Quantum Description of Shuttle Instability in Nanoelectromechanical Single Electron Transistor

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The voltage dependence of nanoelectromechanical effects in a system where the quantized mechanical vibrations of a quantum dot are coupled to coherent tunneling of electrons through a single level in the dot is studied. It is found that there are two different regimes depending on the value of the applied voltage. If the bias voltage is below a certain threshold value, then the state of the mechanical subsystem is located near its ground state. If the bias voltage is above the threshold value then the system becomes unstable which manifests itself in the expectation value of the displacement being an oscillating function of time with an exponentially increasing amplitude. This can be interpreted as a shuttle instability in a quantum regime.

Nanoelectromechanical systems (NEMS), where electronic and mechanical degrees of freedom are coupled is a new and fast growing branch of condensed matter physics. One such a system, a single-electron transistor (SET) where the conducting island has a vibrational degree of freedom associated with its center-of-mass motion (Fig.1), a so-called nanoelectromechanical-SET (NEM-SET), has been attracting a great deal of attention recently, both theoretically and experimentally.

In Ref. 3 it was shown, that the metallic grain placed between the two leads of NEM-SET becomes unstable and the periodic mechanical motion of the grain develops if a large bias voltage is applied between the leads. This phenomenon is usually referred to as a shuttle instability (see the review Ref. 20). A theory of the shuttle instability developed in Ref. 3 was based on the assumptions that both the charge on the island and its trajectory are well defined quantities. When we decrease the island size two different quantum effects manifest themself. Firstly, the electron energy level spacing in a nanometer-size grain is of the order of 10 K and resonant tunneling effects become essential at small enough temperatures. Therefore the single-electron energy spectrum can not be treated as continuous any more as it was done in Ref. 3. 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. This regime has been studied theoretically in Ref. 6.

Diminishing the size of the island further (down to 7 Å in diameter, for C60 molecule) results in the quantization of the mechanical motion of the island. A NEM-SET system in the regime of quantized mechanical motion of the central island was studied theoretically in Ref. 5. It was assumed that the phase breaking processes are strong enough to make the density matrix diagonal in the representation of the eigenstates of the quantum oscillator Hamiltonian |n⟩, which describes the mechanical subsystem. At the same time it is well known that the expectation value of the displacement operator in the eigenstates of a quantum oscillator are zero while it is the coherent state, which is a coherent superposition of all |n⟩, that approaches a description of the classical periodic motion of the oscillator as ħ → 0. The interesting question arises, therefore, how the expectation value of displacement operator evolves in time and what state results when the formal condition of the shuttle instability are satisfied for the quantum NEM-SET.

The approach used in Ref. 5 was further extended in Ref. 7 to include the position dependence of the tunneling matrix elements. However, the possibility of the shuttle instability effects was excluded by assuming a strong external...
dissipation. The case of the weak dissipation was studied in Ref. 6,12 in the limit of large voltages. The effect of a quantized vibrational mode on electron tunneling through a similar structure (a chain of three quantum dots) has been studied in Ref. 8.

In this article we will show that if a bias voltage between the leads is higher then a certain value, then the quantum state of the central island of the NEM-SET evolves in such a way that the expectation value oscillates in time with an increasing amplitude. This results shows that the shuttle instability is a fundamental phenomenon which exists even when the trajectory of the island and the charge on it are no longer well-defined.

We use the following Hamiltonian to model our system

\[ H = \sum_{\alpha,k} \epsilon_{\alpha k} a_{\alpha k}^\dagger a_{\alpha k} + \epsilon_d(X)c^\dagger c + \frac{p^2}{2M} + \frac{Mw_0^2X^2}{2} + \sum_\alpha T_\alpha(X)(A_{\alpha}^\dagger c + c^\dagger A_{\alpha}). \]  

(1)

Here \( A_{\alpha} \equiv \sum_k a_{\alpha k} \),

\[ \epsilon_d(X) = \epsilon_0 - dX, \]  

(2)

where \( d \) is proportional to an electric field between the leads,

\[ T_{L,R}(X) = T_0 \exp\{\mp X/\lambda\}, \]  

(3)

where \( \lambda \) is a characteristic tunneling length. The first term in the Hamiltonian describes the electrons in the leads, the second term relates to the single energy level in the central island, the third and forth terms to the quantized vibrational degree of freedom associated with center-of-mass motion of the central island and the last term describes tunneling between the electrodes and the island. All energies are measured from the Fermi energy of the leads. We assume that the electrons in each electrode are non-interacting with a constant density of states 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 central island is relevant to the problem.

