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Energy pumping in a quantum nanoelectromechanical system

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Fully quantized mechanical motion of a single-level quantum coupled to two voltage biased electronic leads is studied. It is found that there are two different regimes depending on the applied voltage. If the bias voltage is below a certain threshold (which depends on the energy of the vibrational quanta) the mechanical subsystem is characterized by a low level of excitation. Above a threshold the energy accumulated in the mechanical degree of freedom dramatically increases. The distribution function for the energy level population and the current through the system in this regime is calculated.

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During the past few years experimental methods of physics has seen an advancing capability to manufacture smaller and smaller structures and devices. This has lead to many new interesting investigations of nanoscale physics. Examples include, for instance, observation of the Kondo effect in single-atom junctions [1], manufacturing of single-molecular transistors [2], and so on. There has also been a great interest in the promising field of molecular electronics [3]. One of the main features of the conducting nanoscale composite systems is its susceptibility to significant mechanical deformations. This results from the fact that on the nanoscale level the mechanical forces controlling the structure of the system are of the same order of magnitude as the capacitive electrostatic forces governed by charge distributions. This circumstance is of the utmost importance in the so called electromechanical single-electron transistor (EM–SET), which has been in focus of recent research. The EM–SET is basically a double junction system where the additional (mechanical) degree of freedom, describing the relative position of the central island, significantly influences the electronic transport. Experimental work in relation to EM–SET structures range from the macroscopic [5] to the micrometer scale [6–8] and down to the nanometer scale [9]. Various aspects of electronic transport in such systems have been theoretically investigated in a series of articles [11–20].

In Ref. 4 and Ref. 15 it was, among other things, shown that coupling the mechanical degree of freedom of an EM–SET to the nonequilibrium bath of electrons constituted by the biased leads, can lead to dynamical self excitations of the mechanical subsystem and as a result bring the EM–SET to the shuttle regime of charge transfer. This phenomena is usually referred to as a shuttle instability. In these papers the grain dynamics are treated classically and the key issue is that the charge of the grain, $q(t)$, is correlated with its velocity, $\dot{x}(t)$, in a way so that the time average, $\overline{q(t)\dot{x}} \neq 0$.

Decreasing the size of the central island in the EM–SET structure to the nanoscale level results in the quantization of its mechanical motion. Charge transfer in this regime was studied theoretically in Ref. 10. However, the strong additional dissipation in the mechanical subsystem suggested in this paper keeps the mechanical subsystem in the vicinity of its ground state and prevents the developing of the mechanical instability. The aim of our paper is to investigate the behavior of the EM–SET system in the quantum regime when its interaction with the external thermodynamic environment generating additional dissipation processes can be partly ignored in such a manner that the mechanical instability becomes possible. We will show that in this case at relatively low bias voltages, intrinsic dissipation processes bring the

mechanical subsystem to the vicinity of the ground state. But if the bias voltage exceeds some threshold value, the energy of the mechanical subsystem, initially located in the vicinity of the ground state, starts to increase exponentially. We have found that intrinsic processes alone saturate this energy growth at some level of excitation. The distribution function for the energy level population and the current through the system in this regime is calculated.

We will consider a model EM–SET structure consisting of a one level quantum situated between two leads (see Fig. 1). To describe such a system we use the Hamiltonian

$$H = \sum_{k,\alpha} E_{k,\alpha} a^{\dagger}_{k,\alpha} a_{k,\alpha} + (E_0 - D\frac{\hat{X}}{x_0})c^{\dagger}c + \frac{1}{2m}\hat{P}^2 + \\ + \frac{1}{2}m\omega_0^2\hat{X}^2 + T_{k,\alpha}(\hat{X})[a^{\dagger}_{k,\alpha}c + c^{\dagger}a_{k,\alpha}]. \qquad (1)$$

The first term describes electronic states with energies $E_{k,\alpha}$ and where $a^{\dagger}_{k,\alpha}$ ($a_{k,\alpha}$) are creation (annihilation) operators for these noninteracting electrons with momentum k in the left ($\alpha = L$) or right ($\alpha = R$) lead. The second term describes the interaction of the electronic level on the with the electric field so that $c^{\dagger}$ (c) is the creation (annihilation) operator for the level electrons and E_0 is the energy level. The scalar D represents the strength of the Coulomb force acting on a charged grain, $\hat{X}$ is the position operator, and $x_0 = \sqrt{\hbar/m\omega_0}$ is the harmonic oscillator length scale for an oscillator with mass m and angular frequency ω_0. The third and fourth terms describe the center of mass movement of the in a harmonic oscillator potential so that $\hat{P}$ is the center of mass momentum operator. The last term is the tunneling interaction between the lead states and the level and $T_{k,\alpha}(\hat{X})$ is the tunneling coupling strength. We will consider the case when the tunneling coupling depends exponentially on the position operator $\hat{X}$, i.e. $T_{k,R}(\hat{X}) = T_R \exp\{\hat{X}/\Lambda\}$ and $T_{k,L}(\hat{X}) = T_L \exp\{-\hat{X}/\Lambda\}$, where T_R and T_L are constants and Λ is the tunneling length.

