Spintronics of a Nanoelectromechanical Shuttle

D. Fedorets,* 1 L. Y. Gorelik, 2 R. I. Shekhter, 1 and M. Jonson 1

1Department of Physics, Göteborg University, SE-412 96 Göteborg, Sweden
2Department of Applied Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

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We consider effects of the spin degree of freedom on the nanomechanics of a single-electron transistor (SET) containing a nanometer-sized metallic cluster suspended between two magnetic leads. It is shown that in such a nanoelectromechanical SET (NEM-SET) the onset of an electromechanical instability leading to cluster vibrations and "shuttle" transport of electrons between the leads can be controlled by an external magnetic field. Different stable regimes of this spintronic NEM-SET operation are analyzed. Two different scenarios for the onset of shuttle vibrations are found.

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As the downizing of electronic devices reaches the near molecular scale, the Coulomb forces associated with inhomogeneous charge distributions produced during device operation become comparable with the chemical forces that hold the device together. Consequently, the spatial configuration of a device may well change dynamically during its operation. This inherent feature of nanoelectronics can be turned into an advantage by designing the devices with the mechanical degrees of freedom in mind; this is the scope of nanoelectromechanics and the basis for nanoelectromechanical systems (NEMS) [1].

A pronounced nanoelectromechanical phenomenon — electron transport by means of a nanoelectromechanical "shuttle" mechanism — has recently been predicted to occur in certain NEMS systems as a result of a bias voltage-induced nanoelectromechanical instability [2]. The most suitable device for the experimental observation of this phenomenon is a nanoelectromechanical single-electron transistor (NEM-SET). A NEM-SET is a single-electron transistor (SET) with a movable central island whose center-of-mass motion is confined by some potential. Experimental studies of NEM-SET devices can be found in Refs. [3, 4, 5]. They have also been extensively investigated theoretically [6, 7, 8, 9, 10].

Another rapidly developing branch of condensed matter physics is spintronics [11], which deals with devices whose functionality depends on the control and manipulation of the spin rather than the charge of electrons. A recent development of great interest in this context is the demonstration of a magnetic hybrid nanostructure consisting of a single C_{60}-molecule placed between two ferromagnetic electrodes [12]. The possibility to manipulate the spin of mechanically shuttled electrons in a molecular NEM-SET of this kind brings about an exciting opportunity to trigger nanomechanical vibrations in the THz range by means of a weak external magnetic field much smaller than the magnetic anisotropy fields in the leads. This Letter is devoted to exploring this very phenomenon. We will show that the spin-dependent tunneling of electrons between differently polarized leads results in a strong sensitivity to an external magnetic field of the nanoelectromechanical instability that is responsible for the shuttling. Depending on the magnitude of the magnetic field two different scenarios for the onset of nanoelectromechanical shuttling are possible when the electrical field between the leads reaches its critical value. This demonstrates the interesting possibility to develop spintronics in the context of NEMS devices.

We will consider a NEM-SET with fully spin-polarized magnetic leads [12]. All electrons in the left lead are assumed to have spins pointing up while in the right lead all spins are pointing down. The movable central island has a single electron energy level, which is spin-degenerate in the absence of a magnetic field. A symmetric bias voltage is applied, resulting in an electric field $\mathcal{E}$ between the leads. The external magnetic field $B$ is oriented perpendicular to the direction of the magnetization in the leads. We consider a symmetric coupling to the leads, in which the spin polarization in the leads does not contribute to the magnetic field on the island.

The Hamiltonian used to describe our system,

$$H = \sum_{\alpha,k} \epsilon_{\alpha,k} a_{\alpha,k}^\dagger a_{\alpha,k} + \sum_{\alpha,k} T_\alpha(X) \left[ a_{\alpha,k}^\dagger c_\alpha + c_\alpha^\dagger a_{\alpha,k} \right] + \left[ e_0 - e\mathcal{E}X \right] \sum_{\alpha} c_{\alpha}^\dagger c_{\alpha} - \left( g\mu_B B/2 \right) \left[ c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow \right] + U c_\uparrow^\dagger c_\upsilon^\dagger c_\downarrow + H_{osc}$$  \hspace{1cm} (1)

has several terms. The first describes noninteracting electrons in leads ($\alpha = L, R$), whose electron densities of states $D$ are assumed to be energy independent. The operator $a_{\alpha,k}^\dagger (a_{\alpha,k})$ creates (destroys) an electron with momentum $k$ in the lead $\alpha$ with the corresponding spin.

