Parametric excitation of dc current in a single-dot shuttle system via spontaneous symmetry breaking

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We investigate theoretically the dynamics of a spatially symmetric shuttle system subjected to an ac gate voltage. We demonstrate that in such a system parametric excitation gives rise to mechanical vibrations when the frequency of the ac signal is close to the eigenfrequency of the mechanical subsystem. These mechanical oscillations result in a dc shuttle current in a certain direction due to spontaneous symmetry breaking. The direction of the current is determined by the phase shift between the ac gate voltage and the parametrically excited mechanical oscillations. The dependence of the shuttle current on the dc gate voltage is also analyzed.

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Some years ago, a novel form of electron transport—a shuttle mechanism—based on the mechanical vibrations of a metallic nanoparticle coupled to two electrodes via elastic molecular links was proposed in Ref. 1. Since then, the shuttle phenomenon has been a subject of intensive experimental and theoretical research.[2–7]

The main feature of the orthodox shuttle phenomenon is that a constant potential difference, applied between two fixed electrodes, leads to a dynamical instability that causes the metal nanoparticle to oscillate. As a consequence, a dc current through the system, induced by the voltage drop between the electrodes, becomes proportional to the frequency of the mechanical oscillations[1]. The idea of shuttle phenomena was also extended to the quantum realm[8–11].

Nanoelectromechanical shuttle systems have been also studied in the regime of ac excitation and several interesting effects on the transport properties and the dynamics of the shuttle system have been found[12–16]. In particular, a shuttle structure driven by a time-dependent bias voltage has been considered in Refs. 17 and 18. It was shown that in case of *asymmetric* configuration such a setup can act as a rectifier, where the intensity of the dc current depends on the ratio between the frequency of the external oscillating voltage and the eigenfrequency of the mechanical subsystem. Current rectification was also conjectured by Ahn *et al.*[19] (and experimentally verified by Kim *et al.*[20]) for the case of a symmetric double-shuttle structure. They attributed current-rectification phenomena to spontaneous symmetry breaking in the system caused by parametric instability. One of the conclusions of this work is that dynamical symmetry breaking in single shuttle systems does not lead to a dc current. Parametric excitation of nanoelectromechanical systems (NEMS) has been also considered in Refs. 21–23.

In the present work, we investigate the possibility to generate a shuttle dc current, rather than rectifying current, in a completely *symmetric* single-dot shuttle system. We demonstrate that, in this scheme, despite the lack of a bias voltage, a shuttle dc current can still be detected. This charge transport is achieved by applying an ac voltage to a gate electrode which controls the electronic population of a metallic island and, in this form, also the stiffness of the resonator resulting in a parametric mechanical instability at the resonant frequency. This constitutes a new archetype of electron shuttle in which the symmetry breaking effect (direction of the shuttle transportation) does not rely on the presence of any bias voltage. In the phenomena under consideration, the shuttle current is controlled by the phase shift between the mechanical vibrations and gate voltage oscillations. We will show that in this scenario, two different values of the phase shift, which differ from each other by π[24], can correspond to a regime of sustained oscillations. The occurrence of these values for the phase shift depends, in particular, on the initial conditions and, as a result, spontaneous symmetry breaking takes place.

To describe the new shuttling mechanism, we consider a system schematically depicted in Fig. 1, where a single-level quantum dot (D) is connected via elastic links to the left (L) and right (R) electrodes. The characteristic distance between the electrodes and the dot at equilibrium position is d. In this setup the dot is acting as a nano-oscillator, and the deviation of the dot from its equilibrium position is denoted $x(t)$. Both electrodes are grounded, i.e., $V_L = V_R = 0$, while a signal $V_G = V_G^{\rm st} + V_G^{\rm ac}\cos(\omega_G t)$ is applied to the gate (G).

To analyze the electromechanical phenomena in such a structure, in the simplest approximation, we describe the dynamics of the central island by Newton's equation,

$$\ddot{x} + Q^{-1}\omega_0\dot{x} + \omega_0^2 x = \frac{\alpha}{m}e^2 n(t)x. \tag{1}$$

Here, m is the mass, ω_0 is the eigenfrequency, and Q is the quality factor of the oscillator. In Eq. (1), the parameter $\alpha = [1/(2C^2(0))]\partial^2 C(x)/\partial x^2|_{x=0}$, where $C(x)$ is the effective capacitance of the dot is used. We consider the symmetric situation $C(x) = C(-x)$ and one can estimate $\alpha \approx d^{-3}$. Note that, in contrast to Refs. 17–20, there is no force acting on the grain if it is in equilibrium position. The population of the dot $n(t) = 0,1$ is controlled by the stochastic evolution of the charge.

