Quantum Shuttle Phenomena in a Nanoelectromechanical Single-Electron Transistor

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An analytical analysis of quantum shuttle phenomena in a nanoelectromechanical single-electron transistor has been performed in the realistic case, when the electron tunneling length is much greater than the amplitude of the zero point oscillations of the central island. It is shown that when the dissipation is below a certain threshold value, the vibrational ground state of the central island is unstable. The steady state into which this instability develops is studied. It is found that if the electric field $\mathcal{E}$ between the leads is much greater than a characteristic value $\mathcal{E}_q$, the quasiclassical shuttle picture is recovered, while if $\mathcal{E} \ll \mathcal{E}_q$ a new quantum regime of shuttle vibrations occurs. We show that in the latter regime small quantum fluctuations result in large (i.e., finite in the limit $\hbar \to 0$) shuttle vibrations.

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The field of nanoelectromechanics has grown rapidly during the last few years [1–3]. In particular, a nano-electromechanical single-electron transistor (NEM-SET) has been attracting a lot of theoretical [4–20] and experimental [21,22] attention. A NEM-SET is a single-electron transistor (SET) where the position of a central island (a small metal particle or a single molecule) is not rigidly fixed but can oscillate under the influence of an elastic potential. In [4] it was shown that in the regime where the island motion can be treated classically and the electron tunneling can be described by the Pauli master equation, a new phenomenon—a so-called shuttle instability occurs. When a large enough bias voltage is applied between the leads, the island oscillates with an increasing amplitude until it reaches a stable limit cycle where it oscillates with some constant amplitude. The key issue in [4] was that as the island moves along the classical trajectory its charge $q(t)$ correlates with its velocity $\dot{x}(t)$ in such a way that the time average $\overline{q(t)\dot{x}(t)}$ is positive. This results in accumulation of energy in the vibrational degree of freedom and in the development of the shuttle instability (see the review [23])

Further miniaturization of the NEM-SET device brings up quantum effects. In a nanometer-size metal particle, the electron energy level spacing is about 10 K and the discreteness of the electron energy spectrum can no longer be neglected even for temperatures of a few kelvin. In this case the characteristic de Broglie wave length associated with the island can still be much shorter than the length scale of the spatial variations of the "mechanical" potential. If so, the motion of the island can be treated classically. Shuttle phenomena in this regime have been studied theoretically in [7]. However, the classical analysis of the shuttle instability (performed in [7]) is limited to displacements that exceed the amplitude $x_0 \equiv \sqrt{\hbar/(M\omega)}$ of the zero point oscillations of the island (M is the mass of the island and ω its vibration frequency). This quantum limitation raises the question of whether or not a threshold value exists for the displacement in order for a shuttle instability to develop. To answer this question a quantum theory of the shuttle instability must be developed. Moreover, the quantization of the island motion might also effect the steady-state regime that develops.

Different aspects of the NEM-SET in the regime of quantized mechanical motion of the island have already been studied [6,10,13,14,16–19]. However, no shuttle instability was found because either the coupling between electron tunneling and mechanical vibrations was ignored [6] or strong dephasing in the mechanical dynamics was expected [13,14,16–19]. In this Letter we will study the quantum dynamics of a NEM-SET for arbitrary dissipation rates. A study complementary to ours has recently been carried out by Novotny *et al.* (compare [8,15]). However, the numerical analysis reported in Ref. [15] was done only for the case when a relatively small number of excited vibrational states are involved. This is the case only if the amplitude of zero point oscillations x_0 is of the order of the electronic tunneling length $\lambda_\star$ and if the dissipation is large enough. Here we present a complementary analytical study valid under the more realistic condition, $x_0/\lambda_\star \equiv \lambda^{-1} \ll 1$.

