Vibrational instability due to coherent tunneling of electrons

To cite this article: D. Fedorets *et al* 2002 *EPL* **58** 99

View the article online for updates and enhancements.

Vibrational instability due to coherent tunneling of electrons

D. Fedorets(*), L. Y. Gorelik, R. I. Shekhter and M. Jonson

*Department of Applied Physics, Chalmers University of Technology
and Göteborg University - SE-412 96 Göteborg, Sweden*

Abstract. – Effects of a coupling between the mechanical vibrations of a quantum dot placed between the two leads of a single-electron transistor and coherent tunneling of electrons through a single level in the dot has been studied. We have found that for bias voltages exceeding a certain critical value a dynamical instability occurs and mechanical vibrations of the dot develop into a stable limit cycle. The current-voltage characteristics for such a transistor were calculated and they seem to be in reasonably good agreement with recent experimental results for the single-C_{60}-molecule transistor by Park *et al.* (*Nature* **407** (2000) 57).

Introduction. – Nanoelectromechanics [1,2] is a new, quickly developing field in condensed-matter physics. A coupling between strongly pronounced mesoscopic features of the electronic degrees of freedom (such as quantum coherence and quantum correlations) and degrees of freedom connected to deformations of the material produces strong electromechanical effects on the nanometer scale. The mesoscopic force oscillations in nanowires [3–5] observed a few years ago is an example of such a phenomenon. Investigations of artificially made nanomechanical devices, where the interplay between single-electron tunneling and a local mechanical degree of freedom significantly controls the electronic transport, is another line of nanoelectromechanics [6–15]. For one of the nanomechanical systems of this kind, the self-assembled single-electron transistor, a new electromechanical phenomenon —the shuttle instability and a new so-called shuttle mechanism of the charge transport were recently predicted in [12]. It was shown that a small metallic grain attached to two metallic electrodes by elastically deformable links breaks into oscillations if a large enough bias voltage is applied between the leads. For the model system studied in [12], it was also shown that a finite friction is required for the oscillation amplitude to saturate and for a stable regime of oscillations to develop.

An essential assumption made in [12] is that the relaxation mechanisms present are strong enough to keep the electron systems in each of the conducting parts of the transistor in local equilibrium (as assumed in the standard theory of Coulomb blockade [16, 17]). Such
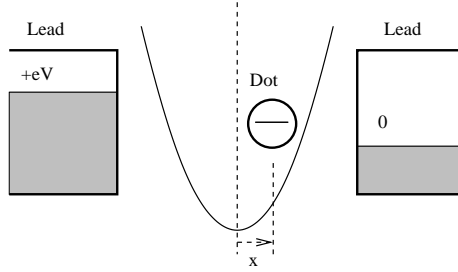
Fig. 1 – Model system consisting of a movable quantum dot placed between two leads. An effective elastic force acting on the dot from the leads is described by the parabolic potential. Only one single electron state is available in the dot and the non-interacting electrons in each have a constant density of states.

relaxation, which destroys any phase coherence between electron tunneling events, allows a description of the whole electronic kinetics by means of a master equation for the occupation probabilities of the dot. It is clear that such an incoherent approach must fail if the size of the grain is small enough. Firstly, a decrease of the grain size results in a decrease of its mass and, consequently, in an increase of the frequency of the mechanical vibrations, which for nanometer-size clusters is of the order of 0.1–1 THz and might exceed the electron relaxation rate in the grain. Secondly, the electron energy level spacing in a nanometer-size grain $\delta \sim \epsilon_{\rm F}/N$, ($N$ is the number of electrons) can be of the order of $10\,{\rm K}$ and exceed the operational temperatures. In this situation the discreteness of the energy spectrum can be very important. What is more, a possibly strong tunneling-induced coupling between electronic states in the grain and in the leads, which results in large quantum fluctuations of the charge in the grain, must be included.

