Shuttle instabilities: semiclassical phase analysis

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Abstract

We present a semiclassical analysis of the instability of an electron shuttle composed of three quantum dots: two are fixed and coupled via leads to electron reservoirs at $\mu_L, R$ with $\mu_L \gg \mu_R$, while the central dot is mounted on a classical harmonic oscillator. The semiclassical analysis, which is valid if the central dot oscillation amplitude is larger than the quantum mechanical zero point motion, can be used to gain additional insight about the relationship of resonances and instabilities of the device.

Key words: NEMS, Quantum Dot, Shuttle transport
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In nano-electromechanical systems (NEMS) the electrical and mechanical properties are deeply interconnected. An archetypal NEMS device consists of a movable object connected to leads [1]. The charge distribution gives rise to an electrical force, which influences the mechanical dynamics, while the position of the movable object determines the tunneling rates from the leads and thus influences the electrical dynamics of the system. A current through the device can sustain mechanical oscillations even in the presence of damping. An interesting regime of transport arises when only one electron per cycle is transferred from the left to the right lead. Due to the position dependent tunneling amplitude the movable part gets charged when near to the left lead, then the electrostatic force pushes it towards the right lead where the now enhanced tunneling rate helps the release of the electron.

We describe the electronic part with the density matrix formalism and couple the master equation to a classical equation of motion for the central dot position [1]. We perform a linear instability analysis of the system to pinpoint where the equilibrium solution for the system becomes unstable leading to Hopf bifurcations; the relative phase between charge, velocity and position of the unstable rotating solution shows the features of shuttling in agreement with the quantum-phase-space description [2].

The semiclassical approach is justified by the quantum-classical correspondence since the dot oscillations are bigger than the minimum quantum amplitude. However the mean field approach for the electric part neglects the effect of shot noise and the damping factor threshold is usually very much reduced compared to the quantum treatment. The semiclassical analysis is also much easier to handle numerically.
1. The model

Consider a simple NEMS consisting a small metallic grain (or a QD) connected to two leads. The grain is moving in a parabolic potential. Two additional dots, one on each side of the oscillating component, fix the energy of the incoming and outgoing electrons \([3]\). The Hamiltonian of the system is \(H = H_{\text{mech}} + H_{el}\), where

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\]

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\[
H_{\text{mech}} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2
\]

\[
H_{el}(x) = \sum_{i,j=L,C,R} |i\rangle \epsilon_{ij}(x) \langle j|
\]

We assume strong Coulomb blockade regime, thus the vectors \(|i\rangle\), \(i = L, C, R\), together with the empty state \(|0\rangle\), span the entire single particle Hilbert space of the device. The matrix elements are explicitly:

\[
\epsilon(x) = \begin{bmatrix}
\frac{\Delta V}{2} & t_L(x) & 0 \\
t_L(x) & -\frac{\Delta V}{2x_0} & t_R(x) \\
0 & t_R(x) & -\frac{\Delta V}{2}
\end{bmatrix}
\]

\(\Delta V\), the device bias, is the difference between the energy of the left and the right dot. \(x_0\) is half the distance between the two outer dots and represents the maximum amplitude of the inner dot oscillation. The three dots are electrically connected only via a tunneling mechanism. The tunneling length is given by \(1/\alpha\) and the tunneling strength depends on the position \(x\) of the inner grain,

\[
t_L(x) = V_0e^{-\alpha(x_0+x)}
\]

\[
t_R(x) = V_0e^{-\alpha(x_0-x)}
\]

The electric part of the NEMS is described in the density matrix formalism. The Hilbert space has dimension four, though the corresponding four-by-four density matrix can be reduced to an effective three-by-three matrix since the elements of the form \(\rho_{0i}, i = L, C, R\) are decoupled from the others and \(\rho_{00}\) can be eliminated using \(\sum_i \rho_{0i} = 1\). This effective density matrix obeys the generalized master equation:

\[
\dot{\rho} = -i[H, \rho] + \Xi \rho
\]

The first term represents the coherent evolution of the electrons in the three dots isolated from the leads.

