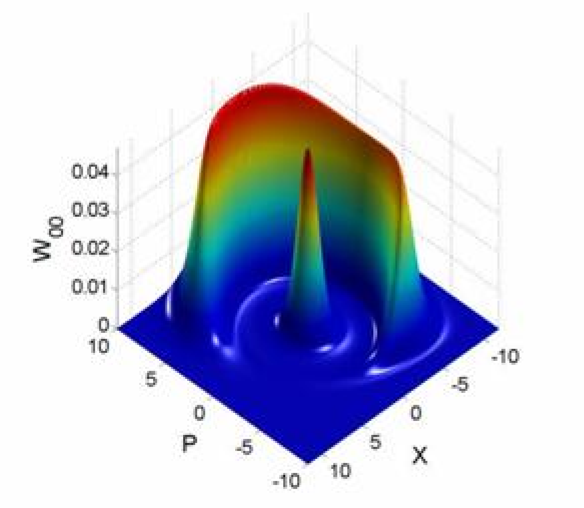
Quantum Shuttles

Andrea Donarini



Windberg, 29th September 2005

Shuttle Device

- Definition of Electron Shuttling
- Experimental implementations
- Model

Investigation Tools

- Phase space
- Current
- Noise

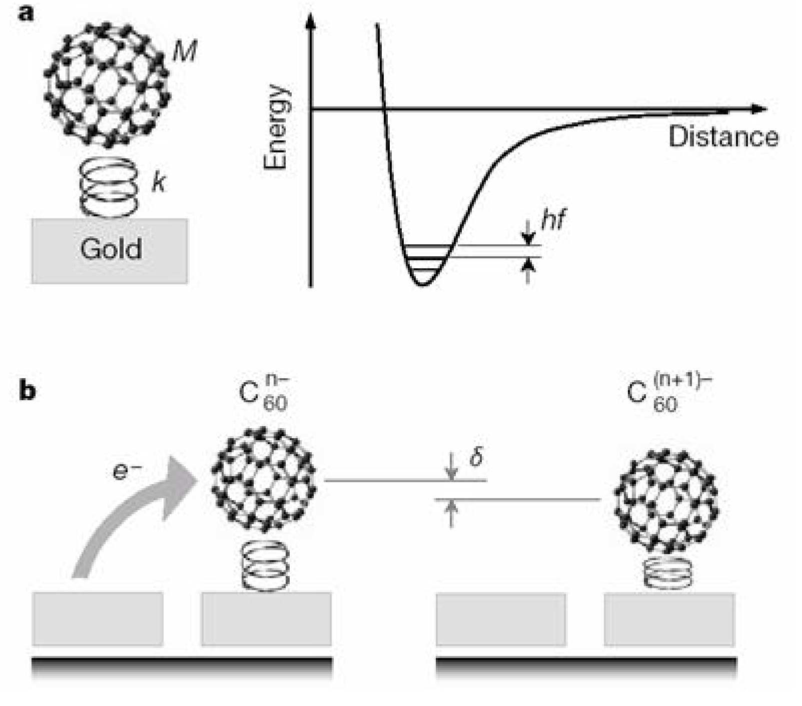
Three Regimes

- Tunneling
- Shuttling
- Coexistence regime

Shuttling

- Is a particular single-electron transport regime
- Occurs in systems with a crucial nanometer scale
- Exhibits a strongly ordered interplay between electrical and mechanical degrees of freedom

