Discrete breathers in ac-driven nanoelectromechanical shuttle arrays

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(Received 21 August 2008; accepted 17 November 2008; published online 5 December 2008)

We investigate the dynamics of electrically ac-driven nanoelectromechanical shuttle arrays. The electromechanical coupling enforces long-range interactions. We find multistability regimes upon changing the voltage and frequency. We show that the instability driven by parametric amplification of sinusoidal mechanical waves leads to the creation of spatially localized mechanical oscillations, discrete breathers, and subsequently to an abrupt change in the electrical transport properties. In particular, we find current rectification, which is induced by the excitation of discrete breathers. This is of potential interest and use for nanomechanical sensor application. © *2008 American Institute of Physics*. [DOI: 10.1063/1.3043434]

Nanomechanical resonators have become of interest to a diverse physics community due to their utility for highly sensitive mass sensing as well as signal processing.[1] A nanomechanical charge shuttle,[2] which is basically a charge carrying mechanical resonator, has interesting dynamics due to its coupling to the electrical degrees of freedom.[3] Further, the multistability of interacting pairs of shuttles[4] (double shuttle) is of potential interest for applications of sensitive measurement and signal processing.

It has been shown that the *left-right symmetry* of an ac-driven double shuttle can be spontaneously broken at certain frequencies, which results in the current rectification.[4] This is due to an instability driven by parametric amplification. The amplification is caused by a time-periodic interaction between the shuttles, which is generated by oscillating charges and the driving voltage. Here, we show that the parametric instability in an array of nanomechanical shuttles leads to the formation of *intrinsic localized modes* or *discrete breathers* (DBs).[5–9]

A DB[8,9] is a time-periodic and spatially localized mode in nonlinear lattice systems. DBs exist in diverse physical systems such as photonic crystals,[10] Josephson junction networks,[11] Bose–Einstein condensates in periodic potentials,[12] and micromechanical systems,[13] among others.[14] In the present study, DBs are spontaneously generated due to parametric instability and abruptly change the electric transport properties, which might be useful for the design of small force detectors.

The N shuttles are arranged in a one-dimensional structure, as shown in Fig. 1. The shuttle array might be realized by miniaturization of semiconductor structures[3,15] or can be produced using molecules (nanopeapod).[16] The displacements from the equilibrium positions $x=(x_1,\ldots,x_N)$ are governed by the equations of motion

$$\ddot{x}_j + \gamma\dot{x}_j + \omega_0^2 x_j = -\frac{V(t)}{mL}Q_j, \qquad (1)$$

where γ, ω_0, m, and Q_j denote the friction constant, the frequency, the mass, and the net charge of the jth shuttle. The drain lead is on the left, and the source lead is at distance L to the right, where the voltage $V(t)=V_0\sin(\omega t)$ is applied. We assume that the capacitance c of an individual shuttle does not depend on its displacement x_i. Charges that pass between shuttles experience a tunneling resistance

$$R_j(x_j - x_{j-1}) = R_j(0)e^{(x_j-x_{j-1})/\lambda}, \qquad (2)$$

with $j=1,\ldots,N$ and $x_0=x_{N+1}=0$. Here, λ is a tunneling length beyond which charge transport is suppressed.

Recent techniques for fabrication of shuttle structures[3,15] yield tunneling resistances R of the order of GΩ, junction capacitances c of the order of 10 aF, and the mechanical oscillation frequency ω_0 of the order of 0.1 GHz. Thus the product $Rc\omega_0 \sim 1$ and the shuttle operates at the border of the adiabatic regime where the electronic relaxation is much faster than the mechanical motion. From now on, for the simplicity of the calculation, we will assume the adiabatic regime $Rc\omega_0 < 1$. The full calculations, which do not rely on the adiabatic assumption, show that the adiabatic approximation is qualitatively valid concerning the parametric instability relevant to this work.[4] For the geometry in Fig. 1, it follows $q_j/R_jc = q_{j+1}/R_{j+1}c$ and $V(t)=\sum_{j=1}^{N+1}\frac{q_j}{c}$, where q_j are the charges accumulated in each capacitor. Then, the net charge of each island $Q_j=q_j-q_{j+1}$ satisfies

$$Q_j(x,t) = c[R_j(x_j - x_{j-1}) - R_{j+1}(x_{j+1} - x_j)]I(x,t), \qquad (3)$$

with the current

$$I(x,t) = \frac{V(t)}{\sum_{j=1}^{N+1} R_j(x_j - x_{j-1})}.$$

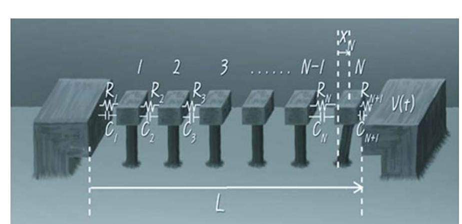

FIG. 1. (Color online) Sketch of N coupled nanoelectromechanical shuttles.