For all of the above reasons a new approach is needed for a description of the electron transport through a nanometer-size movable cluster or quantum dot. The non-trivial question then arises whether or not the coherent electron tunneling through a movable dot causes any electromechanical instability. Such a question is of notable practical significance in view of the recent experiment by Park *et al.* [7], where the current through so-called single-C_{60}-molecule transistors was measured and anomalies —including a few equidistant step-like features— in the *I-V* characteristics observed. This current steps were interpreted in [7] as a manifestation of the coupling between electron tunneling and the center-of-mass vibrational degree of freedom of the molecule.

Theoretical model. – To investigate the influence of the above electromechanical coupling, we consider a model system consisting of a movable quantum dot placed between two bulk leads. An effective elastic force acting on the dot due to interaction with the leads is described by the parabolic potential presented in fig. 1. We assume that only one single-electron state is available in the dot and that the electrons in each lead are non-interacting with a constant density of states. At the same time we treat the motion of the grain classically. The Hamiltonian for the electronic part of the system is

$$H = \sum_{\alpha,k}(\epsilon_{\alpha k} - \mu_\alpha)a_{\alpha k}^\dagger a_{\alpha k} + \epsilon_{\rm d}(t)c^\dagger c + \sum_{\alpha,k} T_\alpha(t)\big(a_{\alpha k}^\dagger c + c^\dagger a_{\alpha k}\big). \tag{1}$$

Here $T_{\rm L,R} = \tau_{\rm L,R}\exp[\mp x(t)/\lambda]$ is the position-dependent tunneling matrix element, $\epsilon_{\rm d}(t) = \epsilon_0 - \mathcal{E}x(t)$ is the energy level in the dot shifted due to the voltage-induced electric field

$\mathcal{E}/e = \chi V$, χ is a parameter characterizing the strength of the electrical field as a function of the bias voltage V, $e < 0$ is the electron charge, x measures the displacement of the dot, $a_{\alpha k}^\dagger$ creates an electron with momentum k in the corresponding lead, $\alpha = \mathrm{L}, \mathrm{R}$ is the lead index, $c^\dagger$ creates an electron in the dot and λ is the characteristic tunneling length [12]. The first term in the Hamiltonian describes the electrons in the leads, the second, the movable quantum dot and the last term, tunneling between the leads and the dot.

The evolution of the electronic subsystem is determined by the Liouville-von Neumann equation for the statistical operator $\hat{\rho}(t)$,

$$i\partial_t \hat{\rho}(t) = \left[\hat{H}, \hat{\rho}(t)\right]_-, \tag{2}$$

while the center-of-mass motion of the dot is governed by Newton's equation,

$$\ddot{x} + w_0^2 x = F/M. \tag{3}$$

Here $w_0 = \sqrt{k/M}$, M is the mass of the grain, k is a constant characterizing the strength of the harmonic potential, $F = -\langle \partial \hat{H}/\partial x \rangle$ and $\langle \bullet \rangle = \mathrm{Tr}\{\hat{\rho}(t)\bullet\}$. The force F on the RHS of eq. (3) is due to the coupling to the electronic subsystem and consists of two terms,

$$F(t) = -i\mathcal{E}G^<(t,t) + 2\lambda^{-1}\sum_{\alpha,k}(-1)^\alpha T_\alpha(t)\,\mathrm{Im}\left[G_{\alpha k}^<(t,t)\right], \tag{4}$$

where $G^<(t,t') \equiv i\langle c^\dagger(t')c(t)\rangle$, $G_{\alpha k}^<(t,t') \equiv i\langle a_{\alpha k}^\dagger(t')c(t)\rangle$ are the lesser Green functions, and $\alpha = 0\,(1)$ for the left (right) lead. The first term describes the electric force that acts on the charge in the dot; the second term is an exchange force, which appears due to the position dependence of the tunneling matrix elements $T_{\mathrm{L,R}}$. The force F depends on the correlation functions $G^<(t,t)$ and $G_{\alpha k}^<(t,t)$, which can be computed exactly in the wide-band limit ($\rho_\alpha = $ const) by using the Keldysh formalism [18].