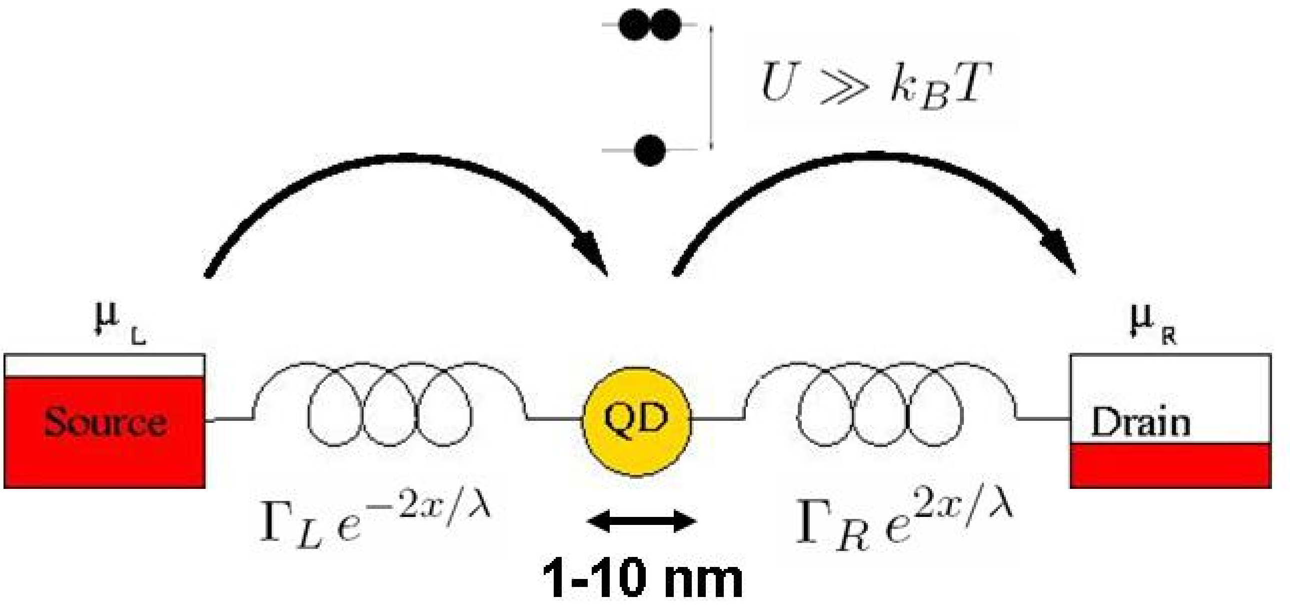
Examples of (quasi-) shuttle devices



A.Erbe, et al Phys. Rev.Lett. 87(2001) 096106

H.Park, et Nature **407** (2000) 57

Simplest model*

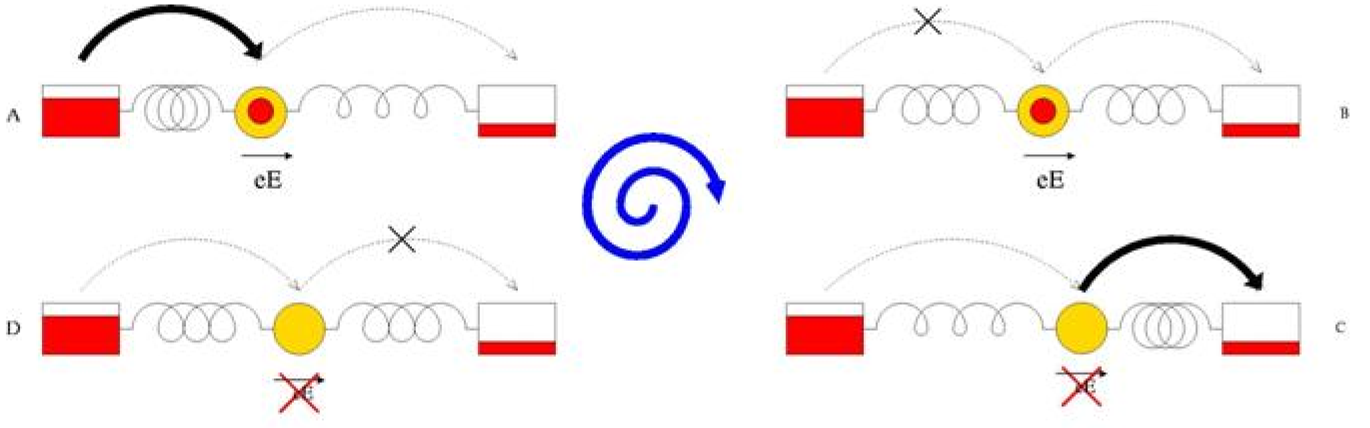


- QD has a nanometric diameter: combined with low temperature, this implies **Coulomb blockade**
- Excess of charge on QD produces an electrostatic force that influences the **mechanical dynamics** of the QD
- Position of the QD influences the **electrical dynamics** via the tunneling amplitudes
- **Energy is conserved** within a cycle due to electrostatic driving and mechanical damping

* L. Y. Gorelik et al., Phys. Rev. Lett. 80, 4526 (1998)

Particular single electron transport regime

Source-drain DC voltage drives the QD to mechanical instability. Eventually the system shows periodic behavior and self-sustained oscillations.



- The current in the shuttling regime is determined by the mechanical frequency:

$$I_{sh} = \frac{\omega e}{2\pi}$$

- The system exhibits charge-position (charge-momentum) correlation

- Injection rates and mechanical frequency are comparable: the process in NON-adiabatic.

Model

The Hamiltonian for the model:

$$H = H_{sys} + H_{leads} + H_{bath} + V + H_{int}$$

where

$$H_{sys} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - eEx|1\rangle\langle 1|$$

$$H_{leads} = \sum_{k;\alpha=L,R} (\epsilon_{k\alpha} - \mu_\alpha) c^\dagger{}_{k\alpha} c_{k\alpha}$$

$$V = \sum_{k;\alpha=L,R} T_{k\alpha}(x) c^\dagger{}_{k\alpha} |0\rangle\langle 1| + h.c.$$

$$H_{bath} + H_{int} = \text{generic heat bath}$$

The tunneling rates from and to the leads:

$$\Gamma_{L,R}(x) = \frac{2\pi}{\hbar} D_{L,R} \exp\left(\mp \frac{2x}{\lambda}\right) |T_{L,R}(0)|^2$$

- λ sets the sensitivity of the mechanical feedback

- $\langle\Gamma(x)\rangle$ is the typical time scale of electrical dynamics

Method

- The time evolution of the density matrix is described by ($\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|$) :

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho]$$

- Since we are not interested in the information about the bath, we introduce the reduced density matrix:

$$\sigma \equiv \mathrm{Tr}_B(\rho)$$

- In the limit of high bias, wide band and low temperature a markovian **Generalized Master Equation** for the reduce density matrix can be written:

$$\begin{aligned}
\dot{\sigma}_{00} =& -\frac{i}{\hbar}[H_{osc}, \sigma_{00}] + \mathcal{L}_{damp}\,\sigma_{00} \\
& - \frac{\Gamma_L}{2}\{e^{-\frac{2x}{\lambda}}, \sigma_{00}\} + \Gamma_R\, e^{\frac{x}{\lambda}}\,\sigma_{11}\, e^{\frac{x}{\lambda}} \\
\dot{\sigma}_{11} =& -\frac{i}{\hbar}[H_{osc} - eEx, \sigma_{11}] + \mathcal{L}_{damp}\,\sigma_{11} \\
& - \frac{\Gamma_R}{2}\{e^{\frac{2x}{\lambda}}, \sigma_{11}\} + \Gamma_L\, e^{-\frac{x}{\lambda}}\,\sigma_{00}\, e^{-\frac{x}{\lambda}}
\end{aligned}$$

Where:

$$\mathcal{L}_{damp}\,\sigma = \frac{i\gamma}{2\hbar}[x, \{p, \sigma\}] + \frac{\gamma m \omega}{\hbar}(\bar{n} + 1/2)[x, [x, \sigma]]$$

