Quantum Precursor of Shuttle Instability

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The effects of a coupling between the quantized mechanical vibrations of a quantum dot and coherent tunneling of electrons through a single level in the dot are studied. The equation of motion for the reduced density operator describing the vibrational degree of freedom is obtained. It is shown that the expectation value of the displacement is an oscillating function of time with an exponentially increasing amplitude, which is the signature of a quantum shuttle instability.

Nanoelectromechanical systems (NEMS), where electronic and mechanical degrees of freedom are coupled, have been attracting a great deal of attention recently. An important example of such a system is the nanoelectromechanical single-electron transistor (NEM-SET) — a structure where the movable conducting island is elastically coupled to the electrodes (Fig.1).

![Model shuttle system consisting of a movable conducting island placed between two leads. An effective elastic force acting on the dot from the leads is described by the parabolic potential.](image)

FIG. 1: Model shuttle system consisting of a movable conducting island placed between two leads. An effective elastic force acting on the dot from the leads is described by the parabolic potential.

In Ref. 3 it was shown, that the NEM-SET becomes unstable with respect to the development of periodic mechanical motion if a large enough bias voltage is applied between the leads. This phenomenon is usually referred to as a shuttle instability. The key issue in Ref. 3 was that the charge on the island, \( q(t) \), is correlated with its velocity, \( \dot{x}(t) \), in such a way that the time average \( \langle q(t)\dot{x}(t) \rangle > 0 \) even if \( \langle \dot{x}(t) \rangle = 0 \) (see the review Ref. 4). A classical theory of the shuttle instability was based on the assumptions that both the charge on the island and its trajectory are well defined quantities.

A decrease of the island size should result in modifications of the electromechnanical phenomena in a NEM-SET as more quantum mechanical effects come into play. There are two different types of quantum effects which manifest itself as the island size decreases. The first one is the discreteness of the energy spectrum. 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. 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. The NEM-SET in this regime has been studied theoretically in Refs. 3 and 7 and the conditions for the shuttle instability to appear have been found.

Diminishing the size of the island further results in the quantization of the mechanical motion of the island. As a result not only the charge on the island but also its trajectory experience strong quantum fluctuations and the picture of the shuttle instability, which was elaborated in Refs. 3 and 7 is no longer valid.

A NEM-SET system in the regime of quantized mechanical motion of the central island was studied theoretically in Ref. 3. 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 \( |\nu\rangle \), 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 \( |\nu\rangle \), that approaches a description of the classical periodic motion of the oscillator as \( \hbar \to 0 \). 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.

In this article we will show that if a large enough bias voltage is applied between the leads, then the quantum state of the central island of the NEM-SET evolves in such a way that the expectation value of the displacement operator is not identically zero. Rather, it 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

\[
H = \sum_{\alpha,k} \epsilon_{\alpha k} a_{\alpha k}^\dagger a_{\alpha k} + \{\epsilon_0 - e\mathcal{E}X\} c^\dagger c + \frac{P^2}{2M} + \frac{M w_0^2 X^2}{2} + \sum_{\alpha,k} T_\alpha(X)(a_{\alpha k}^\dagger c + c^\dagger a_{\alpha k}).
\]

The first term in the Hamiltonian describes the electrons
in the electrodes, 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. Here we assume that only one single electron state is available in the central island and that the electrons in each electrode are non-interacting with a constant density of states.

Let us introduce dimensionless operators for displacement, \( x \equiv X/r_0 \), and momentum, \( p \equiv r_0P/h \), where \( r_0 \equiv \sqrt{\hbar/(Mw_0)} \), and then measure all lengths in units of \( r_0 \) and all energies in units of \( hw_0 \).

In order to transfer the \( x \)-dependence of the island energy level to the term describing tunneling, we make the unitary transformation

\[
\hat{H} = U H U^\dagger, \quad U \equiv e^{i\alpha x/cp} \quad (2)
\]

The Hamiltonian can now be written as

\[
\hat{H} = \hat{H}_e + \hat{H}_v + \Omega, \quad (3)
\]

where

\[
\begin{align*}
\hat{H}_e &\equiv \sum_{\alpha,k} \epsilon_{\alpha k}a_{\alpha k}^\dagger a_{\alpha k} + \hat{\epsilon}_0c^\dagger c \equiv H_a + H_e, \\
\hat{H}_v &\equiv \frac{p^2}{2} + \frac{x^2}{2}, \\
\Omega &\equiv \sum_{\alpha,k} T_{\alpha} \left\{ \Omega^\alpha \epsilon_{\alpha k}^*c + h.c. \right\},
\end{align*}
\]

with \( \Omega^\alpha \equiv e^{i\alpha x}T_\alpha(x) \), \( \hat{\epsilon}_0 \equiv \epsilon_0 - Mw_0^2d^2/2 \) and \( d \equiv e\mathcal{E}/(Mw_0^2) \).