It is convenient to introduce dimensionless operators for displacement, \( x \equiv X/r_0 \), and momentum, \( p \equiv r_0P/\hbar \), where \( r_0 \equiv \sqrt{\hbar/(MW_0)} \), and then measure all lengths in units of \( r_0 \) and all energies in units of \( \hbar w_0 \).

The Hamiltonian can now be written as

\[ H = H_{el} + H_{dot} + H_T, \]  

(4)

where

\[ H_{dot} \equiv \frac{1}{2} \left[ p^2 + x^2 \right] + \epsilon_d(x)c^\dagger c, \]  

(5)

\[ H_{el} \equiv \sum_{\alpha,k} \epsilon_{\alpha k} a_{\alpha k}^\dagger a_{\alpha k}, \]  

(6)

\[ H_T \equiv \sum_\alpha \left[ A_{\alpha}^\dagger C_{\alpha} + C_{\alpha}^\dagger A_{\alpha} \right], \quad C_{\alpha} \equiv T_\alpha(x)c. \]  

(7)

We will use an equation of motion (EOM) approach to study the time evolution of the operator \( x \) in the Heisenberg picture. In this approach we deal with the algebra of the time-dependent operators \( a_{\alpha k}(t), c(t), x(t), p(t) \) in the Heisenberg representation whose evolution can be described by a coupled system of EOMs. The EOM for the operator \( a_{\alpha k}(t) \) can be formally solved and eliminated from the system. The reduced system of EOMs is local in time under the condition of the wide-band approximation (\( D_{\alpha} = \text{const}, \) where \( D_{\alpha} \) is a density of state in the lead \( \alpha \)). It is shown in Appendix A that the evolution of an operator \( S = S(x,p,c^\dagger c) \) is described by the following quantum Langevin equation

\[ i\hbar \partial_t S = -i[S,H_{dot}] - \sum_{\alpha} \left\{ i\sqrt{\eta_{\alpha}} a_{\alpha}^\dagger - \frac{\eta_{\alpha}}{2} C_{\alpha}^\dagger \right\} [S,C_{\alpha}] - \sum_{\alpha} [S,C_{\alpha}^\dagger] \left\{ i\sqrt{\eta_{\alpha}} a_{\alpha} + \frac{\eta_{\alpha}}{2} C_{\alpha} \right\}, \]  

(8)

where

\[ a_{\alpha}(t) \equiv \frac{1}{\sqrt{\eta_{\alpha}}} \sum_k e^{-i\epsilon_{\alpha k}t} a_{\alpha k}(0), \quad \eta_{\alpha} \equiv 2\pi D_{\alpha}. \]  

(9)

For complete description we need also to know the evolution of \( c(t) \), which as shown in Appendix B is given by

\[ c(t) = \sum_{\alpha,k} e^{-i\epsilon_{\alpha k}t} B_{\alpha k}(t,0)a_{\alpha k}(0), \]  

(10)
where
\[ B_{ak}(t, t') = \frac{1}{i} T \int_{t'}^{t} dt_1 e^{i [\hat{t}_d - \epsilon_d + i \frac{\hat{\epsilon}}{2}] t_1} \hat{T}_a(t_1), \tag{11} \]
\( T \) is time-ordering operator, \( \hat{T}(t) \equiv \sum_{\alpha} \eta_a \hat{T}^2_\alpha(t), \hat{T}_a(t) \equiv T_a(x(t)), \epsilon_d(t) \equiv \epsilon_d(x(t)) \) and \( x(t) \) is the operator \( x \) in the Heisenberg picture.

We substitute \( x \) and \( p \) in Eq. (8) and get
\[ \dot{x} = p, \quad \dot{p} = -x + \hat{F}, \tag{12} \]
or
\[ \ddot{x} + x = \hat{F}, \tag{13} \]
where
\[ \hat{F} \equiv dc^\dagger c + 2\lambda^{-1} \sum_{\alpha} (\alpha \epsilon - \alpha \beta) \sqrt{\epsilon} \alpha \beta \alpha \delta_{\alpha \beta} \left\{ a^\dagger_{\alpha \beta} \right\}. \tag{14} \]