We will formulate the problem at hand in terms of the dimensionless displacement $x \equiv X/x_0$ and momentum $p \equiv x_0 P/\hbar$ of the island. If we measure all lengths in units of x_0 and all energies in units of $\hbar\omega$, the Hamiltonian of the system reads

$$H = \sum_{\alpha,k} \epsilon_{\alpha k} a_{\alpha k}^\dagger a_{\alpha k} + [\epsilon_0 - dx]c^\dagger c + H_{\mathrm{osc}}$$
$$+ \sum_{\alpha,k} T_\alpha(x)[a_{\alpha k}^\dagger c + \mathrm{H.c.}] + H_B + H_{B-\mathrm{osc}}, \quad (1)$$

where $a_{\alpha k}^\dagger$ creates an electron with momentum k in the corresponding lead, $\alpha = L, R$ is the lead index, $c^\dagger$ creates an electron on the single energy level in the island, $d \equiv e\mathcal{E}/(M\omega^2 x_0)$ is the shift in the equilibrium position of the oscillator due to the electric field $\mathcal{E}$ between the leads, $H_{\mathrm{osc}} \equiv [p^2 + x^2]/2$ is the free oscillator Hamiltonian, and $T_{L,R}(x) = T_{L,R}(0) \exp[\mp x/\lambda]$. We assume that the electrons in each electrode are noninteracting with a

constant density of states $\mathcal{D}_\alpha$ and that all relevant energies are small compared to the level spacing in the central island which for typical systems under consideration exceeds 100 meV. In this case only one single level in the island is relevant to the problem. The term H_B describes a heat bath and the last term $H_{B-\text{osc}}$ relates to the coupling between the oscillator and the bath [24]. We assume that this coupling is linear in x and treat it in weak-coupling limit. For simplicity we will consider only zero temperature case.

The time evolution of the system is governed by the Liouville–von Neumann equation for the total density operator. After projecting out the leads and the thermal bath we obtain an equation of motion (EOM) for the reduced density operator ρ of the vibrational degree of freedom and the electronic state in the island. Under conditions of large bias ($eV \gg \hbar\omega, \epsilon_0$), the EOM for ρ becomes Markovian (for details, see [8,15,25,26]):

$$
\begin{aligned}
\partial_t \rho = & -i[H_v + (\epsilon_0 - dx)c^\dagger c, \rho] \\
& + \pi \mathcal{D}_L (2\hat{T}_L c^\dagger \rho c \hat{T}_L - \{\hat{T}_L^2 cc^\dagger, \rho\}) \\
& + \pi \mathcal{D}_R (2\hat{T}_R^\dagger c \rho c^\dagger \hat{T}_R - \{\hat{T}_R^2 c^\dagger c, \rho\}) + \mathcal{L}_\gamma \rho, \quad (2)
\end{aligned}
$$

where $\mathcal{L}_\gamma \rho \equiv -(i\gamma/2)[x, \{p, \rho\}] - (\gamma/2)[x, [x, \rho]]$, $\{\bullet, \bullet\}$ denotes the anticommutator, $\gamma \ll 1$ is a dissipation rate, and time is measured in units of ω^{-1}. It follows from Eq. (2) that the time evolution of the electronic off-diagonal elements of the reduced density operator is decoupled from the evolution of the diagonal elements. After shifting the origin of the x axis to the point $x = d/2$ and introducing $\Gamma_\alpha(x) \equiv 2\pi \mathcal{D}_\alpha T_\alpha^2(x + d/2)$ we get the system of EOMs for the diagonal elements $\rho_{00} \equiv \langle 0|\rho|0\rangle$ and $\rho_{11} \equiv \langle 1|\rho|1\rangle$, where $|1\rangle = c^\dagger|0\rangle$:

$$
\begin{aligned}
\partial_t \rho_{00} = & -i\left[H_{\text{osc}} + \frac{d}{2}x, \rho_{00}\right] - \frac{1}{2}\{\Gamma_L(x), \rho_{00}\} \\
& + \sqrt{\Gamma_R(x)}\, \rho_{11} \sqrt{\Gamma_R(x)} + \mathcal{L}_\gamma \rho_{00}, \quad (3)
\end{aligned}
$$

$$
\begin{aligned}
\partial_t \rho_{11} = & -i\left[H_{\text{osc}} - \frac{d}{2}x, \rho_{11}\right] - \frac{1}{2}\{\Gamma_R(x), \rho_{11}\} \\
& + \sqrt{\Gamma_L(x)}\, \rho_{00} \sqrt{\Gamma_L(x)} + \mathcal{L}_\gamma \rho_{11}. \quad (4)
\end{aligned}
$$

In what follows we will deal with the evolution of the density operator $\rho_+ \equiv \rho_{00} + \rho_{11}$, which determines the expectation values of the observables in vibrational space, and $\rho_- \equiv \rho_{00} - \rho_{11}$, which describes the shuttling of electrons.