Following the standard analysis [19] we express the correlation function $G_{\alpha k}^<(t,t)$ in terms of the Green functions of the dot,

$$G_{\alpha k}^<(t,t') = \int \mathrm{d}t_1 T_\alpha(t_1)\left\{G^{\mathrm{r}}(t,t_1)g_{\alpha k}^<(t_1,t') + G^<(t,t_1)g_{\alpha k}^{\mathrm{a}}(t_1,t')\right\}. \tag{5}$$

Here G^{r} is the retarded Green function of the dot and $g_{\alpha k}^{\mathrm{a}(<)}$ is the advanced (lesser) Green function of the leads for the uncoupled system. The Dyson equation for the retarded (advanced) Green function has the following form: $G^{\mathrm{r}(\mathrm{a})} = g^{\mathrm{r}(\mathrm{a})} + g^{\mathrm{r}(\mathrm{a})}\Sigma^{\mathrm{r}(\mathrm{a})}G^{\mathrm{r}(\mathrm{a})}$, where $\Sigma^{\mathrm{r}(\mathrm{a})}(t_1,t_2) = \sum_{\alpha,k} T_\alpha(t_1)g_{\alpha,k}^{\mathrm{r}(\mathrm{a})}(t_1,t_2)T_\alpha(t_2)$. In the wide-band limit $\Sigma^{\mathrm{r}(\mathrm{a})}(t_1,t_2) \propto \delta(t_1 - t_2)$ and this Dyson equation can be solved exactly. The lesser Green function $G^<$ is given by the Keldysh equation $G^< = G^{\mathrm{r}}\Sigma^<G^{\mathrm{a}}$, where $\Sigma^<(t_1,t_2) = \sum_{\alpha,k} T_\alpha(t_1)g_{\alpha k}^<(t_1,t_2)T_\alpha(t_2)$.

As a result, we obtain a general expression for the force F of the form

$$F(t) = \sum_\alpha \rho_\alpha \int \mathrm{d}\epsilon f_\alpha(\epsilon)\left\{\mathcal{E}|B_\alpha(\epsilon,t)|^2 + 2\frac{(-1)^\alpha}{\lambda}T_\alpha(t)\,\mathrm{Re}[B_\alpha(\epsilon,t)]\right\}, \tag{6}$$

where

$$B_\alpha(\epsilon,t) = -i\int_{-\infty}^t \mathrm{d}t_1 T_\alpha(t_1)\exp\left[i\int_{t_1}^t \mathrm{d}t_2\left[\epsilon - \epsilon_{\mathrm{d}}(t_2) + i\frac{\Gamma(t_2)}{2}\right]\right].$$

$\Gamma(t) = 2\pi\sum_\alpha \rho_\alpha T_\alpha^2(t)$, ρ_α is the density of states in the corresponding lead and $f_\alpha(\epsilon) = [\exp[\beta(\epsilon - \mu_\alpha)] + 1]^{-1}$. It is worth mentioning that eq. (6) is valid for arbitrary values of the tunneling matrix elements.

An important question is now whether or not the mechanical stability of the transistor configuration is affected by coherently tunneling electrons.

Instability. – In order to investigate the stability of the equilibrium position of the dot, we expand the RHS of eq. (3) to first order with respect to the displacement: $F(t) = \int_{-\infty}^{t} dt' D(t - t') x(t')$. After a Fourier transformation of the obtained equation, we get the following dispersion equation for the frequency:

$$w^2 - \left(w_0^2 - w_1^2\right) = -D_w/M, \tag{7}$$

where

$$D_w = -\int \frac{d\epsilon}{2\pi} \sum_\alpha \Gamma_\alpha f_\alpha \{R_\alpha G_w^+ + R_\alpha^* G_{-w}^-\},$$

$$R_\alpha = \left\{\left|\mathcal{E}G_0^+ + \frac{(-1)^\alpha}{\lambda}\right|^2 - ig\left[\mathcal{E}|G_0|^2 + G_0^+ \frac{(-1)^\alpha}{\lambda}\right]\right\},$$

$w_1^2 = \sum_\alpha \Gamma_\alpha \int d\epsilon f_\alpha \operatorname{Re}[G_0^+]/(\pi\lambda^2 M)$, $\Gamma_\alpha = 2\pi\rho_\alpha\tau_\alpha^2$, $\Gamma = \sum_\alpha \Gamma_\alpha$, $G_w^\pm(\epsilon) = [\epsilon + w - \epsilon_0 \pm i\Gamma/2]^{-1}$ and $g = (\Gamma_L - \Gamma_R)/\lambda$.