The evolution of the system is described by the Liouville-von Neumann equation for the total density operator \( \sigma \):

\[
i\partial_t \sigma = [\hat{H}, \sigma] = [\hat{H}_e + \hat{H}_v, \sigma] + [\Omega, \sigma]. \quad (7)
\]

It is convenient to transform Eq. (7) into the interaction picture, defined by

\[
\hat{\sigma}(t) \equiv e^{i(H_e+H_v)t}\sigma(t)e^{-i(H_e+H_v)t},
\]

Then

\[
i\partial_t \hat{\sigma}(t) = [\hat{\Omega}(t), \hat{\sigma}(t)], \quad (9)
\]

where

\[
\hat{\Omega}(t) \equiv e^{i(H_e+H_v)t}\Omega(t)e^{-i(H_e+H_v)t}. \quad (10)
\]

In what follows we will assume that electrons in the leads are weakly coupled to the rest of the system and that the leads are so large that their statistical properties are unaffected by the weak coupling. Then the following approximation can be made

\[
\hat{\sigma}(t) \approx \hat{\rho}(t) \otimes \sigma_L \otimes \sigma_R. \quad (11)
\]

Since we are interested in the evolution of the variables describing the central island we need an equation of motion only for the reduced density operator. If we trace over the electrodes degrees of freedom directly in Eq. (11) we obtain zero in the RHS, which means that the effect is of the higher order with respect to \( \Omega \).

If we formally integrate both sides of Eq. (11) and substitute the result back into the RHS of Eq. (11), we obtain an integro-differential equation with RHS of the second order with respect to \( \Omega \).

\[
\partial_t \hat{\sigma}(t) = -i[\hat{\Omega}(t), \hat{\sigma}(0)] - \int_0^t dt_1 [\hat{\Omega}(t_1), [\hat{\Omega}(t_1), \hat{\sigma}(t_1)]]. \quad (12)
\]

We trace out the electrode degrees of freedom and get the integro-differential equation for the reduced density operator

\[
\partial_t \hat{\rho}(t) = -\text{Tr}_a \left\{ \int_0^t dt_1 \left[ \hat{\Omega}(t_1), \left[ \hat{\Omega}(t_1), \hat{\sigma}(t_1) \right] \right] \right\}, \quad (13)
\]

where \( \hat{\rho}(t) \equiv \text{Tr}_a \{ \hat{\sigma}(t) \} \) is the reduced density operator in the interaction representation and the trace is over the electrode degrees of freedom. The first term in Eq. (13) gives zero because we choose such initial condition that \( \sigma(0) = \rho(0) \otimes \sigma_L \otimes \sigma_R \).

By using Eq. (11) we obtain

\[
\partial_t \hat{\rho}_t = -\sum_\alpha \int d\mathcal{D}_\alpha \int_0^t dt_1 e^{i\mathcal{E}(t-t_1)} \times \left\{ \left\{ \Omega_\alpha \epsilon_t^\dagger \Omega_\alpha \epsilon_t \right\}_t \hat{\rho}_t - \left\{ \Omega_\alpha \epsilon_t^\dagger \hat{\rho}_t \Omega_\alpha \epsilon_t \right\}_t \right\} f_\alpha^+ + \left\{ \hat{\rho}_t \left( \Omega_\alpha \epsilon_t^\dagger \Omega_\alpha \epsilon_t \right)_t - \left\{ \Omega_\alpha \epsilon_t^\dagger \hat{\rho}_t \Omega_\alpha \epsilon_t \right\}_t \right\} f_\alpha^- \quad + h.c., \quad (14)
\]

where \( f_\alpha^+ \equiv f_\alpha^\dagger = [1 + e^{\beta(\epsilon_t - \mu_\alpha)}]^{-1} \), \( f_\alpha^- \equiv 1 - f_\alpha \) and \( \mathcal{D}_\alpha \) is the density of states in the corresponding lead.