To introduce a connection to the quantified vibrational states of the oscillator we perform a unitary transformation of the Hamiltonian (1) so that $UHU^{\dagger} = \tilde{H}$, where $U = \exp(i\hat{P}d_0c^{\dagger}c/\hbar)$. In this paper we consider the situation when $\tilde{H}$ has the most symmetric form:

$$\tilde{H} = \sum_{k,\alpha} E_{k,\alpha} a^{\dagger}_{k,\alpha} a_{k,\alpha} + \tilde{E_0}\, c^{\dagger}c + \hbar\omega_0\left(b^{\dagger}b + \frac{1}{2}\right) + \\ + T_0 \sum_k [a^{\dagger}_{k,R} c \exp(x_- b + x_+ b^{\dagger}) + \\ + a^{\dagger}_{k,L} c \exp(-x_+ b - x_- b^{\dagger})] + \text{h.c.} \qquad (2)$$

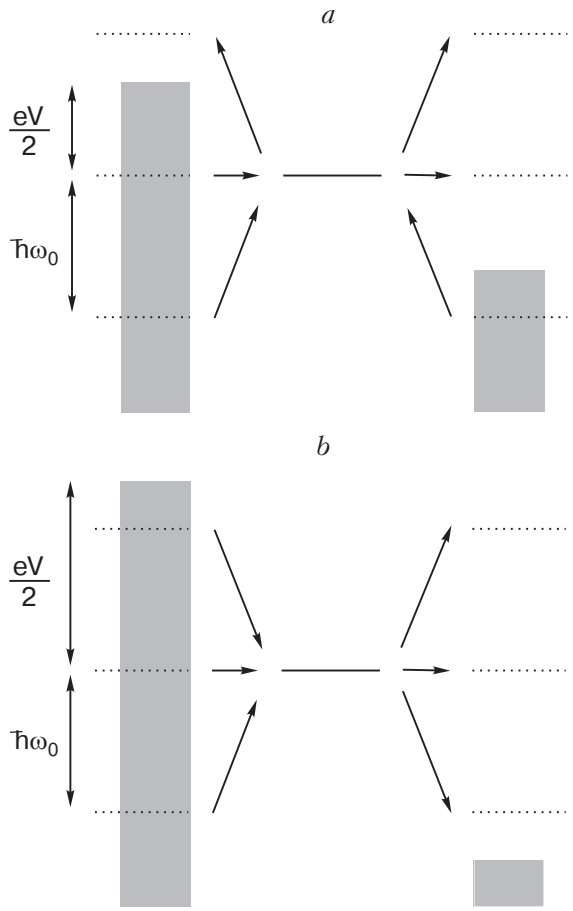

Fig. 1. Model system consisting of a one level quantum dot placed between two leads. The level of the dot equals the chemical potential of the leads and a bias voltage of V is applied between the leads. The center of mass movement of the dot is in a harmonic oscillator potential with the vibrational quanta $\hbar\omega_0$. The applied bias voltage is such that $eV/2 < \hbar\omega_0$ (a). Same as (a) but with the applied bias voltage larger than $2\hbar\omega_0/e$ (b).

Here $b^{\dagger}$ (b) is a bosonic creation (annihilation) operator for the vibronic degree of freedom, and the dimensionless parameters $x_{\pm} = 1/\sqrt{2}(x_0/\Lambda \pm d_0/x_0)$ (where $d_0 = D/(x_0 m\omega_0^2)$) characterize the strength of the electromechanical coupling. Furthermore, T_0 is the renormalized tunneling coupling constant, and $\tilde{E}_0 = E_0 - Dd_0/(2x_0 + m\omega_0^2 d_0^2/2)$ is the shifted dot level. For simplicity, but without loss of generality, we choose $\tilde{E}_0$ equal to the chemical potential of the leads at zero bias voltage.

First let us study the situation when the mechanical subsystem is characterized by a low level of excitation. We will consider the case of small electromechanical coupling. This means that the dimensionless parameters $x_{\pm} << 1$ and that only elastic electronic

transitions and transitions accompanied by emission or absorption of a single vibronic quantum (single-vibronic processes) are important. If the applied voltage is smaller than $2\hbar\omega_0/e$ and the temperature is equal to zero, the six allowed transitions of this type are the ones described in Fig. 1,*a*. Here we see that only elastic tunneling processes and tunneling processes in which the vibronic degree of freedom absorbs one vibronic quantum are allowed and as a result the rate equation for the distribution function of the energy level population $P(n,t)$ has the form:

$$\Gamma^{-1}\partial_t P(n,t) = P(n,t) + (x_+^2 + x_-^2)(n+1)P(n+1,t) - \\ - (1 + n(x_+^2 + x_-^2))P(n,t),$$

where $\Gamma = 2\pi T_0^2 \nu/\hbar$ and ν is the density of states in the leads.