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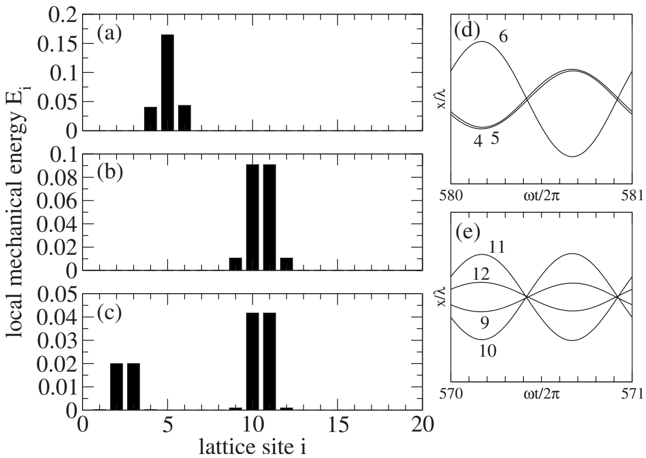

FIG. 2. Mechanical energy of the local oscillators E_i for different initial conditions: (a) single-site breather with total mechanical energy $E=0.248$ and time-averaged current $I_{dc}/I_0=-2.94\times10^{-8}$, where $I_0\equiv V_0/[(N+1)R]$, (b) two-site breather with $E=0.203$ and $I_{dc}/I_0=5.67\times10^{-3}$, and (c) a multisite oscillation with $E=0.126$ and $I_{dc}/I_0=7.35\times10^{-4}$. (d) and (e) show the time evolution of the involved shuttles shown in (a) and (b), respectively. We choose $\omega/\omega_0=1.029$, $L/\lambda=500$, $\eta=V_0\sqrt{c}/(\sqrt{mL\lambda}\omega_0)=0.87$, and $\gamma/\omega_0=0.025$. The unit of energy E is $\frac{1}{2}m\omega_0^2 l^2$.

The dc rectified current is obtained by a time averaging over one period of the ac voltage

$$I_{dc}=\frac{\omega}{2\pi}\int_0^{2\pi/\omega} I(t)dt.$$

We integrate the equations of motion starting with all shuttles close to their rest positions. Depending on the control parameters, this state can be stable or unstable, leading to the formation of new structures. Figure 2 exemplarily depicts some of the outcomes in the multistable regime, which lead to time-periodic and spatially localized oscillations—DBs. In Figs. 2(a)–2(c), we plot the local mechanical energy $E_i=\frac{1}{2}m\dot{x}_i^2+\frac{1}{2}m\omega_0^2x_i^2$ versus lattice site i in units of $\frac{1}{2}m\omega_0^2l^2$, where $l=L/(N+1)$ is the equilibrium distance between two neighboring shuttles. We observe spatially highly localized oscillations. Figures 2(d) and 2(e) show that the dynamics is periodic in time with the same period as and therefore mode locked to the driving voltage.

At some distance from the DB, the shuttles perform small amplitude oscillations. These oscillations, which are unstable in the absence of the DB, are stabilized in its presence due to long-range interactions between the mechanical degrees of freedom, mediated by the electrical current. This follows from Eq. (3) since the net charge Q_j of the jth shuttle is a function of all shuttle displacements.

Single-site breathers do not carry a significant dc current as compared to two-site breathers, see, e.g., Figs. 2(a) and 2(b). This is a natural extension of the finding in Ref. 4 that a symmetric configuration of a pair of shuttles induces a dc current whereas a single shuttle does not.

Let us analyze the parametric instability of the small amplitude oscillations of the array when the displacements are smaller than the tunneling length λ. In that case, the net charge $Q_j=q_j-q_{j+1}$ of the jth shuttle is approximated as

$$Q_j=cV(t)\frac{R_j(x)-R_{j+1}(x)}{\sum_{i=1}^{N+1}R_i(x)}, \tag{4}$$

$$\approx\frac{cV(t)}{\lambda(N+1)}(2x_j-x_{j-1}-x_{j+1}). \tag{5}$$

Then the equations of motion are equivalent to those of one-dimensional coupled harmonic oscillators with time-periodic spring constants

$$\ddot{x}_j+\gamma\dot{x}_j+\omega_0^2x_j+\frac{cV_0^2\sin^2\omega t}{mL\lambda(N+1)}(2x_j-x_{j-1}-x_{j+1})=0. \tag{6}$$

Let us assume periodic boundary condition $x_{j+N}=x_j$ for the convenience of calculations. The equations of motion can be decoupled by introducing normal coordinates y_n, $[n=0,\pm1,\pm2,\ldots,\pm(N/2-1),N/2]$: $x_j=(1/\sqrt{N})\Sigma_n y_n\exp[i(2n\pi/N)j]$.