The problem under consideration can be solved analytically in the limit of a weak electromechanical coupling, $d/\lambda = e\mathcal{E}/(M\omega^2 \lambda_\star) \ll 1$. This limit has already been used in the classical description of shuttle phenomena [4,7], where it assured that an electric force acting on the charged island is much weaker than a typical elastic force. For simplicity, we will also assume that the tun-

neling coupling is symmetric, $\Gamma_L(0) = \Gamma_R(0) \equiv \Gamma/2$ and $\Gamma \ll 1$.

To study the vibrational dynamics near the ground state we use the small parameter $\lambda^{-1} \ll 1$ to linearize the problem with respect to the displacement x. The linearized system of equations, which describes the time evolution of the expectation value of the displacement $\bar{x}(t) \equiv \langle x \rangle$ and the momentum $\bar{p}(t) \equiv \langle p \rangle$, of the island ($\langle \bullet \rangle \equiv \text{Tr}\{\rho_+(t)\bullet\}$) has the following form:

$$
\begin{aligned}
\dot{\bar{x}} = \bar{p}, \qquad \dot{\bar{p}} = -\gamma \bar{p} - \bar{x} - \frac{d}{2} n_-, \\
\dot{n}_- = -\Gamma n_- + \frac{2\Gamma}{\lambda} \bar{x},
\end{aligned}
\quad (5)
$$

where $n_- \equiv 1 - 2\text{Tr}\rho_{11}$. An analysis of Eq. (5) shows that an initial deviation from the equilibrium point grows exponentially in time with rate constant $\alpha = (\gamma_{\text{thr}} - \gamma)/2$ if $\gamma < \gamma_{\text{thr}} = \Gamma d/\lambda$. Therefore, when the dissipation is below the threshold value γ_{thr}, the vibrational ground state becomes unstable.

The exponential increase of the displacement drives the system into the nonlinear regime of the vibrating dynamics, where the system may reach a stable stationary state. In order to study this regime we will use Wigner function analysis suggested in [15]. The Wigner distribution function (WDF) corresponding to the density operator $\rho_\pm$ is defined by

$$
W_\pm(x, p) \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\xi\, e^{-ip\xi} \left\langle x + \frac{\xi}{2}\Big|\rho_\pm\Big|x - \frac{\xi}{2}\right\rangle. \quad (6)
$$

After rescaling the displacement, $X \equiv x/\lambda$, and momentum, $P \equiv p/\lambda$, we obtain the following EOMs for the WDFs:

$$
\partial_t W_+ = [X\partial_P - P\partial_X + \hat{L}_1]W_+ + \hat{L}_2 W_-, \quad (7)
$$

$$
\partial_t W_- = [X\partial_P - P\partial_X + \hat{L}_1 - \Gamma_+]W_- + [\hat{L}_2 + \Gamma_-]W_+, \quad (8)
$$

where $\Gamma_\pm \equiv \Gamma_R(X) \pm \Gamma_L(X)$ and

$$
\hat{L}_1 \equiv \gamma\partial_P P + \frac{\gamma}{2\lambda^2}\partial_P^2 - \frac{\Gamma_+}{2}\sum_{n=1}^{\infty}\frac{(-)^n}{\lambda^{4n}(2n)!}\partial_P^{2n}, \quad (9)
$$

$$
\hat{L}_2 \equiv \frac{d}{2\lambda}\partial_P + \frac{\Gamma_-}{2}\sum_{n=1}^{\infty}\frac{(-)^n}{\lambda^{4n}(2n)!}\partial_P^{2n}. \quad (10)
$$