To study the shuttle instability in the quantum regime we assume that dimensionless parameters \( 1/\lambda \) and \( d \) are small which allows us to linearize the problem with respect to \( x \). Eq. (10) then reads
\[ c(t) = T_0 \sum_{\alpha, k} e^{-i \epsilon_{\alpha k} t} \left\{ G^+_{\alpha k} + i \left[ dG^+_{\alpha k} + \left( -\frac{\alpha}{\lambda} \right)^2 \right] X_{\alpha k}(t) \right\} a_{\alpha k}(0). \tag{15} \]
Here \( G^+_{\alpha k} \equiv [\epsilon_{\alpha k} - \epsilon_0 + i \Gamma/2]^{-1} \), \( \Gamma = \sum_{\alpha} \eta_a T_0^2 \), \( T_0 \) is defined in Eq. (3),
\[ X_{\alpha k}(t) \equiv \int_0^t d\tau e^{i [\epsilon_{\alpha k} - \epsilon_0 + i \frac{\hat{\epsilon}}{2}](t-\tau)} x(\tau) \tag{16} \]
and the linearized force operator \( \hat{F} \) has the following form
\[ \hat{F} \equiv \hat{F}_1 + \hat{F}_2, \tag{17} \]
where
\[ \hat{F}_1 \equiv T_0^2 \sum_{\alpha, k} e^{i [\epsilon_{\alpha k} - \epsilon_{\beta q}]} a^\dagger_{\alpha k}(0) a_{\beta q}(0) \left\{ -\frac{x}{\lambda^2} \left[ G^-_{\alpha k} + G^+_{\beta q} \right] + i \left[ X_{\beta q} - X^*_{\alpha k} \right] \left[ dG^-_{\alpha k} + \left( -\frac{\alpha}{\lambda} \right) \left[ dG^+_{\beta q} + \left( \frac{\beta}{\lambda} \right) \right] \right] \right\} \tag{18} \]
is the term of the first order in the small parameters \( d \) and \( \lambda^{-1} \) and
\[ \hat{F}_2 \equiv T_0^2 \sum_{\alpha, k} e^{i [\epsilon_{\alpha k} - \epsilon_{\beta q}]} a^\dagger_{\alpha k}(0) a_{\beta q}(0) \left\{ -\frac{x}{\lambda^2} \left[ G^-_{\alpha k} + G^+_{\beta q} \right] + i \left[ X_{\beta q} - X^*_{\alpha k} \right] \left[ dG^-_{\alpha k} + \left( -\frac{\alpha}{\lambda} \right) \left[ dG^+_{\beta q} + \left( \frac{\beta}{\lambda} \right) \right] \right] \right\} \tag{19} \]
is the second order term in \( d \) and \( \lambda^{-1} \). Thus the above linearization of the force \( F \) corresponds to its expansion up to second order in \( d \) and \( \lambda^{-1} \).

Averaging Eq. (18) with respect to the initial density operator we obtain EOM for the expectation value of the displacement of the dot. If we only take into account effects up to second order in \( T_0 \) (Born approximation), we can make the following factorization in the RHS of Eq. (18)
\[ \langle x(t) a^\dagger_{\alpha k}(0) a_{\beta q}(0) \rangle \approx \langle x(t) \rangle f_{\alpha k} \delta_{\alpha k, \beta q}, \tag{20} \]
where \( f_{\alpha k} \equiv [1 + e^{(\epsilon_{\alpha k} + \epsilon V/2)/(kT)}]^{-1} \). Then
\[ \bar{x} + \ddot{x} = \hat{F} \left[ x(\tau) \right], \tag{21} \]
where \( \bar{x}(t) \equiv \langle x(t) \rangle - x_0, x_0 \equiv (d/2) \sum_{\alpha} f_{\alpha}(\epsilon_0), f_{\alpha}(E) \equiv [1 + e^{(E + \epsilon V/2)/(kT)}]^{-1} \) and
\[ \hat{F} \left[ x(\tau) \right] \equiv -2T_0^2 \sum_{\alpha k} f_{\alpha k} \text{Im} \left[ X_{\alpha k} \right] \left\{ -\frac{\alpha}{\lambda} \right\}^2. \tag{22} \]
It is remarkable that Eq. (21) with $\bar{F}$ given by Eq. (22) is the same as the Newton’s equation used in Ref. 6. It is well-known that for an isolated quantum harmonic oscillator the equation of motion for the expectation values of displacement and momentum is exactly the same as the classical Hamiltonian equations (Ehrenfest theorem). However, it is not obvious that this statement is valid for the harmonic oscillator coupled to some degrees of freedom. Therefore, it follows from Eq. (22) that the Ehrenfest theorem is valid for the system under consideration if the tunneling is weak.