The criterion for instability is that the frequency ω has a positive imaginary part. When $\Gamma/(Mw_0^2\lambda^2) \ll 1$ and $\mathcal{E}\lambda/(\sqrt{w_0^2 + \Gamma^2}) \ll 1$ (the case of weak electromechanical coupling) we obtain that $\operatorname{Im}[w] \approx -\operatorname{Im}[D_{w_0}]/(Mw_0)$. From now on we consider only the case of weak electromechanical coupling. An analytical analysis cannot be performed in the general case, but for a large symmetrically applied bias voltage and zero temperature one can show that $\operatorname{Im}[D_{w_0}]$ is negative:

$$\operatorname{Im}[D_{w_0}] \asymp -\frac{4\mathcal{E}w_0}{\lambda(w_0^2 + \Gamma^2)} \frac{\Gamma_L\Gamma_R}{\Gamma}. \tag{8}$$

The instability that follows from eq. (8) is in contrast with the behavior at low voltages where it can be shown that $\operatorname{Im}[D_{w_0}]$ is positive. Therefore, a finite threshold voltage for the instability exists in the system. A simple expression for the threshold voltage can be found for a symmetric junction in the case of weak tunneling under the above conditions: $eV_c = 2(\epsilon_0 + w_0)$.

Under the condition of weak electromechanical coupling, the displacement $x(t)$ of the dot can be represented in a harmonic oscillation form $A(t)\cos(wt + \phi(t))$ with an amplitude $A(t)$ and a phase $\phi(t)$ that slowly vary on the scale of w_0^{-1}. By averaging over the fast harmonic oscillations, one can get the following equation for the evolution of the amplitude (see for example [12]):

$$\frac{dA^2}{dt} = \frac{W(A^2)}{M\pi w_0}. \tag{9}$$

Here $W(A^2) = \oint dx F$ is the work done by the force F on the dot during one period of oscillation with a constant amplitude A. We conclude from eq. (9) that the stable regime of oscillations corresponds to $W = 0$ and $dW(A^2)/dA^2 < 0$. Typical $W(A^2)$-curves are depicted in fig. 2 for the parameters taken from the experiment described in [7]. When an applied voltage is lower than the threshold voltage, the work W is negative for all amplitudes. This implies that the equilibrium position of the grain is stable. When the voltage is higher than the threshold voltage, the function $W(A^2)$ is positive for $0 < A < A_c(V)$ (which corresponds to a slow increase of the oscillation amplitude), negative for $A > A_c(V)$ (which corresponds to a slow decrease of the amplitude) and equal to zero at $A = A_c(V)$. This means that when the applied voltage exceeds the threshold value the amplitude of the oscillation slowly increases until it develops into a stable limit cycle with amplitude $A_c(V)$. As one can see from fig. 2, the amplitude of the limit cycle is of the order of $\lambda \sim 0.1$ nm and is considerably larger than the amplitude of zero-point oscillations of the grain, which for the C_{60} molecule in the experiment [7] is approximately 3 pm.
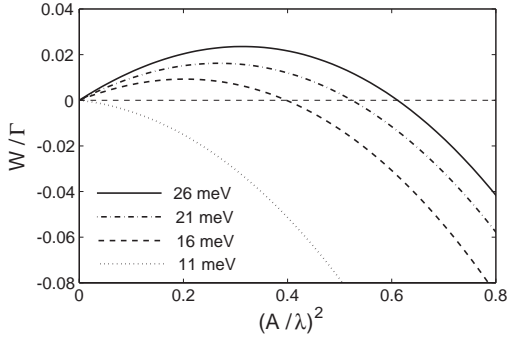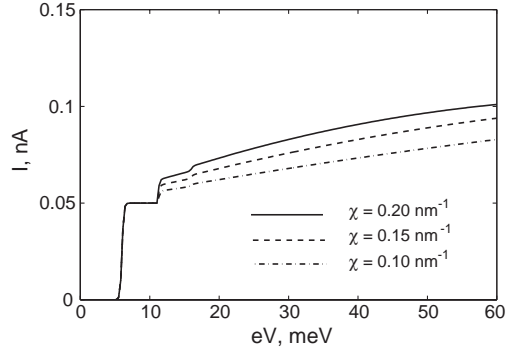
Fig. 2