It is convenient to study the steady-state solution in polar coordinates, $X = A\sin\varphi$, $P = A\cos\varphi$. In these coordinates, the steady-state solution is determined by the system of equations

$$
[\partial_\varphi - \hat{L}_1]W_+ = \hat{L}_2 W_-, \quad (11)
$$

$$
[\partial_\varphi + \Gamma_+ - \hat{L}_1]W_- = [\hat{L}_2 + \Gamma_-]W_+, \quad (12)
$$

with the periodic boundary conditions $W_\pm(A, \varphi + 2\pi) = W_\pm(A, \varphi)$. After eliminating W_- from the system of Eqs. (11) and (12), we get a closed equation for W_+

$$[\partial_\varphi - \hat{L}]W_+ = 0, \qquad (13)$$

where $\hat{L} \equiv \hat{L}_1 + \hat{L}_2[1 - \hat{G}_0\hat{L}_1]^{-1}\hat{G}_0[\Gamma_- + \hat{L}_2]$ and $\hat{G}_0 \equiv [\partial_\varphi + \Gamma_+]^{-1}$ is defined on the space of functions which are 2π periodic in the variable φ. It is convenient to define a projector $\mathcal{P}$ which maps a 2π periodic function $f(\varphi)$ to its mean: $\mathcal{P}f(\varphi) \equiv \int_0^{2\pi} f(\varphi)d\varphi/(2\pi)$ and a projector $\mathcal{Q} \equiv 1 - \mathcal{P}$. We use these projectors to decompose W_+ into two parts: $W_+(A, \varphi) = \bar{W}_+(A) + \tilde{W}_+(A, \varphi)$, where $\bar{W}_+ \equiv \mathcal{P}W_+$ and $\tilde{W}_+ \equiv \mathcal{Q}W_+$. By inserting this decomposition into Eq. (13) and acting on this equation from the left with $\mathcal{P}$ and $\mathcal{Q}$, respectively, we obtain two coupled equations for $\bar{W}_+$ and $\tilde{W}_+$:

$$\mathcal{P}\hat{L}[\bar{W}_+ + \tilde{W}_+] = 0, \qquad (14)$$

$$[\partial_\varphi - \mathcal{Q}\hat{L}]\tilde{W}_+ = \mathcal{Q}\hat{L}\bar{W}_+. \qquad (15)$$

Formally solving Eq. (15) for $\tilde{W}_+$ and substituting the result into Eq. (14) gives a closed equation for $\bar{W}_+(A)$,

$$\mathcal{P}\hat{L}[1 - \hat{g}_0\mathcal{Q}\hat{L}]^{-1}\bar{W}_+(A) = 0, \qquad (16)$$

where $\hat{g}_0 \equiv \partial_\varphi^{-1}$ acts in the space of 2π-periodic functions with zero mean. One can see from Eq. (15) that $\tilde{W}_+$ is of lower order in the small parameters d/λ, λ^{-2}, and γ than $\bar{W}_+$. Therefore, in the leading order approximation we can write $W_+(A, \varphi) \approx \bar{W}_+(A)$. If we write the left-hand side of Eq. (16) in terms of A and φ and expand it to second order in the parameters d/λ, λ^{-2}, and γ, we get

$$A^{-1}\partial_A A[f(A) + D(A)\partial_A]\bar{W}_+(A) = 0, \qquad (17)$$

where

$$f(A) \approx \frac{A}{2}\left[\gamma - \frac{d}{\lambda}\alpha_0(A) - \frac{1}{2\lambda^4}\alpha_1(A)\right], \qquad (18)$$

$$D(A) \approx \frac{\gamma}{4\lambda^2} + \frac{1}{4\lambda^4}\beta_1 + \left[\frac{d}{2\lambda}\right]^2\beta_2 + \gamma\frac{d}{2\lambda}\beta_3 > 0, \qquad (19)$$

$\alpha_0 \equiv -A^{-1}\mathcal{P}\cos\varphi\, G$, $\alpha_1 \equiv A^{-1}\mathcal{P}\cos\varphi\,\Gamma_-\,\partial_P G$, $G \equiv \hat{G}_0\Gamma_-$, and $\beta_k = \beta_k(A, \Gamma)$.