This integro-differential equation becomes a differential equation if we consider the case of zero temperature, \( T = 0 \), and large bias voltage, \( eV \to \infty \).

\[
\partial_t \hat{\rho}_t = \pi \mathcal{D}_L \left[ 2(\Omega_L \epsilon_t^\dagger)_{t} \hat{\rho}_t (\Omega_L \epsilon_t)_{t} - \left\{ (\Omega_L \epsilon_t^\dagger)_{t} (\Omega_L \epsilon_t)^{\dagger} \right\}_{t} \hat{\rho}_t \right] \\
+ \pi \mathcal{D}_R \left[ 2(\Omega_R \epsilon_t^\dagger)_{t} \hat{\rho}_t (\Omega_R \epsilon_t)_{t} - \left\{ (\Omega_R \epsilon_t^\dagger)_{t} (\Omega_R \epsilon_t)^{\dagger} \right\}_{t} \hat{\rho}_t \right] \quad (15)
\]

To describe the evolution of the oscillator variables we need only \( \hat{\rho}_0 = \rho(0) \otimes \sigma_L \otimes \sigma_R \) and \( \hat{\rho}_{1,1} = \rho(1) \otimes \sigma_L \otimes \sigma_R \), where \( |1\rangle \equiv c^\dagger |0\rangle > \). The corresponding equations for \( \rho_{0,0} \) and \( \rho_{1,1} \) are given by

\[
\partial_t \hat{\rho}_{0,0} = -\pi \mathcal{D}_L \left\{ \Omega_L^\dagger \Omega_L \hat{\rho}_{0,0} \right\} + 2\pi \mathcal{D}_R \Omega_R^\dagger \hat{\rho}_{1,1} \Omega_R, \quad (16)
\]

\[
\partial_t \hat{\rho}_{1,1} = -\pi \mathcal{D}_L \left\{ \Omega_L^\dagger \Omega_L \hat{\rho}_{1,1} \right\} + 2\pi \mathcal{D}_L \Omega_L \hat{\rho}_{0,0} \Omega_L^\dagger, \quad (17)
\]

It is convenient to change from \( \rho_{0,0} \) and \( \rho_{1,1} \) to \( R_0 \) and \( R_1 \) given by

\[
R_0(t) \equiv e^{i\mathcal{E}t} e^{-i\mathcal{E}t} \rho_{0,0} e^{i\mathcal{E}t} e^{-i\mathcal{E}t}, \quad (18)
\]

\[
R_1(t) \equiv e^{i\mathcal{E}t} e^{-i\mathcal{E}t} \rho_{1,1} e^{i\mathcal{E}t} e^{-i\mathcal{E}t}. \quad (19)
\]
Then
\begin{align*}
\partial_t R_0 &= -i \left[ H_v \left( x + \frac{d}{2} \right), R_0 \right] - \frac{1}{2} \left\{ \hat{\Gamma}_L(x), R_0 \right\} \\
&\quad + \sqrt{\hat{\Gamma}_R(x) R_1 \sqrt{\hat{\Gamma}_R(x)}}, \quad (20) \\
\partial_t R_1 &= -i \left[ H_v \left( x - \frac{d}{2} \right), R_1 \right] - \frac{1}{2} \left\{ \hat{\Gamma}_R(x), R_1 \right\} \\
&\quad + \sqrt{\hat{\Gamma}_L(x) R_0 \sqrt{\hat{\Gamma}_L(x)}}, \quad (21)
\end{align*}
where \( \hat{\Gamma}_{L,R}(x) \equiv \Gamma_{L,R}(x+d/2) \) and \( \Gamma_\alpha(x) \equiv 2\pi D_\alpha T^\alpha_0(x) \). These two equations completely describe the evolution of the vibrational degree of freedom.

By using Eqs. (20) and (21) we can obtain the equations of motion for any momenta with respect to the density operators \( R_+ \equiv R_0 + R_1 \) and \( R_- \equiv R_0 - R_1 \). We expand \( \hat{\Gamma}_{L,R}(x) \) to first order with respect to the displacement, \( \hat{\Gamma}_{L,R}(x) = (1 \mp x/\lambda)\hat{\Gamma}_{L,R}(0) \), where \( \lambda \) is characteristic tunneling length, and leave only terms of the first order with respect to \( \lambda^{-1} \).