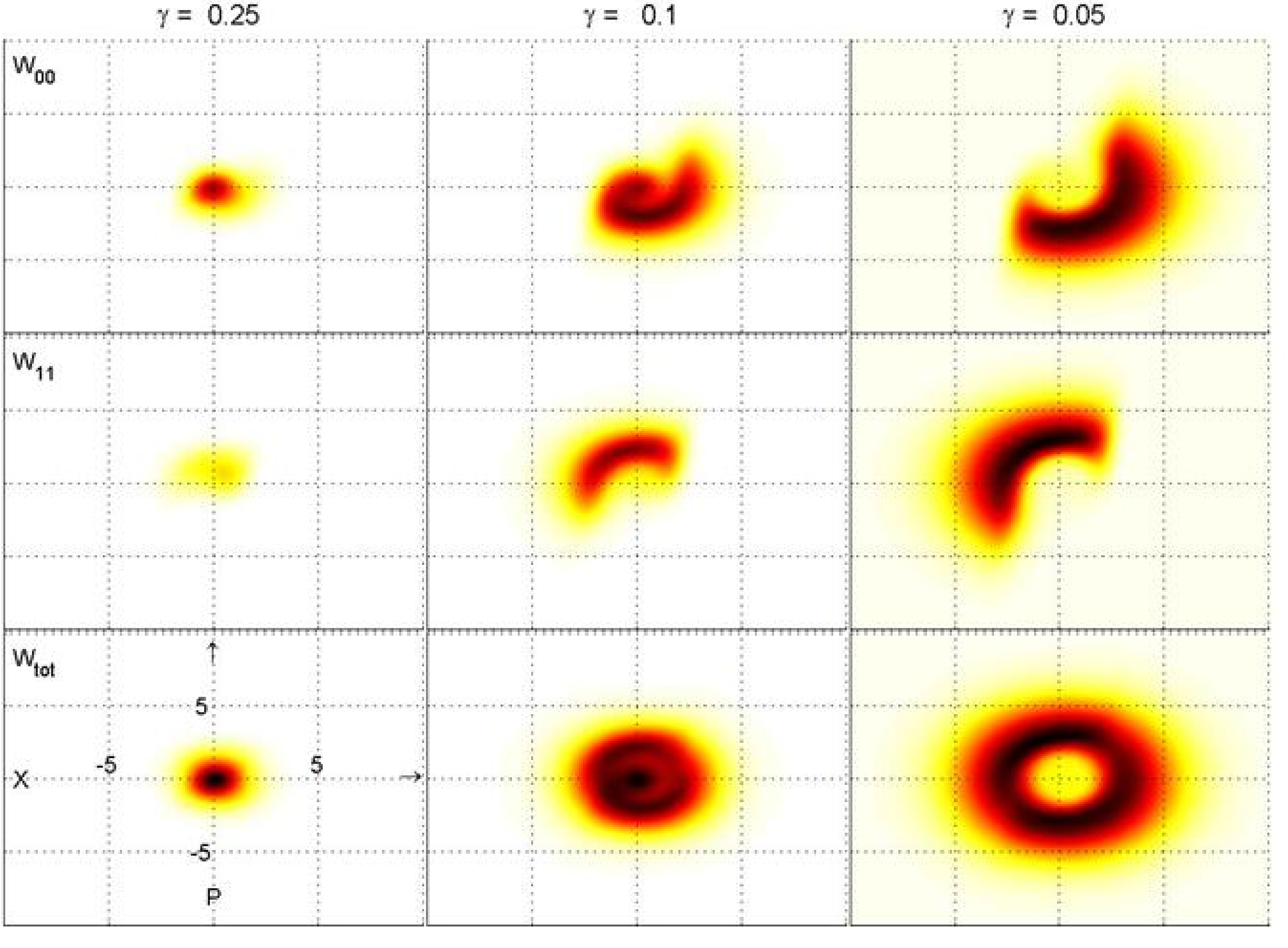
Charge-position correlation

We look for the stationary solution of the GME:

$$\mathcal{L}\sigma^{stat} = 0$$

And represent it in the phase space of the system:

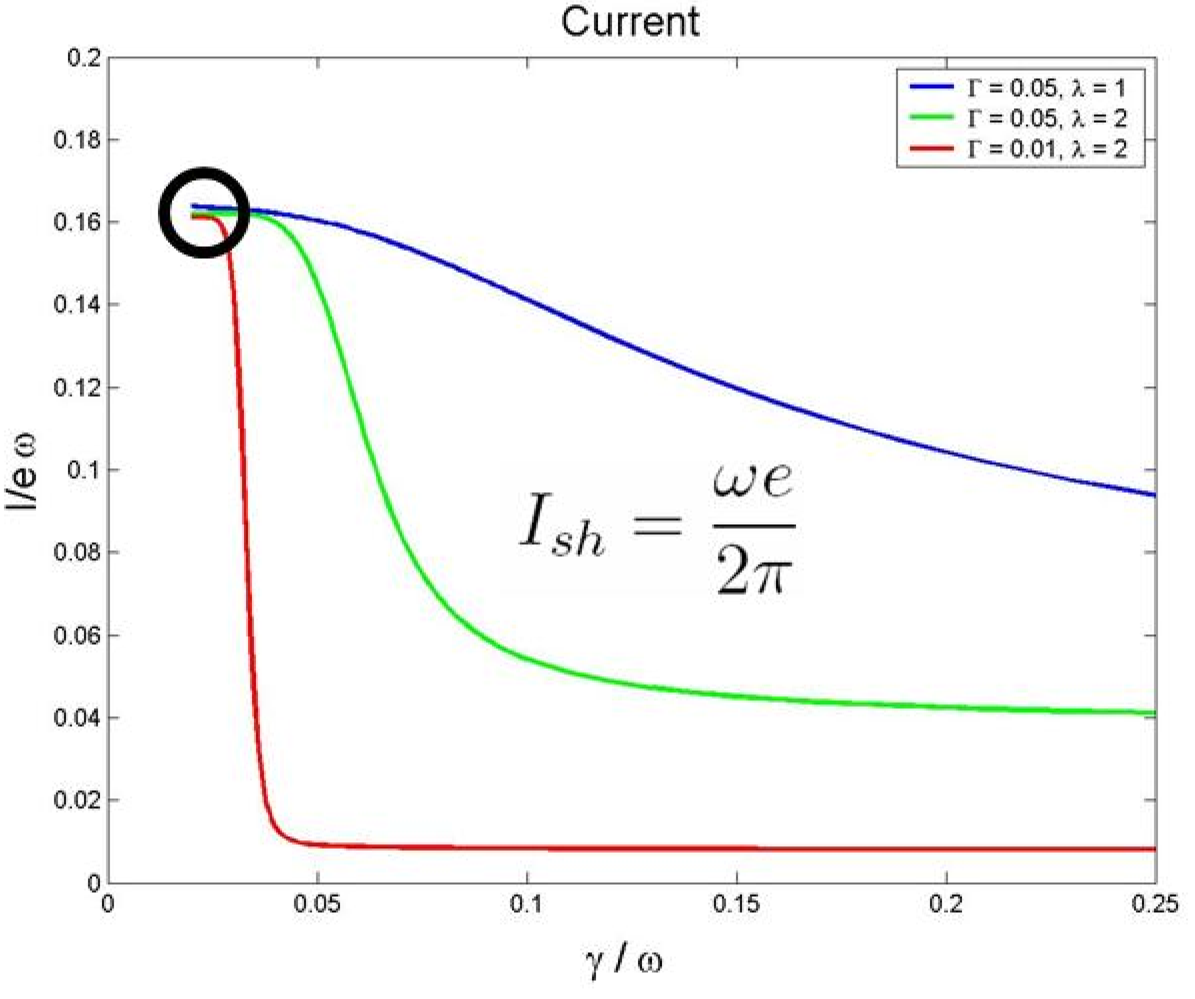
$$W_{ii}(X,P) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{d}\xi \left\langle X - \frac{\xi}{2}\right| \sigma_{ii}^{stat} \left| X + \frac{\xi}{2}\right\rangle \exp\left(i\frac{P\xi}{\hbar}\right)$$



Current

Given the stationary state σ^{stat} we can calculate the average current:

$$I = \Gamma_R \, \mathrm{Tr}_{osc}\left(e^{\frac{2x}{\lambda}} \, \sigma_{11}^{stat}\right) = \Gamma_L \, \mathrm{Tr}_{osc}\left(e^{-\frac{2x}{\lambda}} \, \sigma_{00}^{stat}\right)$$



In the deep shuttling regime the current has a value which only depends on the mechanical frequency.