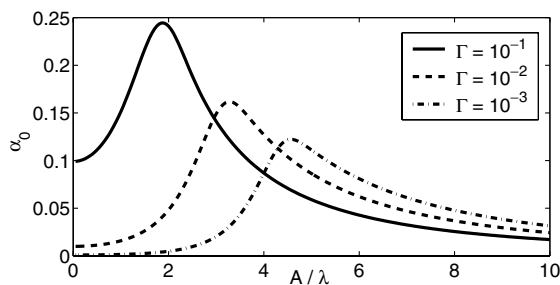We will see later that the functions $\alpha_0(A)$ and $\alpha_0(A)$ determine the behavior of $\bar{W}_+$. The positive function $\alpha_0(A)$ (see Fig. 1) behaves as $\Gamma(1 + A^2/2)$ in the vicinity of $A = 0$ and for large A it decreases as $\ln[2A/\Gamma]/(\pi A^2)$. The function $\alpha_1(A)$ (see Fig. 2) is positive and grows as $4A^2\Gamma^3/9$ for small A. For large A it is negative and goes to zero as $-2/(\pi A^2)$.

Solving Eq. (17) gives

$$\bar{W}_+(A) = Z^{-1}\exp\left\{-\int_0^A dA\,\frac{f(A)}{D(A)}\right\}, \qquad (20)$$

where Z is a normalization constant determined by the condition $2\pi\int_0^\infty dA\,A\,\bar{W}_+(A) = 1$.

The steady-state solution W_+ is localized in the phase space around points of maxima of $\bar{W}_+$. From Eq. (20) one can see that $\bar{W}_+$ has maxima at points A_M, where $f(A_M) = 0$ and $f'(A_M) > 0$. In the vicinity of these points, $\bar{W}_+$ is bell shaped and can be approximated by a Gaussian distribution function with variance $\sigma^2 \equiv D(A_M)/f'(A_M)$. Expanding Eq. (18) around $A = 0$, we find that $f \sim A(\gamma - \gamma_{\text{thr}})/2$ as $A \to 0$. Thus, $\bar{W}_+$ always has an extremum at $A = 0$: a maximum if $\gamma > \gamma_{\text{thr}}$ and a minimum if $\gamma < \gamma_{\text{thr}}$. This reflects the fact that the vibrational ground state is unstable when the dissipation is below the threshold value (the shuttle instability discussed above).

The global behavior of $\bar{W}_+$ depends on the electric field $\mathcal{E}$. We have found two different regimes: an electric field driven "classical" regime, where $\mathcal{E} \gg \mathcal{E}_q \equiv C(\Gamma)\hbar^2/(eM\lambda_x^3)$ and a "quantum" regime, when the electric field is weak, $\mathcal{E} \ll \mathcal{E}_q$. The dimensionless $C(\Gamma) \approx \max[\alpha_1(A)]/\max[\alpha_0(A)]$ depends only weakly on Γ (for $\Gamma = 10^{-3}$–10^{-1}, it is of the order of 10^{-2}).

In the classical regime, $\bar{W}_+$ has a maximum at finite $A = A_{\text{cl}}$, if the dissipation is sufficiently weak, $\gamma < \gamma_0 \equiv \max[\alpha_0(A)]d/\lambda > \gamma_{\text{thr}}$. The width of the WDF around A_{cl} is of the order of $\max\{d/\lambda, \lambda^{-3}d^{-1}\} \ll 1$, which allows for a classical interpretation of that regime. The value of A_{cl} corresponds to the stable limit cycle amplitude of the classical shuttle oscillations obtained in [4]. This amplitude increases as the value of the dissipation decreases and since $\alpha_0 > 0$, no stable state with finite A_{cl} is possible without external dissipation.

In the quantum regime, the structure of $\bar{W}_+$ is determined by the quantum fluctuations of the island energy driven by inelastic tunneling processes. In this

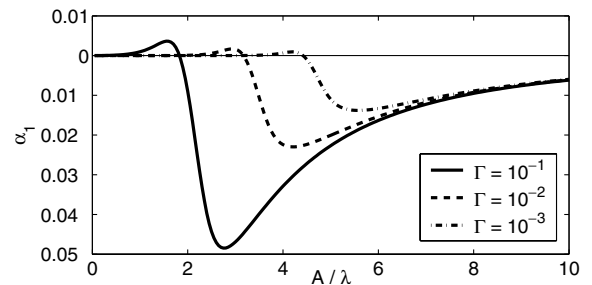FIG. 1. Function $\alpha_0(A)$ for $\Gamma/(\hbar\omega) = 10^{-1}, 10^{-2}, 10^{-3}$.