In the quasisymmetric case, \( \hat{\Gamma}_L(0) = \hat{\Gamma}_R(0) \), the equations for \( n_- \), \( x_+ \) and \( p_+ \) are decoupled from the rest,
\begin{align*}
\dot{x}_+ &= p_+, \quad (22) \\
\dot{p}_+ &= -x_+ - d n_-, \quad (23) \\
\dot{n}_- &= -\hat{\Gamma} n_- + \frac{2\gamma}{\lambda} x_+ \quad (24)
\end{align*}
and equations for the second momenta are decoupled from the higher momenta,
\begin{align*}
\partial_t \langle x^2 \rangle_+ &= \langle \{p, x\} \rangle_+, \quad (25) \\
\partial_t \langle p^2 \rangle_+ &= -\langle \{p, x\} \rangle_+ - 2dp_-, \quad (26) \\
\partial_t \langle \{p, x\} \rangle_+ &= -2\langle x^2 \rangle_+ + 2\langle p^2 \rangle_+ - 2dx_-, \quad (27) \\
\dot{x}_- &= p_+ - \hat{\Gamma} x_- + \frac{2\gamma}{\lambda} \langle x^2 \rangle_+, \quad (28) \\
\dot{p}_- &= -x_- - d - \hat{\Gamma} p_- + \frac{\hat{\Gamma}}{\lambda} \langle \{p, x\} \rangle_+, \quad (29)
\end{align*}
where \( \langle \bullet \rangle_+ \equiv \text{Tr} \{ R_\pm \bullet \} \), \( n_- \equiv \langle 1 \rangle_- \), \( x_\pm \equiv \langle x \rangle_\pm \) and \( p_\pm \equiv \langle p \rangle_\pm \) and \( \hat{\Gamma} \equiv \hat{\Gamma}_L(0) + \hat{\Gamma}_R(0) \).

The characteristic equation for the system of Eqs. (22-24) is given by
\begin{equation}
(\alpha^2 + 1)(\alpha + \hat{\Gamma}) + 2\gamma = 0, \quad \gamma \equiv \frac{d}{\lambda} \ll 1 \quad (30)
\end{equation}
and has three roots
\begin{equation}
\alpha_1 \approx -\hat{\Gamma} \left[ 1 + \frac{2\gamma}{\hat{\Gamma}^2 + 1} \right], \quad (31)
\end{equation}
\begin{equation}
\alpha_2 \approx i + \frac{\gamma}{1 - i\hat{\Gamma}}, \quad \alpha_3 \approx \alpha_2^*, \quad (32)
\end{equation}
The first root is a negative real number, which corresponds to a solution which exponentially goes to zero. The last two roots have positive real parts and non-zero imaginary parts, which gives rise to oscillating solutions with exponentially increasing amplitudes. The expectation value \( \tau(t) \equiv \text{Tr} \{ U^\dagger \sigma(t) U x \} \) of the displacement operator \( x \) depends on \( x_+ \) as follows: \( \tau(t) = x_+ + d/2 \). This means that when we apply a high enough bias voltage between the leads the expectation value of the displacement starts to oscillate with an increasing amplitude with respect to the point \( x = d/2 \) of the original coordinate system.

The characteristic equation for the system of Eqs. (23-24) is given by
\begin{equation}
\alpha^4 + (\hat{\Gamma} + \alpha^2)[1 + (\hat{\Gamma} + \alpha^2)] + 2\gamma[4\hat{\Gamma} \alpha + 5\alpha^2 - 4] = 0, \quad (33)
\end{equation}
and has five roots
\begin{align*}
\alpha_1 &\approx \frac{2\gamma}{\hat{\Gamma}^2 + 1}, \quad (34) \\
\alpha_2 &\approx 2i + \frac{2\gamma}{1 - i\hat{\Gamma}}, \quad \alpha_3 \approx \alpha_2^*, \quad (35) \\
\alpha_4 &\approx -\hat{\Gamma} + i, \quad \alpha_5 \approx \alpha_4^*. \quad (36)
\end{align*}
The first root gives a non-oscillatory solution of exponentially growing amplitude. The remaining four roots correspond to oscillatory solutions with increasing \( \alpha_2 \) and \( \alpha_3 \) and decreasing amplitudes \( \alpha_4 \) and \( \alpha_5 \), respectively. Thus the energy of the oscillator, which is given by the sum of the two second momenta \( \langle x^2 \rangle_+ \) and \( \langle p^2 \rangle_+ \), exponentially grows with time.

The importance of the position dependence of \( T_\alpha(x) \) can be seen if we let \( \lambda \rightarrow \infty \) in the above treatment. Then we find that the energy grows linearly with time, while the average displacement does not grow.

In conclusion, we have studied a quantum shuttle system where the quantized mechanical vibrations of a quantum dot are coupled to coherent tunneling of electrons through a single level in the dot. We have obtained the equation of motion for the reduced density operator describing the vibrational degree of freedom. It was shown that the expectation value of the displacement is an oscillating function of time with an exponentially increasing amplitude, which is the signature of a quantum shuttle instability.
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9 As this article was prepared for submission we learned that an approach similar to ours is used by T. Novotny and A.-P. Jauho (private communication) to analyze the stationary behaviour of a quantum shuttle system.