We solve Eq. (21) by Laplace transforms and obtain

$$\ddot{x}(t) \approx -x_0 e^{rt} \cos t,$$

where

$$r \equiv \frac{\Gamma}{8} \sum_{\alpha} \left\{ \left[ d + \frac{1}{\lambda} \right]^2 f_{\alpha, +1} - \left[ d - \frac{1}{\lambda} \right]^2 f_{\alpha, -1} \right\},$$

and $f_{\alpha, \pm 1} \equiv f_{\alpha}(\epsilon_0 \pm 1)$. The sign of $r$ depends on the bias voltage and can be easily analyzed if the temperature is zero. If the bias voltage is below the threshold value $V_c$, defined by $eV_c = 2(\epsilon_0 + 1)$, then $f_{\alpha, +1} = 0$ and $r \leq 0$. In this case $\ddot{x}(t)$ exponentially goes to zero (point $\bar{x} = 0$ is stable). If the voltage is above the threshold value, then $f_{\alpha, \pm 1} = 1$, $f_{\alpha, \pm 1} = 0$ and $r = \Gamma d/(2\lambda)$. In this case $\ddot{x}(t)$ oscillates with exponentially growing amplitude (point $\bar{x} = 0$ is unstable) and the corresponding state of the mechanical subsystem moves further and further from the ground state.

In conclusion, we have studied stability of a system where the quantized mechanical vibrations of a quantum dot are coupled to coherent tunneling of electrons through a single level in the dot. Two different regimes have been found. For bias voltages above a certain threshold value (which, in the case of zero temperature, is defined by the position of the level in the dot plus the energy of a vibrational quantum) the system is unstable. In this regime the expectation value of the displacement is an oscillating function of time with an exponentially increasing amplitude, which is the signature of a shuttle instability in a quantum regime. Below the threshold the system is stable even without any external damping of the dot’s motion.

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**APPENDIX A**

The equation of motion for $a_{\alpha k}(t)$ is given by

$$\partial_t a_{\alpha k} = i[H, a_{\alpha k}] = -i\epsilon_{\alpha k}a_{\alpha k} - iC_\alpha.$$

We formally solve Eq. (A1) to obtain

$$a_{\alpha k}(t) = e^{-i\epsilon_{\alpha k}t}a_{\alpha k}(0) - i \int_0^t dt_1 e^{-i\epsilon_{\alpha k}(t-t_1)}C_\alpha(t_1).$$

Then by using the wide-band approximation ($D_\alpha = \text{const}$) we get

$$A_\alpha(t) = \sqrt{\eta_\alpha}a_\alpha(t) - i \frac{\eta_\alpha}{2}C_\alpha(t),$$

where

$$a_\alpha(t) \equiv \frac{1}{\sqrt{\eta_\alpha}} \sum_k e^{-i\epsilon_{\alpha k}t}a_{\alpha k}(0), \quad \eta_\alpha \equiv 2\pi D_\alpha.$$

If $S = S(x, p, c^\dagger c)$, then its equation of motion is

$$\dot{S} = -i[S, H_{\text{dot}}] - i \sum_\alpha \{ A^\dagger_\alpha [S, C_\alpha] + [S, C^\dagger_\alpha]A_\alpha \}.$$

Combining Eqs. (A3) and (A5) yields Eq. (8).
APPENDIX B

The equation of motion for $c(t)$ reads

$$\dot{c}(t) = i[H, c] = -i\dot{c}_d(t)c(t) - i\sum_\alpha \hat{T}_\alpha(t)A_\alpha(t), \quad (B1)$$

where $\dot{c}_d(t) \equiv c_d(x(t))$, $\hat{T}_\alpha(t) \equiv T_\alpha(x(t))$ and $x(t)$ is operator $x$ in the Heisenberg picture. Combining Eqs. (A3) and (B1) gives

$$\dot{c}(t) = -i \left[ \dot{c}_d(t) - i\frac{\dot{\Gamma}(t)}{2} \right] c(t) - i\sum_\alpha \sqrt{\eta_\alpha} \hat{T}_\alpha(t)a_\alpha(t). \quad (B2)$$

The solution of Eq. (B2) for $t \gg \|\dot{\Gamma}\|^{-1}$ is given by Eq. (10).