Fig. 3

Fig. 2 – The energy W pumped into the mechanical degree of freedom during one period of oscillation for different values of the applied voltage V: $w_0 = 5\,\text{meV}$, $T = 0.13\,\text{meV}$, $\epsilon_0 = 6\,\text{meV}$, $\Gamma = 1\,\mu\text{eV}$ and $\Gamma_\text{R}/\Gamma_\text{L} = 9$.

Fig. 3 – *I-V* curves for different values of the parameter χ which characterizes the strength of the electric field between the leads for a given voltage: $w_0 = 5\,\text{meV}$, $T = 0.13\,\text{meV}$, $\epsilon_0 = 6\,\text{meV}$, and $\Gamma = 2.3\,\mu\text{eV}$. Best fit to [7] is obtained for an asymmetric coupling to the leads; here we use $\Gamma_\text{R}/\Gamma_\text{L} = 9$.

Current. – In the regime where the stable limit cycle oscillations have developed the vibration-induced inelastic tunneling of electrons can significantly contribute to the current. The time-averaged current through the system in the stable regime where oscillations of the limit cycle amplitude $A_\text{c}(V)$ and frequency $w_0 = \sqrt{k/M}$ have developed, has the following form:

$$I = -\frac{e\Gamma_\text{L}}{2\pi T} \int_0^T \mathrm{d}t \int \mathrm{d}\epsilon \left\{ e^{-\frac{2x}{\lambda}} \sum_\alpha \Gamma_\alpha f_\alpha \left| \frac{B_\alpha}{\tau_\alpha} \right|^2 + 2e^{-\frac{x}{\lambda}} f_\text{L} \,\text{Im}\left[\frac{B_\text{L}}{\tau_\text{L}} \right] \right\}, \tag{10}$$

where $x(t) = A_\text{c} \cos(w_0 t)$ and $T = 2\pi/w_0$ is the period of oscillations. This expression is valid under the same general conditions as eq. (6).

Under the condition that the effective level broadening $\tilde{\Gamma} \ll w_0$ (where $\tilde{\Gamma} = \Gamma J_0(i2A_\text{c}/\lambda)$) eq. (10) can be simplified to

$$I \approx \frac{e\Gamma_\text{L}\Gamma_\text{R}}{\Gamma} \sum_{m=-\infty}^{+\infty} \{f_{\text{L},m}\xi_\text{L}^{2m} - f_{\text{R},m}\xi_\text{R}^{2m}\} J_m^2(A_\text{c}\eta), \tag{11}$$

where $f_{\alpha,m} = f_\alpha(\epsilon_0 + mw_0)$, $\eta = \sqrt{(\mathcal{E}/w_0)^2 - \lambda^{-2}}$, $\xi_\alpha = -[(\mathcal{E}/w_0) + (-1)^\alpha/\lambda]/\eta$ and J_m are Bessel functions of the first kind. The typical *I-V* curves are shown in fig. 3, where we assume that voltage has been applied only to the left lead (according to the experiment [7]). The main characteristic feature of all obtained *I-V* curves is that they show only a few equidistant steps which are followed by stepless behavior of the curves. The distance between the steps is given by the vibrational frequency w_0 and their heights can vary depending on the parameters. The steps following the first one is due to the development of a vibrational instability and a transition into the associated charge transfer regime. The obtained behavior of the *I-V* curves is in reasonably good agreement with the experimental data [7]. Best fit to the published experimental *I-V* curves is obtained for an asymmetric coupling to the leads ($\Gamma_\text{R}/\Gamma_\text{L} \approx 9$). When the ratio $\Gamma_\text{R}/\Gamma_\text{L}$ decreases both the vibration-induced current jumps and a high-voltage slope of the *I-V* curve increase deviating from the experimental data.