The electrons in each lead are held at a constant electrochemical potential $\mu_{L,R} = -eV/2$, where $e < 0$ is the electron charge and $V > 0$ is the bias voltage. Since the leads are fully spin-polarized the lead index $\alpha$ can

*Present address: Kavli Institute of Nanoscience, TU Delft, Lorentzweg 1, 2628 CJ Delft, The Netherlands.
also be used as a spin index: $L = \uparrow$ and $R = \downarrow$. The second term represents tunneling of electrons (without spin flip) between the island and the leads. The operator $c_\alpha^\dagger (c_\alpha)$ creates (destroys) an electron with spin $\alpha$ in the dot. The tunneling amplitudes depend exponentially on the displacement $X$: $T_{LR}(X) = T_0 \exp(\mp X/\lambda)$. The third and fourth terms describe the single electronic state in the dot and its coupling to the electric field $E$ and the magnetic field $B$. The Zeeman splitting is given by $g \mu_B B$, where $g$ is the electronic $g$-factor and $\mu_B$ is the Bohr magneton. The fifth term represents the Coulomb repulsion between two electrons on the island and the last term $H_{osc} = \frac{P^2}{2M} + M\omega_0^2 X^2/2$ describes the vibrational degree of freedom associated with the center-of-mass motion of the island. Here $M$ is the mass of the island and $\omega_0$ its vibration frequency. For simplicity, we assume that the temperature is zero.

In the absence of an external magnetic field, electronic tunneling through the system described by the Hamiltonian is blocked. Applying a bias voltage and a magnetic field allows the electronic transport to be externally manipulated by lifting this “spin-blockade”. By deblocking electron tunneling the mechanical degree of freedom is also greatly influenced, the equilibrium position of the island becoming unstable if the rate of energy transfer from the electronic subsystem to the nanooscillator exceeds a critical value.

The coupled electronic and mechanical dynamics of the dot is governed by a quantum master equation for the corresponding reduced density operator $\rho(t)$. It can be derived from the Liouville-von Neumann equation for the total system by projecting out the degrees of freedom associated with the leads and the thermal bath. The reduced density operator $\rho(t)$ obtained in this way acts on the Hilbert space of the dot, which is a tensor product of the Hilbert space of the oscillator and the electronic space of the dot. The latter is spanned by the four basis vectors $|0\rangle$, $|\uparrow\rangle \equiv c_0^\dagger |0\rangle$, $|\downarrow\rangle \equiv c_\uparrow^\dagger |0\rangle$, and $|2\rangle \equiv c_\uparrow^\dagger c_\downarrow^\dagger |0\rangle$. In the electronic basis the operator $\rho(t)$ can be written as a $4 \times 4$ matrix whose elements are operators in vibration space. The diagonal elements $\rho_0 \equiv \langle 0|\rho|0\rangle$ and $\rho_2 \equiv \langle 2|\rho|2\rangle$ represent the density operators of the empty and doubly occupied oscillator correspondingly. The singly occupied oscillator is described by the $2 \times 2$ block $\rho_1 \equiv \{\rho_{1s,1s} \equiv \langle s_1|\rho|s_2\rangle\}$, where $s_1, s_2 = |\uparrow\rangle, |\downarrow\rangle$. The time evolution of the density operators $\rho_0$, $\rho_1$ and $\rho_2$ is determined by the coupled system of dimensionless equations of motion

$$\begin{align}
\partial_t \rho_0 &= -i [H_{osc} + xd, \rho_0] - \{\Gamma_L(x), \rho_0\}/2
+ \text{Tr}_s \sqrt{\Gamma_L \rho_1} \sqrt{\Gamma_R} + \mathcal{L}, \rho_0, \\
\partial_t \rho_1 &= -i [H_{osc} - \frac{h}{2} \hat{\sigma}_x, \rho_1] - \{\Gamma^+_L, \rho_1\}/2
+ \text{Tr}_s \sqrt{\Gamma_L \rho_1} \sqrt{\Gamma_R} + \mathcal{L}, \rho_1.
\end{align}$$