It is straightforward to solve these equations and find that the solution exponentially fast approaches the stable solution $P(0) = 1$ and $P(n) = 0$ for all $n > 0$. As a result, the dimensionless average extra energy excited in the vibronic subsystem,

$$E(t) = \sum_{n=0}^{\infty} nP(n,t), \qquad (3)$$

goes to 0.

If the applied bias voltage is increased above the threshold value $V_c = 2\hbar\omega_0/e$ we instead get the allowed transitions described in Fig. 1,*b*, i.e. two absorption processes has changed into emission processes where the energy quantum $\hbar\omega_0$ is transferred to the vibronic degree of freedom. These transitions lead to the following equation for $P(n)$:

$$\Gamma^{-1}\partial_t P(n,t) = -(1 + x_-^2 + (n+1)x_+^2)P(n,t) + \\ + x_-^2(n+1)P(n+1,t) + P(n,t) + x_+^2 nP(n-1,t). \quad (4)$$

One can find from this equation that the time evolution of the exited energy is given by the formula:

$$E(t) = \frac{x_+^2}{x_+^2 - x_-^2}[\exp(\Gamma(x_+^2 - x_-^2)t) - 1], \qquad (5)$$

i.e. energy is continuously pumped into the mechanical subsystem, which is strong evidence that the low exited regime is unstable if the bias voltage exceeds the critical value V_c. Furthermore, it is necessary to remark here that for this case we thus have a linear increase in the energy as a function of time even when x_+^2 approaches x_-^2.

As the excitation of the vibronic subsystem increases multi-vibronic processes become important. They give rise to an additional dissipation which saturates the energy growth induced by the single-vibronic processes. As a result the system comes to a stationary regime which is characterized by a significant level of excitation of the vibronic subsystem. To demonstrate this we will now expand our analysis by taking into account electronic transitions accompanied by the emission or absorption of two vibronic quanta (two-vibronic processes). To describe such transitions one has to take into account second order terms in $b^\dagger$ and b in the tunneling part of the Hamiltonian (2). As illustrated in Fig. 2 these terms will generate four processes in which two vibrational quanta are absorbed by the electron during the tunneling event. There is also a renormalization of the elastic channel coming from the inclusion of these terms. Now the equation for the distribution function of the energy level population has the form:

$$\Gamma^{-1}\partial_t P(n,t) = nP(n-1,t) - [\varepsilon n^2 + (\alpha - \varepsilon + 1)n + 1] \times \\ \times P(n,t) + \alpha(n+1)P(n+1,t) + \\ + \varepsilon(n+1)(n+2)P(n+2,t) = 0, \qquad (6)$$

where we have introduced the constants $\varepsilon = (x_+^4 + x_-^{4)})/(4x_+^2)$ and $\alpha = x_-^2/x_+^2$.

To find the stationary solution of this equation we introduce the generating function:

$$\mathcal{P}(z) = \sum_{n=0}^{\infty} z^n P(n),$$

where z is a complex number inside the unit circle. Rewriting Eq. 6 we find the equation for $\mathcal{P}(z)$

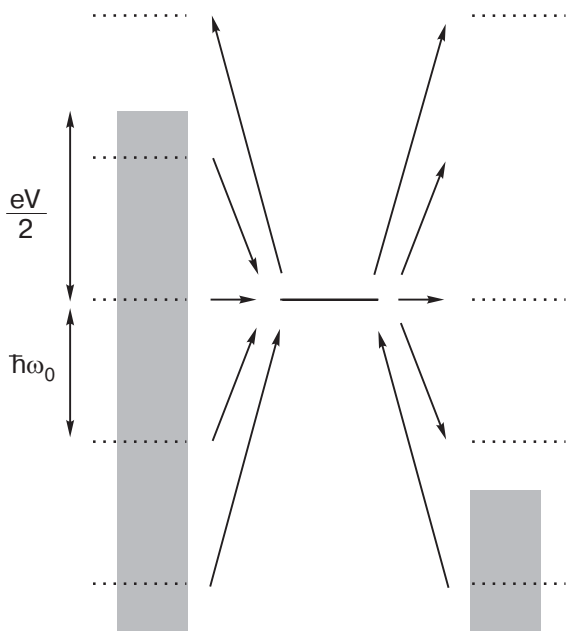

Fig. 2. Illustration of the second order case where elastic tunneling and inelastic tunneling exchanging two or less vibrational quanta are included. The level of the dot is equal to the chemical potential and the bias voltage is set so that $2\hbar\omega_0/e < V < 4\hbar\omega_0/e$.