Noise Calculation

For the noise calculation it is useful to introduce the GME resolved with respect to the number of electrons collected in the right lead:

$$\begin{aligned}\dot{\sigma}_{00}^{(n)} &= -\frac{i}{\hbar}[H_{osc}, \sigma_{00}^{(n)}] + \mathcal{L}_{damp}\, \sigma_{00}^{(n)} \\ &\quad - \frac{\Gamma_L}{2}\{e^{-\frac{2x}{\lambda}}, \sigma_{00}^{(n)}\} + \Gamma_R\, e^{\frac{x}{\lambda}}\, \sigma_{11}^{(n-1)}\, e^{\frac{x}{\lambda}} \\ \dot{\sigma}_{11}^{(n)} &= -\frac{i}{\hbar}[H_{osc} - eEx, \sigma_{11}^{(n)}] + \mathcal{L}_{damp}\, \sigma_{11}^{(n)} \\ &\quad - \frac{\Gamma_R}{2}\{e^{\frac{2x}{\lambda}}, \sigma_{11}^{(n)}\} + \Gamma_L\, e^{-\frac{x}{\lambda}}\, \sigma_{00}^{(n)}\, e^{-\frac{x}{\lambda}}\end{aligned}$$

The probability that ***n*** electrons have passed through the device at time ***t*** reads:

$$P_n(t) = \mathrm{Tr}_{osc}[\sigma_{00}^{(n)}(t) + \sigma_{11}^{(n)}(t)] \quad *$$

Current and noise can be expressed in terms of these probabilities:

$$I = e\frac{d}{dt}\sum_n nP_n(t)\Big|_{t\to\infty} = e\sum_n n\dot{P}_n(t)\Big|_{t\to\infty}$$

$$S(0) = 2e^2\frac{d}{dt}\left[\sum_n n^2 P_n(t) - \Big(\sum_n nP_n(t)\Big)^2\right]\Bigg|_{t\to\infty}$$

* B. Elattari and S. A. Gurvitz, Physics Letters A 292, 289 (2002).

Using the GME for the number resolved density matrix $\sigma_{ii}^{(n)}$ one can recover the expression for the current:

$$I = \Gamma_R \,\mathrm{Tr}_{osc}\left(e^{\frac{2x}{\lambda}}\,\sigma_{11}^{stat}\right) = \Gamma_L \,\mathrm{Tr}_{osc}\left(e^{-\frac{2x}{\lambda}}\,\sigma_{00}^{stat}\right)$$

The zero frequency noise spectrum, measured by the Fano factor, reads:

$$F = \frac{S(0)}{2eI} = 1 - \frac{2e\Gamma_R}{I}\mathrm{Tr}_{osc}\left(e^{\frac{2x}{\lambda}}\left[\mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}\begin{pmatrix} \Gamma_R e^{\frac{x}{\lambda}}\,\sigma_{11}^{stat}\,e^{\frac{x}{\lambda}} \\ 0 \end{pmatrix}\right]_{11}\right)$$

Where

$$\mathcal{Q} = 1 - \mathcal{P} \quad \text{and} \quad \mathcal{P}\bullet = \begin{pmatrix} \sigma_{00}^{stat} \\ \sigma_{11}^{stat} \end{pmatrix} \mathrm{Tr}_{sys}(\bullet)$$

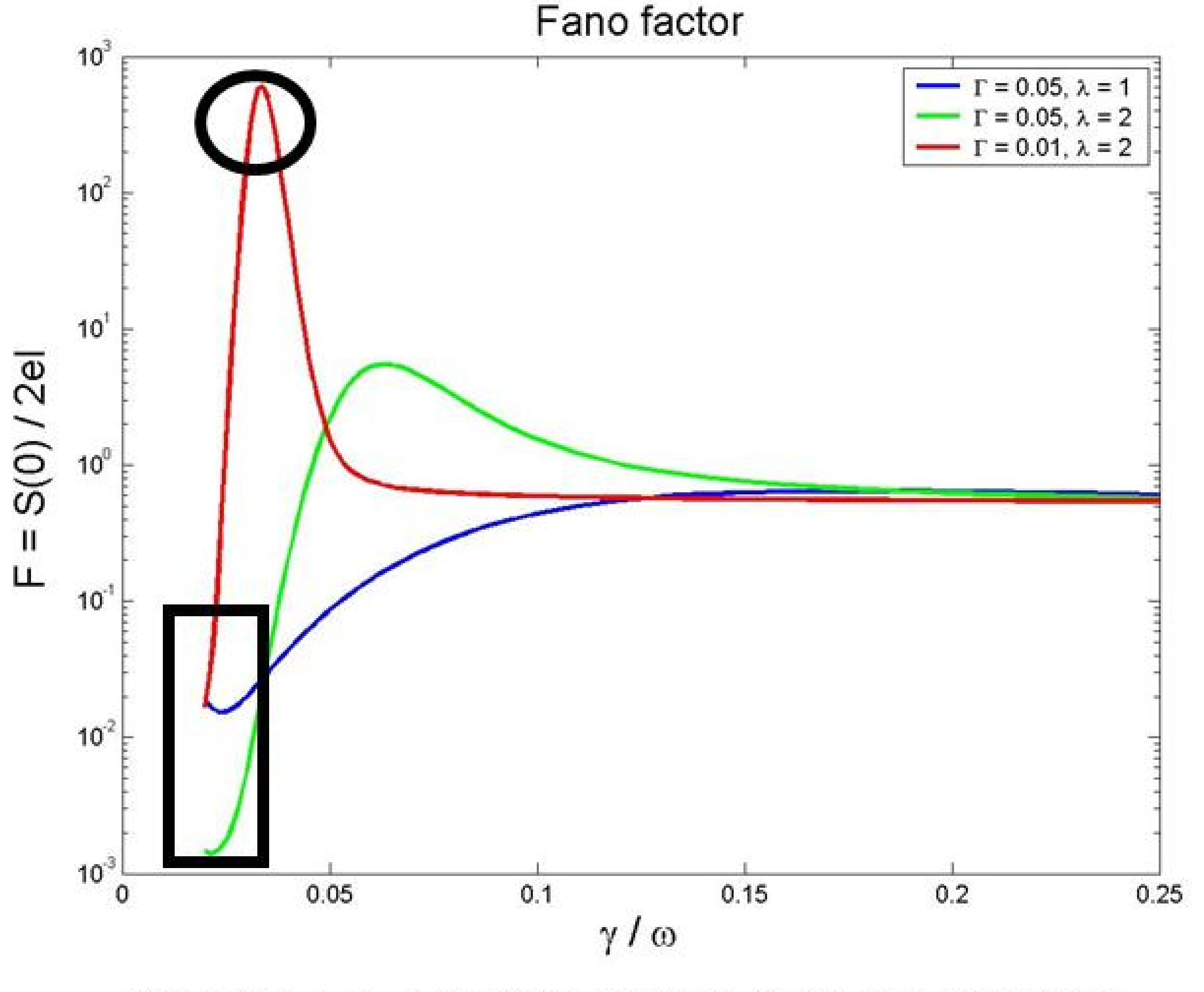
Even if the Liouvillian has no inverse, the expression

$$\mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}$$

Has the meaning of a pseudo inverse.