The coupling to the leads is introduced in the wide band approximation following Gurvitz \([4]\) and gives the second term of the equation \((\Xi \rho)\):

\[
\Xi \rho = \Gamma \begin{bmatrix}
1 - \rho_{LL} - \rho_{CC} - \rho_{RR} & 0 & -\rho_{LR}/2 \\
0 & 0 & -\rho_{PC}/2 \\
-\rho_{RL}/2 & -\rho_{RC}/2 & -\rho_{PP}
\end{bmatrix}
\]

where \(\Gamma\) is the injection rate to the leads. The equation of motion for the central dot position has a conservative part deduced from the (quantum-)averaged Hamiltonian \(\langle H \rangle = H_{\text{mech}} + \text{Tr}(\rho H_{el}(x))\) and a phenomenological damping term:

\[
\dot{x} = \frac{\partial \langle H \rangle}{\partial p} = \frac{p}{m}
\]

\[
\dot{p} = -\frac{\partial \langle H \rangle}{\partial x} - \gamma p = -m\omega^2 x + \frac{\Delta V}{2x_0}\rho_{CC} - \gamma p + \alpha t_L(\rho_{CL} + \rho_{LC}) - \alpha t_R(\rho_{CR} + \rho_{RC})
\]

2. Instability analysis

In the shuttling regime the electrical and the mechanical component of the system evolve with the same time scale. Thus it is important to treat all degrees of freedom on equal footing: we introduce a set of generalized coordinates \(q\), and write the Eqs. \((5,7)\) as

\[
\dot{q}_i = F_i(q)
\]

and linearize around the equilibrium, \((0 \equiv F(q^0)):\)

\[
\dot{q}_i = \mathcal{M}_{ij}(q_j - q^0_j) + ...
\]

where \(\mathcal{M}_{ij} = \partial_i F_j|_{q=q^0}\). In general, even if the velocity of the central dot is zero, a current can flow through the system and is given by \(I = \Gamma \rho_{RR}\). Let us study the equilibrium position and electronic configuration of the three dot system as a function of the device bias. At \(\Delta V = 0\) the central dot is at rest in the middle (we will take this as zero position). This unique solution appears natural, but in fact is not obvious if one recognizes the presence of an exchange force that acts on the dot \(i.e.\) the last line of Eq. 7 \(^2\). As the difference between the energy of the left and right dot is increased the equilibrium position of the central dot shifts to the

\(^2\) We thank the Chalmers group for suggesting this point during private communications.
right, but then returns to zero again for high device biases (Fig. 1a). This reveals a competition between the electrostatic force and the progressively dominating decoupling of the three dots due to the mismatch of their energy levels. The equilibrium occupation of the three dots also reflects this decoupling (Fig. 1b).

In the limit of high device biases the left dot has the highest probability of being occupied while the others are almost empty. At small biases the equilibrium occupation is strongly dependent on the injection rate $\Gamma$. In this regime the ratio between the injecting rate and the bare tunneling probability $r = \Gamma/(V_0e^{-\alpha x_0})$ accurately describes the scenario. If $r \ll 1$ the three dots are almost isolated and their coherent oscillations are damped by the contacts, but so slowly that the three dots tend to a uniform stationary occupation. In the opposite limit ($r \gg 1$) the left dot is continuously refilled and the right emptied at a rate which overcomes the dot’s dynamical response. The left and central dot share the occupation probability while the right dot is empty and the empty state occupation probability vanishes.

The quantum description of the shuttle device shows that the central dot can oscillate with an amplitude which is much bigger than the minimum uncertainty length $\Delta x$. We expect the equilibrium solution of the semiclassical description to be unstable in the same parameter range (except for the damping: the lack of noise sources in the present semiclassical approach reduces the instability threshold). The vector $\mathbf{q} = [p_L, p_C, p_R, \rho_L, \rho_C, \rho_R, \rho_{LR}, \rho_{CR}, \rho_{RR}]$ has an electrical part (the first 9 components) and a mechanical part (the last 2 components). The matrix $\mathcal{M}$ is written in a block form, consistent with this natural separation:

$$\mathcal{M} = \begin{bmatrix} A & C \\ D & B \end{bmatrix}$$

The eigenvalues of $\mathcal{M}$ represent the characteristic frequencies and damping for small oscillation of the position and the density matrix around the equilibrium configuration. If at least one of the eigenvalues of $\mathcal{M}$ has a positive real part then the equilibrium solution is unstable. In the general case all the four blocks of the matrix $\mathcal{M}$ depend on both the electrical and mechanical degree of freedom. But if we set $x_0 = 1/\alpha$ and take the limit $\alpha \to 0$, the off-diagonal blocks of the $\mathcal{M}$ ($C$ and $D$) vanish and the eigenvalues are those of $A$ (electrical) and $B$ (mechanical). The imaginary part of the spectrum consists of the Bohr frequencies (i.e., all possible differences between the eigenvalues) of the isolated electron system and the mechanical frequency of the oscillator (Fig. 2a). The real part of the spectrum, though, is negative due to the presence of the leads and the mechanical damping (Fig. 2b). As $\alpha$ is increased, the spectrum of $\mathcal{M}$ gets a positive real part: two instability regions appear (Fig. 2b). They have the form of Hopf bifurcations: for these parameters the solution of Eq. 8 is a limit cycle. Correspondingly, in the unstable regime, the imaginary part of the spectrum shows crossings between the “electrical” and “mechanical” frequencies (arrows in Fig. 2a). These are resonances between the oscillator and the electrical modes of the three dots. They appear $\Delta V \simeq \omega$ and $2\omega$. The slight shift from the exact values is due to the bare interaction $V_0$ which modifies the electronic spectrum of the Hamiltonian from the decoupled 0, $\pm \Delta V/2$ (which remains as asymptotic behavior).

Only an analysis of the eigenvectors can demonstrate the actual oscillation of both the electric and mechanical components in the limit cycle solution. For this reason we have studied the electrical and mechanical weight of the eigenvectors in the unstable regime (Fig. 3a). The larger the real part of the unstable eigenvalue, the higher is the mixing of the two components.

![Fig. 1. Equilibrium position (a) and equilibrium electronic configuration (b) as a function of the device bias for three different injection rates $\Gamma = 0.05, 0.5, 5$.](image-url)
In the quantum description [2], the shuttling instability is characterized by a strong correlation between charge, position and velocity of the oscillating dot. Therefore we study next the relative phase between charge, velocity and position of the unstable solution, even if a priori it is not clear whether this property will be maintained in the limit cycle stationary solution. The phase analysis shows, for a given charge configuration (that for definiteness we take maximal) a decrease in the position and velocity phase: for both resonances the charged dot passes from maximal position and zero velocity to minimal position and zero velocity. The range of phase rotation is decreasing together with the instability in the case with $\Delta V \approx \omega$ (Fig. 3b). This rotation of the charged dot configuration in phase space is also in qualitative agreement with the quantum analysis.

Fig. 2. Imaginary (a) and real (b) part of the spectrum of $M$ for different values of tunneling length. $\alpha = 0, 0.1, 0.2, 0.5$. The instability grows with $\alpha$. Only the four eigenvalues with positive imaginary part are plotted. The system is symmetric to complex conjugation. The three eigenvalues with zero imaginary part are omitted for simplicity: they represent always damped modes.

Fig. 3. Eigenvector analysis as a function of device bias. a) The relative amplitude of the electrical (full) and mechanical (dot dashed) components of the unstable eigenvector. The relative amplitude of the two components tends to be equal in the instability region and the effect is more prominent for higher $\alpha$. b) The phase of position (full) and velocity (dot dashed) with respect to the phase of the charge in the central dot for the unstable eigenvector.

framework to identify the correspondence between instability and resonance in the NEMS. Also the rotation of the phase space configuration of the charged dot in the shuttling regime was detected. More work is needed to understand whether other characteristics of the system such the higher order instabilities ($\Delta V \approx 3\omega, 4\omega, ...$) are pure quantum phenomena.

3. Conclusions

In this work we have analyzed the instabilities of a triple-dot shuttle using a semiclassical approach, motivated by the “semiclassical behavior” of the quantum description. We were able in this simple and intuitive

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References

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