FIG. 2. Function $\alpha_1(A)$ for $\Gamma/(\hbar\omega) = 10^{-1}, 10^{-2}, 10^{-3}$.

case, the maximum of $\bar{W}_+$ appears at finite $A = A_q$, when the dissipation is below the critical value $\gamma_1 \equiv \max[\alpha_1(A)] x_0^4/(2\lambda_*^4)$. In contrast to the classical regime, A_q at low dissipation is determined by the zero of the function $\alpha_1(A)$ (see Fig. 2) and is still of the order of 1 even when the dissipation is zero. Despite the fact that the amplitude of the shuttle oscillations corresponding to the maximum of WDF is much greater then the amplitude of the zero point oscillations, the underlying steady state can not be interpreted as classical because the width of $\bar{W}_+(A)$ around A_q is no longer small compared to A_q.

The Wigner function W_+ describes the state of the vibrational degree of freedom, while W_- relates to the correlations between the charge state of the island and the state of the oscillator. It follows from Eq. (12) that $W_-(A, \varphi) \approx G(A, \varphi)\bar{W}_+(A)$. The WDF for the charged island is given by $W_{11} \equiv [W_+ - W_-]/2 \approx N(A, \varphi) \times \bar{W}_+(A)$, where $N \equiv \hat{G}_0\Gamma_L$ is the occupation of the classical shuttle with an amplitude A and frequency ω [7]. The WDF for the charged island exhibits qualitatively the same behavior as was observed numerically in [15].

The steady-state current through the system is given by $I = e\text{Tr}[\Gamma_L(x)\rho_{00}] \equiv \frac{e}{2}\int dX dP\,\Gamma_L(X)[W_+ + W_-]$ (see [15]). Using that $W_+ \approx \bar{W}_+$ and $W_- \approx G\bar{W}_+$, we get

$$I \approx \langle I_{cl}(A) \rangle, \qquad \langle \bullet \rangle \equiv 2\pi \int_0^\infty dA\, A\bar{W}_+(A)[\bullet], \quad (21)$$

where $I_{cl}(A) \equiv e\mathcal{P}\Gamma_L(X)\hat{G}_0\Gamma_R(X)$ is the time-averaged current through the classical shuttle [7]. Therefore, the current I is given by the classical expression $I_{cl}(A)$ averaged over the probability distribution $\langle \bullet \rangle$ of the amplitude A. The function $I_{cl}(A)$ grows monotonically from the tunneling current $e\Gamma/4$ at $A = 0$ to the shuttle current $I_{\text{shuttle}} \equiv e\omega/(2\pi)$, which is reached already at the amplitudes $A_{\text{shuttle}} \simeq 1$. In the classical regime the distribution is narrow and $I \approx I_{cl}(A_{cl})$, where A_{cl} is the stable limit cycle amplitude of the classical shuttle oscillations. Thus, in the classical regime the steady-state current is the same as in the classical shuttle case [7]. In the quantum regime, A_q grows (as the dissipation decreases) only as far as the zero A_0 of the function $\alpha_1(A)$, but since $I_{cl}(A_0) \approx I_{\text{shuttle}}$, one can see that the small quantum fluctuations result in a large shuttle current even at $\mathcal{E} = 0$ (as was observed numerically in [15]). This amplification is another manifestation of the mechanical instability in a nonequilibrium NEM-SET.

In conclusion, we have studied quantum shuttle phenomena in the NEM-SET in the realistic limit, when the electron tunneling length is much greater then the amplitude of the zero point oscillations of the island. It is shown that when the dissipation is sufficiently low, the vibrational ground state of the central island is unstable. This shuttle instability develops into the steady state corre-

sponding to pronounced shuttle vibrations. For large electrical fields between the leads this steady-state regime can be interpreted in classical terms. At low field a new quantum regime has been found.

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