(2)

Here all lengths are measured in units of zero point oscillation amplitude $x_0$, all energies in units of $\hbar \omega_0$ and time in units of $\hbar \omega_0^{-1}$: $x \equiv X/x_0$ and $p \equiv x_0 P/\hbar$ are dimensionless operators for the oscillator displacement and momentum correspondingly. Dimensionless electric ($d$) and magnetic ($h$) fields are defined by

$$d \equiv eE/(M\omega_0^2 x_0), \quad h \equiv g \mu_B B/(\hbar \omega_0).$$

(5)

$$\mathcal{L}, \rho \equiv -i \gamma \{x, \rho\}/2 - \gamma (n_{\omega_0} + 1/2) \{x, \rho\}/2, \quad \gamma = 1/\tau_{\omega_0}$$

(6)

where $\gamma \ll 1$ is a dimensionless dissipation rate and $n_{\omega_0} \equiv 1/[e^{h\omega_0/\kappa} - 1]$ is the Bose distribution function. One can formally derive Eq. (6) by weakly connecting the oscillator to an Ohmic heat bath by adding the terms $H_{heat} = \sum_q \hbar \omega_q b^\dagger_q b_q$ and $H_{osc-heat} = X \sum_q g_q (b^\dagger_q + b_q)$ to the Hamiltonian (1) and then eliminate the bath variables in the Born-Markov approximation.

The mechanical degree of freedom alone is described by the density operator $\rho_+ \equiv \rho_0 + \text{Tr}_s \rho_1 + \rho_2$, which is conveniently analyzed in the Wigner representation defined by

$$W(\rho(x, p)) \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\xi e^{-ip\xi} \langle x + \xi/2 | \rho | x - \xi/2 \rangle$$

(7)

for a density operator $\rho$.

In an experimentally relevant regime $\xi$ where the electromechanical coupling parameter

$$\eta \equiv d/\lambda \sim 1/\lambda \ll 1$$

(8)

is small, one can find the stationary solution of the system of Eqs. (2) perturbatively in terms of the small parameters $\eta$ and $\gamma$.

Rescaling the phase variables $X \equiv x/\lambda$, $P \equiv p/\lambda$ and changing to the polar coordinates $X = A \sin \varphi$, $P = A \cos \varphi$, one obtains the steady-state equation for the Wigner function $W_+ \equiv W_{\rho_+}$ of the oscillator as

$$\partial_\varphi W_+ = \{ -\Gamma_+(X) \mathcal{C}/2 + \mathcal{L}, \}
W_+
+ \{\eta \partial_P + \Gamma_-(X) \mathcal{C}/2\} W_{0-2} - \Gamma_+(X) \mathcal{C} W_{-1-1/2}.$$

(9)

Equation (9) couples to the steady state equation for the vector-function $W \equiv [W_{0-2}, W_{-1-1}, W_{-2}, W_{+2}]^T$, where $W_{0\pm 2} \equiv W_{\rho_0} \pm W_{\rho_2}$, $W_{1-1} \equiv W_{\rho_1} - W_{\rho_{1\uparrow}}$ and
\[ W_{\pm c} \equiv W_{\rho \pm} \pm W_{\rho \pm}. \] Here \( \Gamma_{\pm}(X) \equiv \Gamma_{R}(X) \pm \Gamma_{L}(X), \) \( \Gamma_{0} \equiv \eta [\partial_{\phi} P + (1/2A^{2})\partial_{\phi}^{2}] \) and \( C \equiv \cosh \left[ (\lambda - \eta \partial_{P}) \right] - 1. \)