We focus on the case in which the mechanical vibration frequency of the dot is very low in comparison to the tunneling rates between the quantum dot and the electrodes and the electric force is much lower than the mechanical one, $\alpha e^2/m\omega_0^2 \equiv \epsilon \ll 1$. Under such conditions, the force generated by the stochastic variable $n(t)$ can be taken into

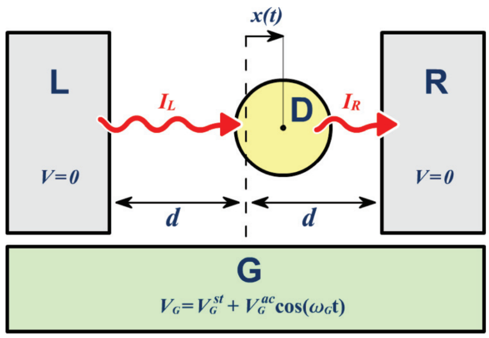

FIG. 1. (Color online) Schematic diagram of the three-terminals shuttle device investigated in this work. A quantum dot D can oscillate between two grounded metallic leads L,R. The dot is capacitevely coupled to a gate electrode G, to which a voltage V_G is applied. Electron tunneling takes place between the dot and the leads. I_L and I_R are the currents between the left and right leads L,R and the dot D.

account only on average by substituting in Eq. (1) its mean value $\langle n(t)\rangle = P(t)$. The variable $P(t)$ represents the probability of finding one electron in the quantum dot at time t. As a consequence, the electronic state of the central island can be described in terms of this probability through the following master equation:

$$\dot{P} = [\Gamma_L(x) + \Gamma_R(x)](f(x,t) - P). \tag{2}$$

Here, the position-dependent tunneling rates between the left or right electrodes and the dot are $\Gamma_{L,R}(x) = \Gamma_0 e^{\mp x/\lambda}$, with λ the tunneling length, and $f(x,t) = f(E_D(x,t)) = [1 + e^{(E_D-\mu)/k_BT}]^{-1}$ is the Fermi-Dirac thermal distribution, where μ is the chemical potential of the leads. The energy of the electron inside the dot is $E_D = \varepsilon_\alpha + E_C$, where ε_α is the energy associated with space quantization and $E_C(x,t) = e^2/2C(x) - e\beta V_G(t)$ is the electrostatic energy, with $\beta \approx 1$ being the transmission coefficient. Finally, considering $\mu = \varepsilon_\alpha + e^2/2C(0)$ and small displacements of the dot, $x \ll d$, we can rewrite $E_D(x,t) - \mu = -(\alpha/2)e^2 n(t) x^2 - eV_G(t)$.

The variation in time of the number of electrons in the leads depends on the applied oscillating voltage $V_G(t)$ and on the position of the vibrating dot $x(t)$. Therefore, the instantaneous current through the system, averaged over fast fluctuations due to the discrete nature of charge tunneling, is[1,17]

$$\frac{I_a(t)}{e} = [\Gamma_L(x(t)) - \Gamma_R(x(t))]\{f(x(t),t) - P(t)\}, \tag{3}$$

and the dc component of this instantaneous current can be calculated as

$$\begin{aligned}\frac{I_{\rm dc}}{e} &= -\lim_{T\to\infty}\frac{2\Gamma_0}{T}\int_0^T dt \sinh\left(\frac{x(t)}{\lambda}\right)[f(x(t),t) - P(t)]\\ &= \lim_{T\to\infty}\frac{1}{T\lambda}\int_0^T dt \frac{\dot{x}(t)P(t)}{\cosh^2(x(t)/\lambda)}.\end{aligned} \tag{4}$$

Here, in writing Eq. (4) we use Eq. (2). From this expression one can observe that the dc current between the leads is defined by the correlations between the velocity and the population of the dot. To find these correlations one should analyze the dynamical system described by Eqs. (1) and (2).