An alternative theoretical description of the experiment based on a photon-assisted tunneling-like picture [15] also shows reasonable agreement with the experimental data [7]. Therefore it is difficult to conclude with certainty that it is the above instability which is responsible for the specific features observed in the experiment. Further experiments are needed to clarify the picture. Such experiments may involve an investigation of the charge fluctuation on the grain or of current noise.

Conclusion. – We have studied the effect of a coupling between coherent tunneling of electrons through a single quantized energy level in the central island —or dot— of a single-electron transistor and vibrations of the dot. We have found that for bias voltages exceeding a certain critical value a dynamical instability occurs and mechanical vibrations of the center of mass of the dot develop into a stable limit cycle. The effect of this vibrations on the current through the system were also studied. *I-V* characteristics calculated in our model were found to be in reasonably good agreement with recent experimental results of Park *et al.* [7] for the single-C_{60}-molecule transistor.

$$* * *$$

REFERENCES

[1] ROUKES M. L., Technical Digest of the 2000 Solid-State Sensor and Actuator Workshop.
[2] CRAIGHEAD H. G., *Science*, **290** (2000) 1532.
[3] RUBIO G., AGRAÏT N. and VIEIRA S., *Phys. Rev. Lett.*, **76** (1996) 2302.
[4] IIJIMA S., BRABEC C., MAITI A. and BERNHOLC J., *J. Chem. Phys.*, **104** (1996) 2089.
[5] YAKOBSON B. I., BRABEC C. J. and BERNHOLC J., *Phys. Rev. Lett.*, **76** (1996) 2511.
[6] TUOMINEN M. T., KROTKOV R. V. and BREUER M. L., *Phys. Rev. Lett.*, **83** (1999) 3025.
[7] PARK H, PARK J., LIM A. K. L., ANDERSON E. H., ALIVISATOS A. P. and MCEUEN P. L., *Nature*, **407** (2000) 58.
[8] ERBE A., BLICK R. H., TILKE A., KRIELE A. and KOTTHAUS J. P., *Appl. Phys. Lett.*, **73** (1998) 3751.
[9] WEISS C. and ZWERGER W., *Europhys. Lett.*, **47** (1999) 97.
[10] KRÖMMER H., ERBE A., TILKE A., MANUS S. and BLICK R. H., *Europhys. Lett.*, **50** (2000) 101.
[11] ERBE A., WEISS C., ZWERGER W. and BLICK R. H., *Phys. Rev. Lett.*, **87** (2001) 096106.
[12] GORELIK L. Y., ISACSSON A., VOINOVA M. V., KASEMO B., SHEKHTER R. I. and JONSON M., *Phys. Rev. Lett.*, **80** (1998) 4526; ISACSSON A., GORELIK L. Y., VOINOVA M. V., KASEMO B., SHEKHTER R. I. and JONSON M., *Physica B*, **255** (1998) 150.
[13] ISACSSON A., *Phys. Rev. B*, **64** (2001) 035326.
[14] NORD T., GORELIK L. Y., SHEKHTER R. I. and JONSON M., cond-mat/0106589.
[15] BOESE D. and SCHOELLER H., *Europhys. Lett.*, **54** (2001) 668.
[16] SHEKHTER R. I., *Sov. Phys. JETP*, **36** (1973) 747.
[17] KULIK I. O. and SHEKHTER R. I., *Sov. Phys. JETP*, **41** (1975) 308.
[18] KELDYSH L. V., *Sov. Phys. JETP*, **20** (1965) 1018.
[19] JAUHO A. P., WINGREEN N. S. and MEIR Y., *Phys. Rev. B*, **50** (1994) 5528.