Noise Results

$$F = \frac{S(0)}{2eI} = 1 - \frac{2e\Gamma_R}{I}\mathrm{Tr}_{osc}\left(e^{\frac{2x}{\lambda}} \left[\mathcal{QL}^{-1}\mathcal{Q} \left(\begin{array}{c} \Gamma_R e^{\frac{x}{\lambda}}\, \sigma_{11}^{stat}\, e^{\frac{x}{\lambda}} \\ 0 \end{array} \right) \right]_{11} \right)$$



- Shuttling is a highly ordered single electron transport regime
- "Divergent" Fano factor in coexistence regimes are reported in literature:

  A. Isacsson and T. Nord, cond-mat/0402228

  E. Sukhorukov, G.Burkard, D. Loss Phys. Rev. B 63, 125315 (2001)

Three regimes

Changing the external damping the single dot shuttle device goes into three different regimes:

- **Tunneling regime – high damping**

  Wigner function shows the oscillator in its ground state and almost no charge resolution

  Current is dependent on injection rates and tunneling length

  Fano factor approaches the characteristic value of 0.5 typical for 2-state model describing the sequential tunneling

- **Shuttling regime – low damping**

  Wigner function shows the oscillator in a quasi-classical ring shape and exhibits strong correlation between charge and position

  Current is determined by the mechanical frequency of the oscillator and corresponds to one electron per cycle

  Extremely low **Fano** factors give a measure for the highly ordered regime

- **Coexistence regime – intermediate damping**

  Wigner function shows the coexistence of ground state and excited ring

  Current is intermediate between the shuttling and the tunneling values

  The HUGE values of the **Fano** factor suggest the presence of slow switching independent current channels.

Tunneling regime

Between a charging or discharging event of the QD the oscillator has time to relax into its ground state.

$$\left\langle \Gamma_{L,R} \exp\left(\mp\frac{2x}{\lambda}\right)\right\rangle_{stat} \ll \gamma$$

The current and Fano factor are given by:

$$I = e\frac{\tilde{\Gamma}_L\tilde{\Gamma}_R}{\tilde{\Gamma}_L+\tilde{\Gamma}_R} \qquad F = \frac{\tilde{\Gamma}_L^2+\tilde{\Gamma}_R^2}{(\tilde{\Gamma}_L+\tilde{\Gamma}_R)^2}$$

where

$$\tilde{\Gamma}_L = \Gamma_L \mathrm{Tr}_{osc}\left(e^{-\frac{2x}{\lambda}}\sigma_{osc}(0)\right)$$

$$\tilde{\Gamma}_R = \Gamma_R \mathrm{Tr}_{osc}\left(e^{\frac{2x}{\lambda}}\sigma_{osc}(eE)\right)$$

$$\sigma_{osc}(l) = \frac{1}{Z}e^{-\beta(H_{osc}-lx)}$$

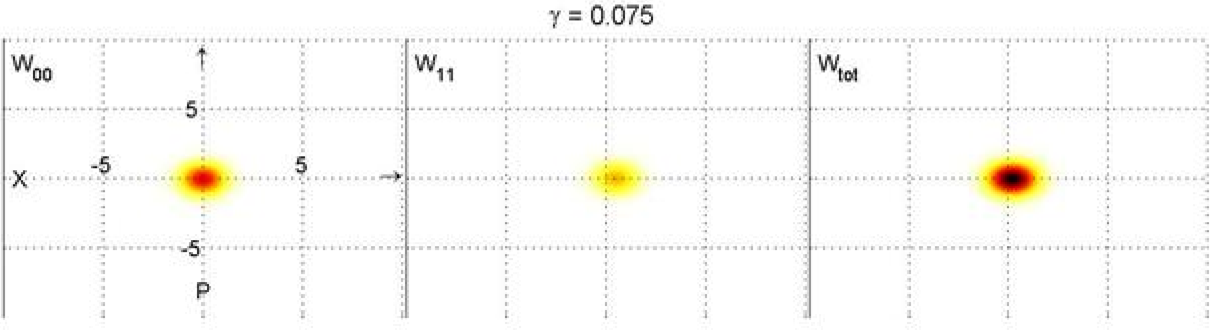
In the limit of classical oscillator ($\lambda \gg x_0 = \sqrt{\frac{\hbar}{m\omega}}$), small electric field and equal left and right rates:

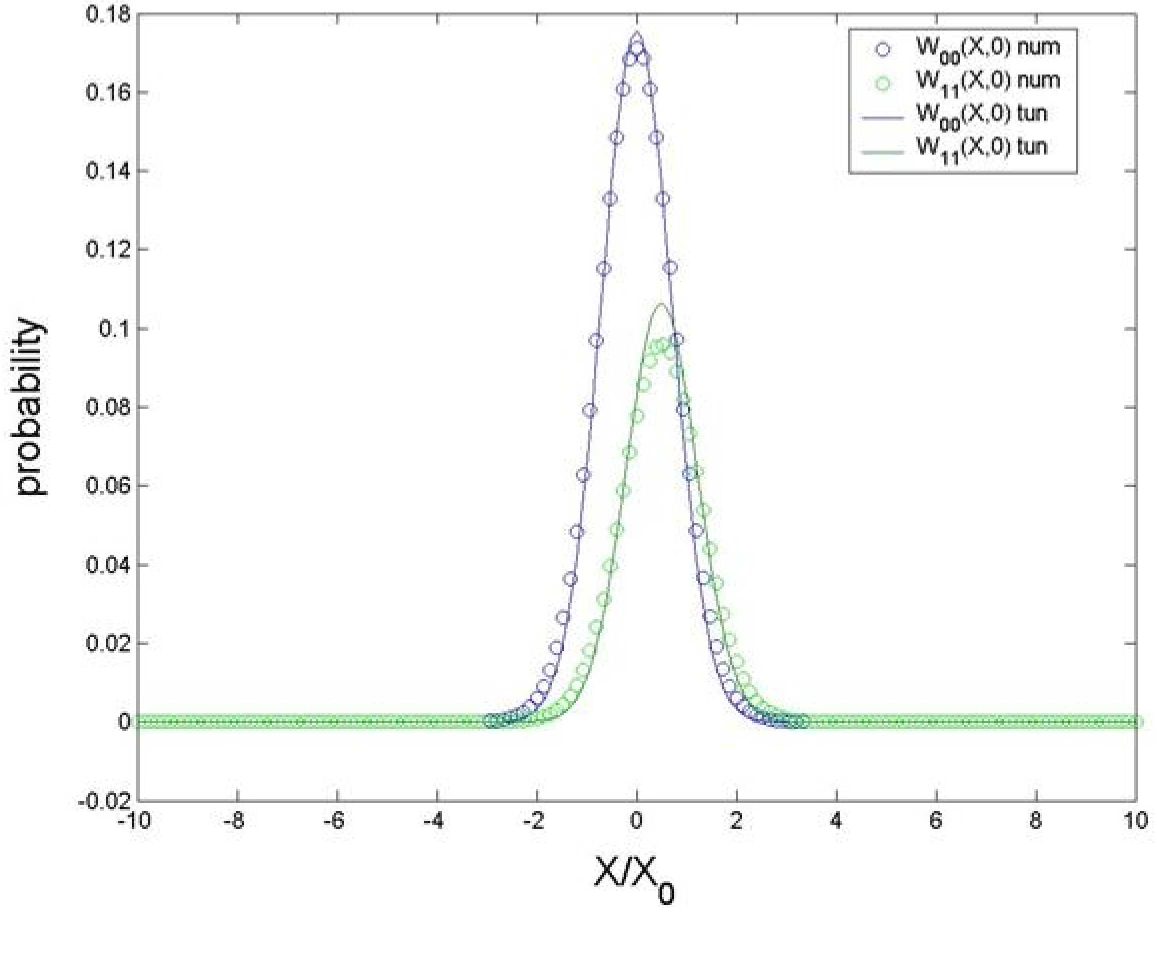
$$I = e\Gamma/2 \qquad F = 1/2$$

Comparison (i)

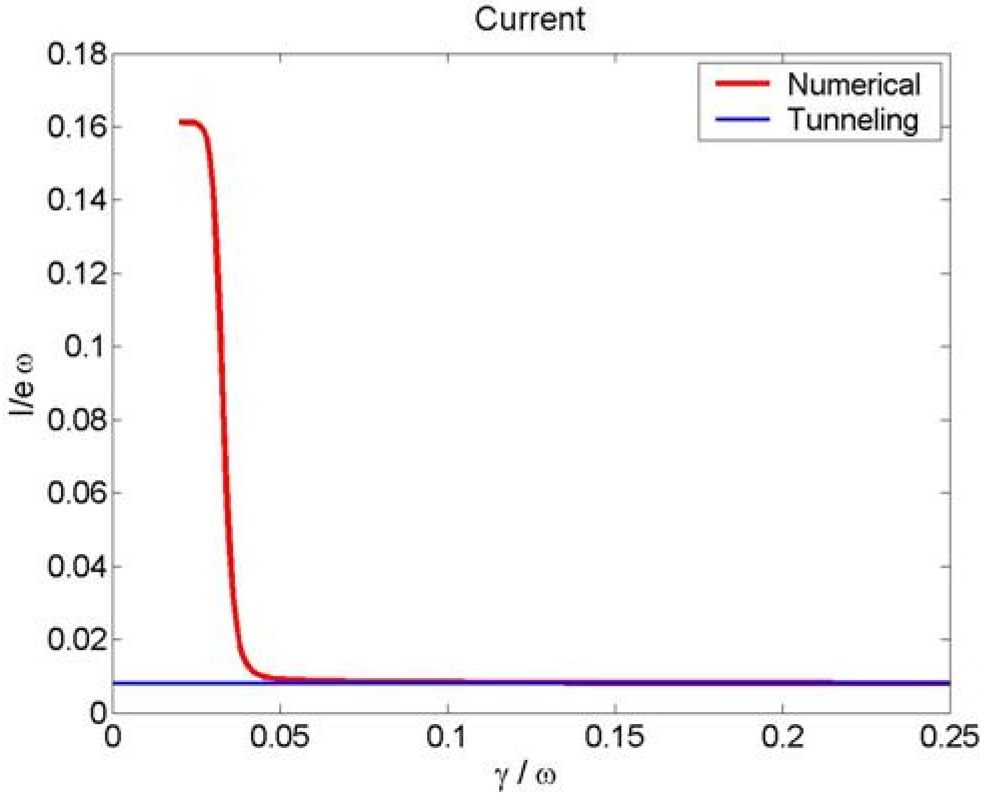
We verify the results predicted by the tunneling regime model in the "most classical" parameters' set up. The tunneling regime condition is there best fulfilled.

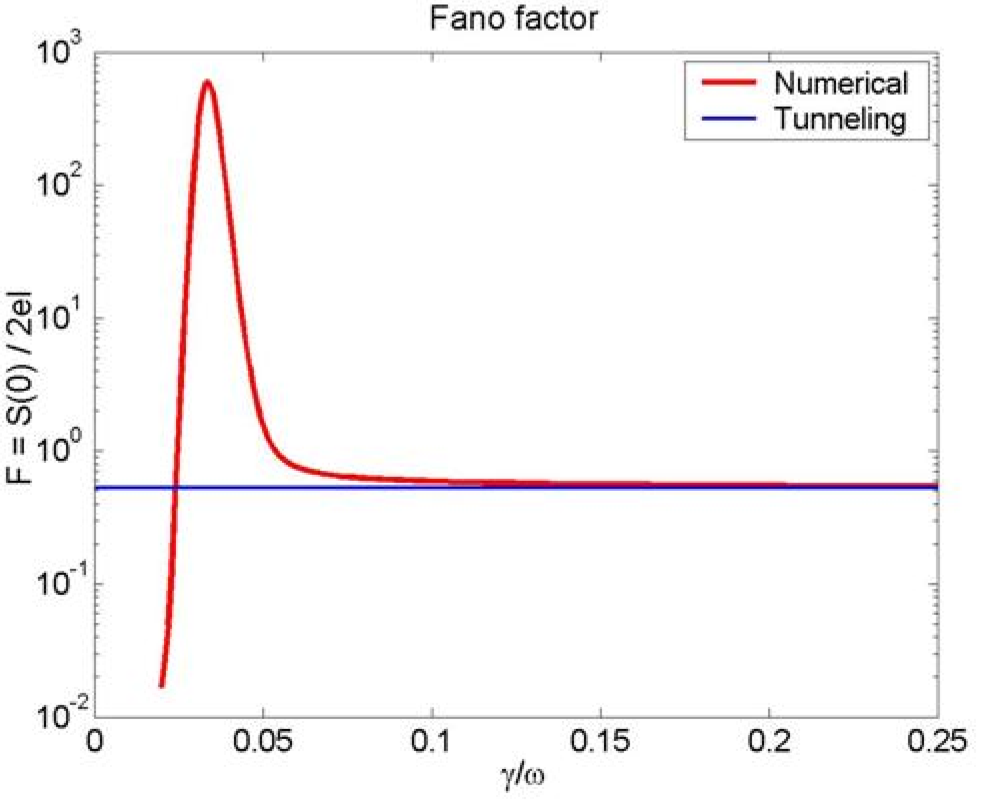
Phase space





Comparison (ii)





