to Fig. 6. However, \emph{the single shuttle systems does not allow a symmetry-broken DC current}. The absence of the DC current in the symmetric single shuttle is clear from the time-averaged current formula of the system

\[
I_{\text{DC}} = I_0 \frac{\omega}{4\pi} \int_{t_0}^{t_0+2\pi/\omega} \frac{\sin \omega t}{\cosh x/\lambda} dt. \tag{17}
\]

Note that the symmetry of the periodic solution \( x(t + \pi/\omega) = \pm x(t) \) always ensures \( \cosh |x(t + \pi/\omega)/\lambda| = \cosh |x(t)/\lambda| \) confirming that the above integral is zero.

In experimental systems, the charge and displacement fluctuations exist due to the discreetness of charges and finiteness of temperature. Noise properties of two colloidal particles in DC source-drain bias have been numerically investigated in Ref. 12 where the shot noise produces random telegraph noise. The noise properties in the presence of oscillating source-drain voltage are expected to contain interesting information on the mechanical properties, which is currently under study. For instance, the shuttles are expected to show enhanced noise power in the bistable regimes we studied in this work.

Our results are robust against the finite temperature effect which modifies the tunneling rate in Eq. (2). This is because the dynamical symmetry breaking appears as a classical effect. While the perfect left/right symmetry does not exist when the tunnel resistances differ by multiple \( 5 \) or \( 10 \), we find the effects are still visible from the enhancement of the net current. The enhanced net current is also visible when the resonance frequencies and tunneling coefficients differ by 10 percents. This robustness comes from the nonlinear phenomenon, \emph{mode-locking}, where the mechanical motions are locked to the driving voltage in spite of small variations of the system parameters. One may also note that the tunneling length \( \lambda \) enters the instability condition through \( \mu \), so the net current can exist in a reasonable range of \( \lambda \) if \( \mu \) and \( \omega \) belongs to the Arnol’d tongue.

In summary, the transport through two tunnel-coupled symmetric charge shuttles has been studied. We found that the oscillation frequencies of the two shuttles are mode-locked to the applied oscillating voltage. Moreover, we observed a dynamical bistability which allows for non-zero electric currents. The origin of this phenomenon has been traced back to parametric instability induced by the nonlinear coupling of the mechanical and electrical degree of freedom.

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