One can show that in the leading order approximation the Wigner function \( W_{+}(A, \varphi) \) is \( \varphi \)-independent and determined by

\[ \partial_{A}A \left[ f(A) + D(A) \partial_{A} \right] W_{+}(A) = 0, \]

where \( f(A) = \left( A/2 \right) \left[ \gamma - \eta \beta_{0}(A) \right], \) \( A\beta_{0}(A) = -\int_{0}^{2\pi} (d\varphi/\pi) \cos \varphi G^{(0)}_{0-2}(\varphi) \geq 0 \) and \( D(A) > 0 \) is of second order in \( \eta \) and \( \gamma. \) The function \( G^{(0)}_{0-2}(\varphi) \) is determined by the system of differential equations:

\[ D_{\varphi}G^{(0)}_{0-2} = \Gamma_{-}(X)G^{(0)}_{0-1} + \Gamma_{-}(X), \]
\[ D_{\varphi}G^{(0)}_{0-1} = \Gamma_{-}(X)G^{(0)}_{0-2} - 2hG^{(0)}_{0-1} - \Gamma_{+}(X), \]
\[ D_{\varphi}G^{(0)}_{0-2} = 2hG^{(0)}_{0-1}, \] \( D_{\varphi} = 2\partial_{\varphi} + \Gamma_{+}(X) \)

It follows from Eq. (10) that the Wigner function \( W_{+} \) has the form \( W_{+}(A) \approx 2^{\frac{-1}{2}} \exp \left\{ -\int_{0}^{A} dA f(A) \right\} \) and is peaked for amplitudes \( A_{M} \) determined by the conditions \( f(A_{M}) = 0 \) and \( f'(A_{M}) > 0. \) In the vicinity of these amplitudes \( W_{+}(A) \) can be approximated by a narrow Gaussian of variance \( \sigma^{2} = D(A_{M})/f'(A_{M}). \) The behavior of the stationary solution \( W_{+}(A) \) is determined by the structure of the positive definite function \( \beta_{0}(A) \), which is bounded, has only one maximum and decreases monotonically for large \( A. \) One can show that if \( h < h_{c} \), the function \( \beta_{0}(A) \) has its only maximum at \( A = 0, \) while if \( h > h_{c} \) it has a minimum there. In the vicinity of \( A = 0, \) one finds that \( \beta_{0}(A) = \gamma_{thr}/(\eta + O(A^{2}), \) where

\[ \gamma_{thr} \equiv \frac{2\Gamma_{0}}{\eta \left( 1 + \frac{h^{2}}{\Gamma_{0}} \right)} \]

From this equation it follows that the electromechanical properties for a low-transparency junction (with a resistance in the Gohm range) is sensitive to very weak magnetic fields of order 1-10 Oe. Such weak fields have a negligible effect on the internal magnetization of the leads, which is why this effect was not considered here.

The presence of various stationary regimes can be illustrated by a “phase diagram” in the \((d, h)\)-plane. Figure 1 shows three domains that correspond to three different types of behavior of the nanomechanical oscillator. In the “vibronic” domain \((v)\), defined by the condition \( \eta/\gamma < 1/[\max \beta_{0}(A)](h), \) the NEM-SET system is stable with respect to mechanical displacements of the island from its equilibrium position. The “shuttle” domain \((s)\) is determined by the condition \( \gamma < \gamma_{thr} \) and corresponds to developed island vibrations of a classical nature. The third domain is the “mixed” domain \((m)\). It appears because the \( v\) - and \( s\)-regimes become unstable at different combinations of electric \((d)\) and magnetic \((h)\) fields if \( h \) exceeds a critical value \( h_{c} \) (cf. [12, 14]).

Hence, while the shuttle regime is unstable below the line \( v \) in Fig. 1, the vibronic regime becomes unstable above the line \( s \). Between these lines (in the \((m)\)-domain) both states can be stable. The oscillator “bounces” between the \( v\) - and \( s\)-regimes due to random electric forces caused by stochastic variations of the grain charge associated with tunneling events.