The normal modes y_n satisfy damped Mathieu equations[4,17]

$$\ddot{y}_n+\gamma\dot{y}_n+\Omega_n^2\left[1-\frac{\mu_n^2}{1+\mu_n^2}\cos(2\omega t)\right]y_n=0, \tag{7}$$

where $\mu_n=\eta\sqrt{2/N+1}\,\sin(n\pi/N)$, $\eta=V_0\sqrt{c}/(\sqrt{mL\lambda}\omega_0)$, and Ω_n is the dressed harmonic frequency for the nth normal mode

$$\Omega_n=\omega_0\sqrt{1+\mu_n^2}=\sqrt{\omega_0^2+\frac{2cV_0^2}{\lambda mL(N+1)}\sin^2\left(\frac{n\pi}{N}\right)}. \tag{8}$$

The principal instability arises in the interval $\omega_-<\omega<\omega_+$,[17] where

$$\omega_\pm=\Omega_n\left(1\pm\frac{1}{2}\sqrt{M_n^2-\gamma^2/\Omega_n^2}+\frac{11}{16}M_n^2\right), \tag{9}$$

with $M_n=\mu_n^2/[2(1+\mu_n^2)]$.

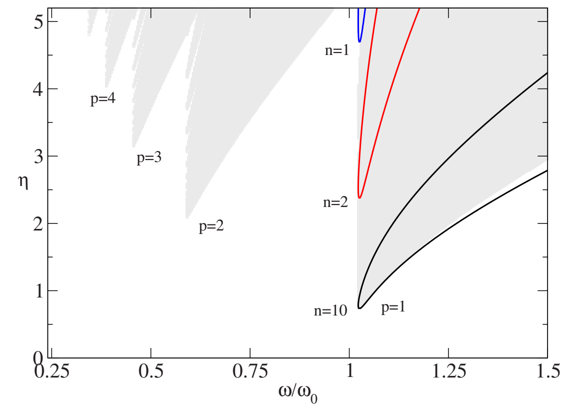

FIG. 3. (Color online) Phase diagram in the plane of the (scaled) amplitude η and the frequency of the applied ac voltage: $N=20$, $\gamma/\omega_0=0.025$. Shaded regions are multistable regions in which DBs emerge. The curves denote the boundary of the unstable regimes given by Eq. (9).

The phase diagram of η and ω/ω_0 in Fig. 3 reveals the existence of different multistable regions. The shaded regions in Fig. 3 correspond to numerical runs of the original equations, which yield instability of the small amplitude state. We plot the border of the multistable regime using Eq. (9) for different n which show good agreement with full numerical data. The collection of the unstable regimes of the Mathieu equation, also coined *Arnol'd tongues*,[18] corresponds to the multistable regimes in Fig. 3. Therefore we confirm that the formation of the DB originates from the instability of driven extended wave in the system. Especially, one can see that the instability for the smallest driving voltage amplitude V_0 is due to the largest wave number $n=N/2$.

The Arnol'd tongues can be characterized by topological numbers $p=1,2,\ldots$ (Fig. 3). It is interesting to note that the low frequency border of the tongues is a straight vertical line where the multistability is independent of the driving voltage and sensitive only to the driving voltage amplitude. The frequency ω_c, defining the left border of the principal multistable regime ($p=1$), is $\omega_c \approx \omega_0 + \gamma$ if $\gamma \ll \omega_0$. This condition can be obtained by imposing the condition $\omega_c = \omega_+ = \omega_-$ in Eq. (9).

The electromechanical shuttle array is characterized by long-range interactions. In case a breather is created, a large amplitude oscillation arises at the core and the total resistance $\Sigma_j R_j$ strongly increases. Then the net charge at the shuttles away from the breather is not given by Eq. (5) but by the much smaller expression

$$Q_j \approx \frac{cV(t)}{\lambda} \frac{(2x_j - x_{j-1} - x_{j+1})}{2\cosh\left(\frac{x_{j_0}(t)}{\lambda}\right)}, \tag{10}$$

where x_{j_0} is the displacement of the jth shuttle, which is at the core of the breather. As seen in Fig. 2, the oscillation amplitude of the core shuttle of the breather is significantly larger than λ, thus the shuttle interactions are strongly suppressed.

In experiments, to initiate the mechanical motion of the single breather, one can impose an oscillating voltage on the gate, which is close to one of the shuttles. It would be difficult to make identical shuttles in the array but it is not a serious problem because our results are robust against the mismatch of the resonance frequency within a few percent ranges (not shown). While we showed the numerical results for $N=20$, a small number of shuttles like $N=6$ are enough to observe the DB. We believe that the predicted Arnold' tongue structure can be observed as observed in coupled mechanical systems.[19]

In summary, we investigated the dynamics of an array of tunnel-coupled charge shuttles. The nonlinear coupling of the mechanical and the electrical degrees of freedom gives rise to a parametric instability and a corresponding multistable regime. In this regime, we demonstrate the existence of DBs, which in turn strongly affect the charge transport through the array of shuttles. We found that small changes in the system parameters give rise to abrupt changes in transport properties if the system is tuned to be close to the multistable regime.

This work was supported by Korea Research Foundation Grant funded by the Korea Government (MOEHRD, Basic Research Promotion Fund) (Grant No. KRF-2006-311-C00311).

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