We perform a perturbative analysis of these equations exploiting the small values of parameters $\omega_0/\Gamma_0 \simeq \omega_G/\Gamma_0 \ll 1$ and $\epsilon, Q^{-1} \ll 1$. In doing so, we take

$$P(t) = f(x,t), \tag{5}$$

in the leading order of the parameter ω_G/Γ_0. Substituting this relation in Eq. (1), we obtained a nonlinear and time-dependent equation for x,

$$\ddot{x} + Q^{-1}\omega_0\dot{x} + \omega_0^2 x = \epsilon\omega_0^2 f(x,t)x, \tag{6}$$

where $f(x,t)$ is a periodic function of time. From this equation, one can find that the mechanical subsystem may experience a parametric instability if $|\omega_G - \omega_0| \ll \omega_0$, when considering the second harmonic term in the Fourier expansion of $f(x,t)$.[25]

Note that Eqs. (2) and (6) are invariant under the transformation $[x(t),P(t)] \to [-x(t),P(t)]$, and it is clear that the only static stationary solution $x(t) = 0$ is invariant under this transformation. If mechanical excitation takes place, it will result in, at least, two different stable periodic (with period $T_G = 2\pi/\omega_G$) solutions: $[x_{st}(t),P_{st}(t)]$ and $[\tilde{x}_{st}(t),\tilde{P}_{st}(t)] \equiv [-x_{st}(t),P_{st}(t)]$. From Eq. (4), it immediately follows that these two stationary regimes generate shuttle currents in opposite directions. Which regime arises from the ac-voltage switching will depend on spontaneous forces accompanying transient processes.

To analyze the regime of parametric excitations one can use the ansatz

$$x(t) = A(t)\cos(\omega_G t + \chi(t)), \tag{7}$$

where the amplitude $A(t)$ and $\chi(t)$ (the phase shift between the mechanical and the gate voltage oscillations) are supposed to be slowly varying functions of time: $\dot{A}/A, \dot{\chi} \simeq \epsilon\omega_G, \omega_G/Q$.

To analyze the dynamics of the amplitude $A(t)$ and the relative phase shift $\chi(t)$, it is convenient to introduce the following dimensionless variables: $\tau = \omega_G t$, $\xi = x/\lambda$, and $E = A^2/2\lambda^2$. Then, after substituting the ansatz given by Eq. (7) into Eq. (6) and averaging over the fast oscillations,[26] one obtains the following coupled differential equations for $E(\tau)$ and $\chi(\tau)$:

$$\frac{\partial E}{\partial \tau} = \frac{\partial \mathscr{H}}{\partial \chi} - Q^{-1}E, \tag{8a}$$

$$\frac{\partial \chi}{\partial \tau} = -\frac{\partial \mathscr{H}}{\partial E}. \tag{8b}$$

Here, $\mathscr{H}$ is the generating Hamiltonian function,

$$\begin{aligned}\mathscr{H}(E,\chi) = (\tilde{\omega}_0 - 1)E + \frac{\epsilon}{2\eta\pi}\int_{-\pi}^{\pi} d\theta\\ \times \ln\left\{1 + e^{[\eta E\cos^2(\theta) + \nu_{\rm st} + \nu_{\rm ac}\cos(\theta-\chi)]}\right\},\end{aligned} \tag{8c}$$

with $\tilde{\omega}_0 = \omega_0/\omega_G$, $\eta = \alpha e^2\lambda^2/2k_BT$, $\nu_{\rm st} = eV_G^{\rm st}/k_BT$, $\nu_{\rm ac} = eV_G^{\rm ac}/k_BT$. Different stationary oscillation regimes of the dot (labeled with subscript i) are defined by the different stationary solutions of Eqs. (1), i.e., $E_i = $ const, $\chi_i = $ const.

In order to find the dc current corresponding to a given stationary regime of oscillations, $2I_{\rm dc}(E_i,\chi_i) \equiv I_i e\omega_G$, we substitute Eq. (5) and Eq. (7) into the expression for the dc current given by Eq. (4). As a result, it reads

$$I_i = \int_{-\sqrt{2E_i}}^{\sqrt{2E_i}} \frac{d\xi}{\cosh^2(\xi)} \times \frac{\sinh[b_i \upsilon_i(\xi)\sin(\chi_i)]}{\cosh[a_i(\xi)] + \cosh[b_i \upsilon_i(\xi)\sin(\chi_i)]}, \tag{9a}$$

with

$$a_i(\xi) = \eta\xi^2 + \nu_{st} + b_i\xi\cos(\chi), \quad b_i = \nu_{ac}/\sqrt{2E_i}. \tag{9b}$$

Here, $\upsilon_i(\xi)$ is the modulus of the dot velocity as a function of its position given by $\upsilon_i(\xi) = \sqrt{2E_i - \xi^2}$. From Eqs. (9), we can conclude that the dc current solely exists at nonzero amplitude of oscillation, while its sign (symmetry breaking signature) is controlled by the phase difference χ_i, $\mathrm{sgn}(I_i) \propto \sin(\chi_i)$.