$$\varepsilon(z+1)\partial_z^2\mathcal{P}(z) + (\alpha - z)\partial_z\mathcal{P}(z) - \mathcal{P}(z) = 0.$$

The solution to this equation is

$$\mathcal{P}(z) = \exp\left(-\int_1^z dz' \frac{\alpha - \varepsilon - z'}{\varepsilon(z'+1)}\right) \times$$

$$\times \left\{\int_{z_0}^z dz' \exp\left(\int_1^{z'} dz'' \frac{\alpha - \varepsilon - z''}{\varepsilon(z''+1)}\right)\frac{C_1}{\varepsilon(z'+1)}\right\},$$

where C_1 and z_0 are constants. Since the probabilities $P(n)$ are positive and normalized, the sum $\sum_{n=0}^{\infty}(-1)^n P(n) = \mathcal{P}(z=-1)$ converges absolutely. This is true only for $z_0 = -1$. The second constant C_1 can be determined from the normalization condition $\mathcal{P}(z=1) = 1$ to be $C_1 = \varepsilon 2^{\gamma} / \int_{-1}^{1} dx \exp((1-x)/\varepsilon) \times$ $\times (x+1)^{\gamma-1}$, where we have introduced the constant $\gamma = (\alpha - \varepsilon + 1)/\varepsilon$. Therefore the final expression for $\mathcal{P}(z)$ is

$$\mathcal{P}(z) = \frac{C_1}{\varepsilon}\frac{\exp\left(\frac{z-1}{\varepsilon}\right)}{(z+1)^{\gamma}}\int_{-1}^{z} dz' \exp\left(\frac{1-z'}{\varepsilon}\right)(z'+1)^{\gamma-1}. \quad (7)$$

We can now calculate the average energy excited in the harmonic oscillator, which is just $\partial_z\mathcal{P}(z)$ calculated at $z = 1$,

$$E = \frac{1}{2\varepsilon}(2 + C_1 - \varepsilon\gamma). \quad (8)$$

One can show that $C_1(\varepsilon)$ decays exponentially as $\exp(-\text{const}/\varepsilon)$ when $\varepsilon \to 0$ so for small ε we get $E = (1-\alpha)/2\varepsilon + O(1)$.

To see how the energy pumped into the harmonic oscillator affects the charge transport we calculate the current I through the system in units of $e\Gamma$. For voltages below V_c the current is only mediated by the elastic channel and is thus $I = 1/2$.

For voltages in the range $2\hbar\omega_0/e < V < 4\hbar\omega_0/e$ the current can be calculated to leading order in ε as

$$I = \left(\frac{1}{4}(x_-^4 - x_+^4) + x_+^2 x_-^2\right)\mathcal{P}''(z=1) +$$

$$+ (x_+ - x_-)^2 P'(z=1) + 1. \quad (9)$$

In Fig. 3 we have chosen a set of numerical values and plotted (solid line) the calculated current as a function of the bias voltage. For comparison we have also plotted (dashed line) the current as given in the high dissipation limit where the harmonic oscillator goes to the ground state between tunneling events. It is clear that the current in the regime characterized by a high level of excitation is much greater than the one in the regime of low level of excitation.

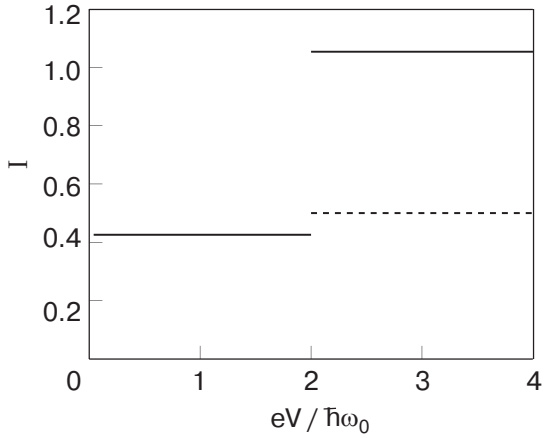

Fig. 3. The current as plotted as a function of the bias voltage (solid line). The current makes a jump as the non-elastic channel is opened at $V = 2\hbar\omega_0/e$. We have also plotted (dashed line) the current as a function of voltage for the high dissipation limit where the harmonic oscillator goes to the ground state between tunneling events.

In conclusion, we have studied fully quantized mechanical motion of a single-level quantum coupled to two voltage biased electronic leads. We have shown that above a certain threshold voltage the energy accumulated in the mechanical subsystem increases dramatically. We have also shown that second order inelastic tunneling events are enough to stabilize this pumping of energy. Finally the current through the system was calculated and it was found that the development of the mechanical instability is accompanied by a dramatic increase in the current.

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