The transition time between the two locally stable regimes of the \((m)\)-domain is given by \( \tau_{v\leftrightarrow s} = \omega_{0}^{-1} \exp (S_{v\leftrightarrow s}/\eta), \) where \( S_{v\leftrightarrow s}(d, h) \sim 1. \) Since \( S_{v\leftrightarrow s} \neq S_{v\leftrightarrow v} \) and \( \eta \ll 1, \) the difference between the switching rates \( \tau_{v\leftrightarrow s} \) and \( \tau_{v\leftrightarrow v} \) can be exponentially large. This implies that the probabilities for the system to be in one or the other of the two regimes can be very different. The line \( p \) in Fig. 1 corresponds to \( S_{v\leftrightarrow s} = S_{v\leftrightarrow v} \) and therefore to equal rates for the transitions \( v \rightarrow s \) and \( s \rightarrow v. \) Below this line, the probability for the system to be in the \( v\)-regime is exponentially larger than for it to be in the \( s\)-regime, while above the dominance of the \( s\)-regime is exponentially large. Due to the smallness of the electromechanical coupling, \( \eta \ll 1, \) the transition between the two regimes is very sharp. Hence the change of vibration regime can be regarded as a “phase transition”. Such a transition will manifest itself if the variation of the external fields is adiabatic on the time scale of \( \max \{ \tau_{v\leftrightarrow v} \}. \) One can expect enhanced low-frequency noise, \( \omega \gtrsim \tau_{v\leftrightarrow v}^{-1}, \) around the line \( p \) as a hallmark of the transition.

In the opposite non-adiabatic limit, either the \( s\)- or the \( v\)-regime is “frozen in” in the mixed domain after crossing the line \( p. \) Thus if one starts in the \( v\)-domain the \( v\)-regime persists until the system crosses the line \( s, \) and if one starts from the \( s\)-domain the \( s\)-regime persists until the system crosses the line \( v. \) Hence, one observes a hysteretic behavior of the non-adiabatic shuttle transition.

As one can see from Fig. 1 there are two different sce-
narios for the onset of shuttle vibrations. If one crosses over from the $v$- to the $s$-domain when $h < h_c$, i.e. avoiding the mixed domain, the onset is soft. In this scenario the vibration amplitude grows gradually from zero to some finite value after crossing the border line (Fig. 2). If $h > h_c$, on the other hand, the onset is hard. In this case the vibration amplitude shows a step at the transition point (Fig. 3), which corresponds to crossing either the $p$- or the $s$-line depending on whether the transition is adiabatic or not.

FIG. 2: Steady-state amplitude $A_C$ of shuttle vibrations and current $I$ through the NEM-SET device for parameters corresponding to a "soft" transition between the vibronic and shuttle domains of Fig. 4 $(\Gamma_+(0) = 0.1$ and $d/(\gamma \lambda) = 14.3)$.

FIG. 3: Hysteretic behavior of the steady-state shuttling amplitude $A_C$ and current $I$ through the NEM-SET device for parameters corresponding to a "hard" transition between the vibronic and shuttle domains of Fig. 4 $(\Gamma_+(0) = 0.1$ and $d/(\gamma \lambda) = 11.1)$.

One can show that the expression for the steady state current through the system is

$$I = e \int \int dX dP \Gamma_L(X)[W_+ + W_{0-2} + W_{1-}] / 2. \quad (15)$$

Typical plots of the current in the cases of soft and hard transitions are shown in Figs. 2 and 4 respectively.

In conclusion, we have considered "shuttle" phenomena in a nanoelectromechanical single-electron transistor (NEM-SET) system consisting of a metallic island suspended between spin-polarized leads. We have shown, that a coupling between the transport of spin-polarized electrons and the center-of-mass motion of the island allows us to control the dynamics of the mechanical degree of freedom of the island by an external magnetic field. Different stable operating regimes of the magnetic NEM-SET were found and transitions between them induced by varying the electric and magnetic fields were analyzed. We have hence demonstrated that magnetic-field-controlled spin effects can lead to a very rich behavior of nanomechanical systems.

Although we have considered fully spin-polarized leads and assumed a symmetric set-up, the overall qualitative picture does not change if these conditions are relaxed. A partial polarization, allowing a shuttle instability even at zero external magnetic field, makes the system sensitive to the magnetic field in a more narrow interval of electric fields. An asymmetric coupling to the leads induces an additional magnetic field along the direction of their spin-polarization. This field reduces the rate of energy pumping into the oscillator, moving the domains in Fig. 1 to higher values of electric and magnetic fields.

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