To proceed further, we consider the case of exact resonance,

$$\omega_G = \omega_0\left\{1 + (\epsilon/4\pi)\int_{-\pi}^{\pi} d\theta[e^{-\nu_{st}} + e^{\nu_{ac}\cos(\theta-\chi)}]^{-1}\right\}. \tag{10}$$

In Eq. (10), we have taken into account the renormalization of the frequency due to Coulomb interactions, which is proportional to ϵ.

In this situation, the solution $E = 0$ is a stationary point. However, in the frame of a perturbative analysis for small E, from Eqs. (1) one finds that this solution is unstable (parametric mechanical instability) if the condition,

$$\frac{1}{Q\epsilon} \leqslant \frac{\sin(2\chi_i)}{4\pi}\int_{-\pi}^{\pi} d\theta \cos(2\theta)\tanh\left(\frac{\nu_{st} + \nu_{ac}\cos(\theta)}{2}\right), \tag{11}$$

is fulfilled. In the above instability criterion, χ_i is defined through the relation $\mathscr{H}(E,\chi_i)/\partial E|_{E=0} = 0$.

From Eq. (11) one can find that there is a critical amplitude for the ac voltage, $\nu_{ac}^*(\nu_{st})$, above which the system becomes excited. Moreover, if the static voltage tends to 0, $\nu_{st} \to 0$, the critical ac voltage becomes infinite, $\nu_{ac}^* \to \infty$.

This threshold ac voltage is shown in Fig. 2, where (red) bars correspond to results obtained from numerical integration of Eqs. (1) and (2), while (blue) curves refer to Eq. (11).

Due to the periodicity of the generating Hamiltonian function, $\mathscr{H}(E,\chi) = \mathscr{H}(E,\chi+\pi)$, the stationary solutions of Eq. (1) come in pairs: to any solution $S_i = \{E_i,\chi_i\}$ corresponds a conjugated solution $\bar{S}_i = \{E_i,\chi_i+\pi\}$. This

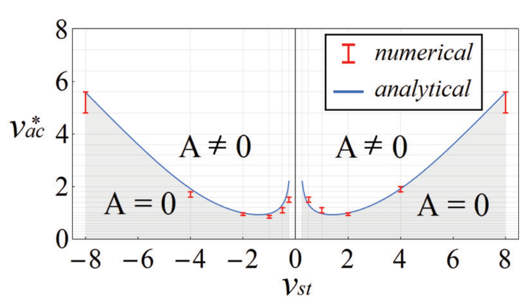

FIG. 2. (Color online) Threshold ac voltage ν_{ac}^* as a function of static dc voltage ν_{st}. The (red) bars correspond to results obtained from numerical integration of Eqs. (1) and (2), while the solid (blue) lines refer to Eq. (11). The plot is calculated for a gold quantum dot of radius $r = 4$ nm and mass $m = 5 \times 10^{-21}$ kg with $\omega_0 = 10$ GHz, $Q = 1000$, $d \sim 2$ nm, $\lambda = 0.1$ nm, $\Gamma_0 = 100$ GHz, $\omega_G = 10$ GHz, and $T = 10$ K. Consequently, $\epsilon = 0.1$, $\alpha = 8.37$, $\tilde{\omega} \sim 1$.

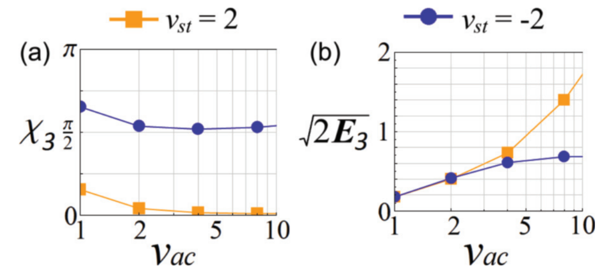

FIG. 3. (Color online) Stationary phase (a) and amplitude (b) of the system as a function of the applied static dc voltages $\nu_{st} = 2$ [(orange) squares] and $\nu_{st} = -2$ [(blue) circles] for different ac voltages ν_{ac}. The phase is almost 0 for the positive dc voltage, while it is nonvanishing for the negative one. As a result, current transport is more feasible at negative dc voltages [see Eqs. (1)]. The plot is calculated for $\epsilon = 0.1$, $\alpha = 8.37$, $\tilde{\omega} \sim 1$.

fact is a clear manifestation of the symmetry properties of Eqs. (2) and (6) discussed above. In the nonexcited regime, i.e., $\nu_{ac} < \nu_{ac}^*(\nu_{st})$, the system defined by Eqs. (1) possesses four formal stationary points: $S_1 = \{0,\pi/4\}$, $S_2 = \{0,3\pi/4\}$, and their conjugates. For $\nu_{st} > 0$, the stationary points $[S_1,\bar{S}_1]$ and $[S_2,\bar{S}_2]$ are stable and unstable, respectively. In the opposite case, $\nu_{st} < 0$, these points exchange stability.

In the regime of oscillations, $\nu_{ac} > \nu_{ac}^*(\nu_{st})$, besides the stationary points $[S_1,\bar{S}_1,S_2,\bar{S}_2]$, two more points, $[S_3 = \{E_3,\chi_3\},\bar{S}_3 = \{E_3,\chi_3+\pi\}]$, appear in the phase diagram. The original stationary points S_1 and S_2 (and their conjugates) become unstable, while the new solutions are stable.

In Fig. 3, the phase shift and amplitude of the stable periodic solution $S_3 = \{E_3,\chi_3\}$ are shown as a function of the applied ac voltage (ν_{ac}) for two static dc voltages: $\nu_{st} = 2$ [(blue) circles] and $\nu_{st} = -2$ [(orange) squares]. From this graph, one can observe that the phase shift and, as a consequence, the dc current [see Eqs. (1)] are almost 0 for the positive dc amplitude. However, the plot indicates that the phase is nearly $\chi \sim \pi/2$ and a nonzero dc current is flowing through the nanostructure for the negative dc voltage.

We also investigated the behavior of the dc current as a function of the applied voltages, $I_3 = I_3(\nu_{st},\nu_{ac})$, and the results are displayed in Fig. 4. From the contour map, the asymmetric behavior of the dc current with respect to the static dc voltage ν_{st} is evident. Therefore, in light of

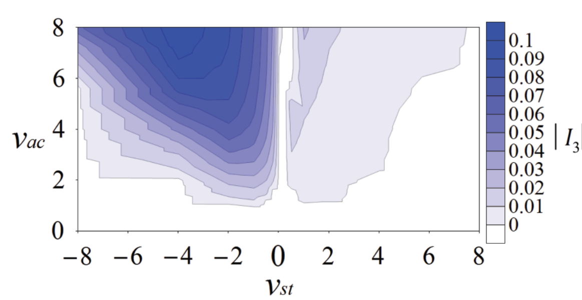

FIG. 4. (Color online) Contour plot of the dc current as a function of the applied voltages, $I_3 = I_3(\nu_{st},\nu_{ac})$. Current through the nanostructure is significant for negative dc voltage values, ν_{st}. In the plot $\epsilon = 0.1$, $\alpha = 8.37$, $\tilde{\omega} = 1$.

the result previously discussed, the values of the applied voltages should be chosen in order to maximize the charge transport, i.e., look for a stationary phase $\chi_3 = \pi/2$; this condition is attainable for negative values of ν_{st} as shown in Fig. 4.

To conclude, we have analyzed the dynamics of a completely symmetric single-dot shuttle structure under the influence of an alternating gate voltage. In this system, we have found that parametric excitation gives rise to two regimes of sustained mechanical oscillations characterized by the same amplitudes but different phases (they differ by π), when the frequency of the ac gate voltage is approximately equal to the mechanical eigenfrequency of the nano-oscillator. These mechanical vibrations result in shuttle transportation of electrons through the nanostructure. We have shown that the two distinct stationary regimes of oscillations generate shuttle currents in opposite directions. Which regime arises from the ac-voltage switching will depend on spontaneous forces accompanying transient processes.

In our considerations we have not taken into account noise forces. Such forces will result in fluctuations of the phase around the stationary values,[27] and infrequent transitions between them. When the amplitude of fluctuations is much lower than π, the switching probability is exponentially low, and the results discussed above are still valid during time intervals less than the characteristic switching time. However, strong fluctuations will lead to transitions between stationary points and, by this, restore the symmetry in the system. A complete study of the noise properties of the considered system is to be discussed elsewhere.

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[27] We would like to emphasize that the amplitude of shot-noise fluctuations at the driving frequency ω_G is low due to the fact $\Gamma_0 \gg \omega_G$ and its contribution is negligible.