Shuttling Regime

$$\left\langle \Gamma_{L,R} \exp\left(\mp\frac{2x}{\lambda}\right)\right\rangle_{stat} \approx \omega \gg \gamma$$

A classical treatment is justified when $\Gamma_{L,R} \ll \omega$ and $\lambda \gg x_0$ since the amplitude of the self-sustained oscillation must also be much larger than the oscillator zero-point uncertainty.

In the limit $\hbar \to 0$ and $k_B T \to 0$ the GME can be written as a system of coupled Fokker-Planck equations:

$$\begin{aligned}
\dot{W}^{cl}_{00}(X,P,t) =& \{H_{osc}, W^{cl}_{00}\}_P - \gamma\frac{\partial}{\partial P}(PW^{cl}_{00}) \\
& - \Gamma_L e^{-\frac{2X}{\lambda}} W^{cl}_{00} + \Gamma_R e^{\frac{2X}{\lambda}} W^{cl}_{11} \\
\dot{W}^{cl}_{11}(X,P,t) =& \{H_{osc} - eEX, W^{cl}_{11}\}_P - \gamma\frac{\partial}{\partial P}(PW^{cl}_{11}) \\
& - \Gamma_R e^{\frac{2X}{\lambda}} W^{cl}_{11} + \Gamma_L e^{-\frac{2X}{\lambda}} W^{cl}_{00}
\end{aligned}$$

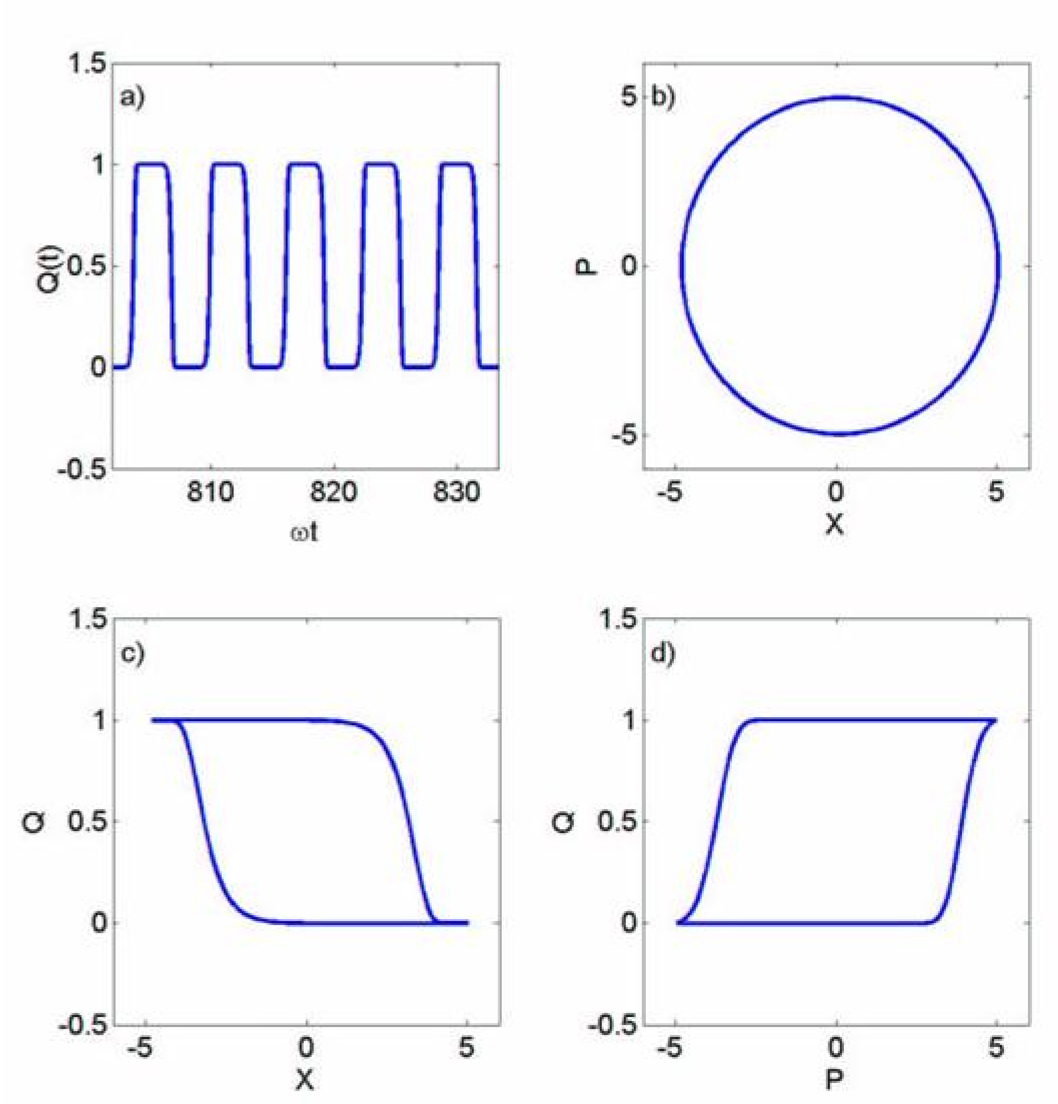
We can at this point introduce a separation Ansatz:

$$W^{cl}_{00}(X,P,t) = \rho_0(t)\,\delta(X - X_{cl}(t))\delta(P - P_{cl}(t))$$
$$W^{cl}_{11}(X,P,t) = \rho_1(t)\,\delta(X - X_{cl}(t))\delta(P - P_{cl}(t))$$

As far as $\rho_1(t)\rho_0(t) \approx 0$ the system of coupled Fokker-Panck equations is reduced to a trajectory equation:

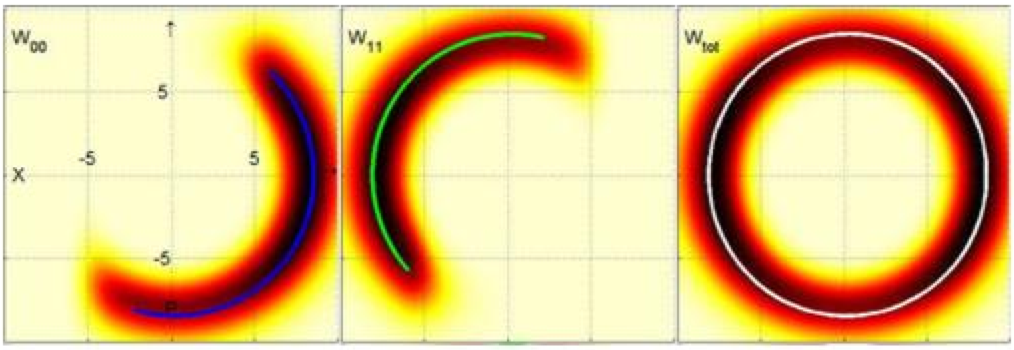
$$
\begin{aligned}
\dot{\rho}_1 &= -\Gamma_L(X_{cl})\rho_0 + \Gamma_R(X_{cl})\rho_1 \\
\dot{\rho}_0 &= \Gamma_L(X_{cl})\rho_0 - \Gamma_R(X_{cl})\rho_1 \\
\dot{X}_{cl} &= P_{cl} \\
\dot{P}_{cl} &= -\omega^2 X_{cl} + eE\rho_1 - \gamma P_{cl}
\end{aligned}
$$

The full- time solution is a stable limit cycle that shows self-sustained oscillations of the central dot occupation and charge-position correlation

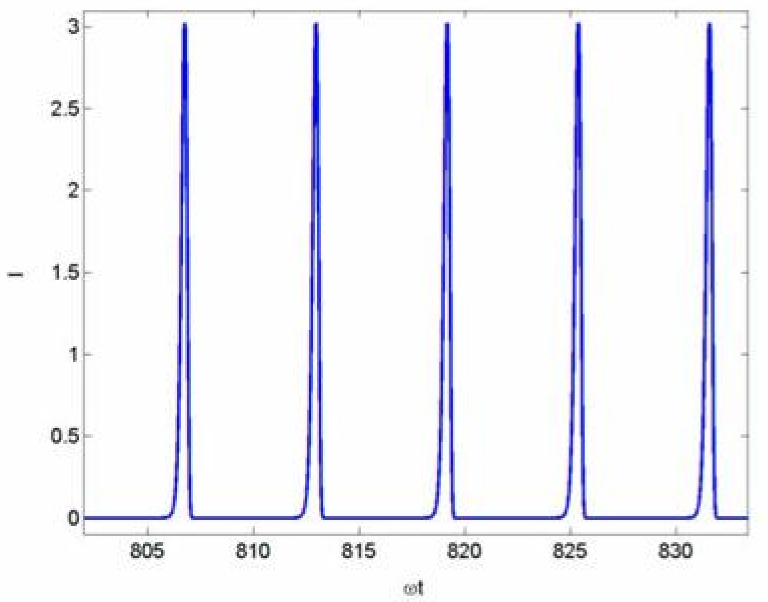


Comparison (iii)

The phase space picture of the stationary solution of GME corresponds to the time average of the classical distribution along the trajectory :



The current is given as a function of time by a series of spikes that well represent the single electron being shuttled by the oscillating dot.



The time average of this time resolved current is:

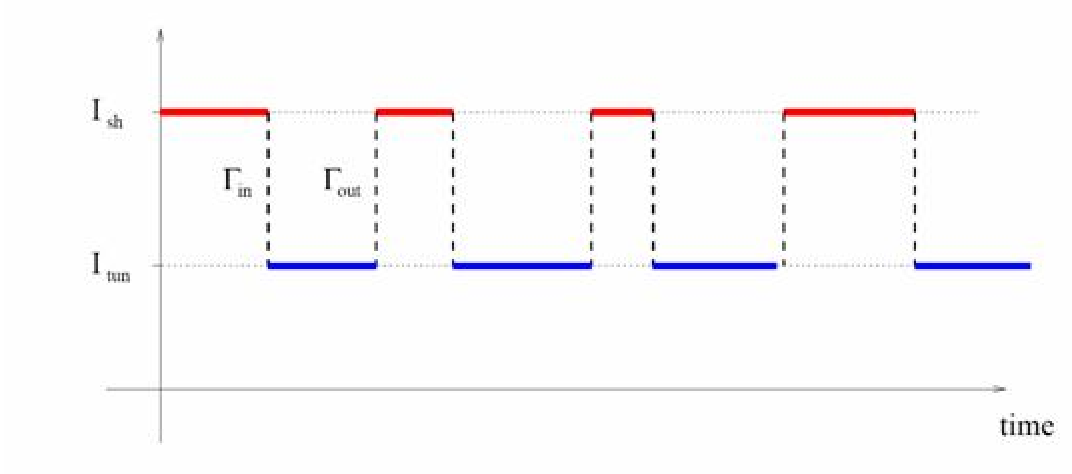
$$I^{\mathrm{stat}} = \frac{1}{2\pi}\int_{\tau}^{\tau+2\pi} d\tau'\, I_R(\tau') \;= 0.15916$$

Coexistence regime*

In the coexistence regime the system switches continuously between the tunneling and shuttling state.

IF the switching rate is much smaller than the oscillator frequency and the average tunneling rate,

THEN the dynamics resembles:
Dichotomous process between current channels



In this limit current and Fano factor read:

$$I = e\frac{I_{sh}\Gamma_{out} + I_{tun}\Gamma_{in}}{\Gamma_{in} + \Gamma_{out}}$$

$$F = \frac{S(0)}{2eI} = \frac{(I_{sh} - I_{tun})^2}{eI}\frac{\Gamma_{in}\Gamma_{out}}{(\Gamma_{in} + \Gamma_{out})^3}$$

* Ya. M. Blanter, O.Usmani and Yu. V. Nazarov cond-mat/0404615

Kramers' equation *

Once again we consider the most classical case. In this limit, the dynamics of the system can be described by a one dimensional radial Kramers' equation:

$$\frac{\partial \bar{W}_{+}(A,t)}{\partial t} = \frac{1}{A}\frac{\partial}{\partial A}A\left[V'(A) + D\frac{\partial}{\partial A}\right]\bar{W}_{+}(A,t)$$

where

$$\bar{W}_{+}(A,t) \equiv \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\varphi\,[W_{00}(A,\varphi) + W_{11}(A,\varphi)]$$

The diffusion constant and the effective potential contain the parameters of the system. The stationary solution reads:

$$\bar{W}_{+}^{stat} = Z^{-1}\exp\left\{-\frac{V}{D}\right\}$$

It is useful to introduce the radial probability density $\mathcal{W}(A,t) \equiv A\bar{W}_{+}(A,t)$ which satisfy the Kramers equation:

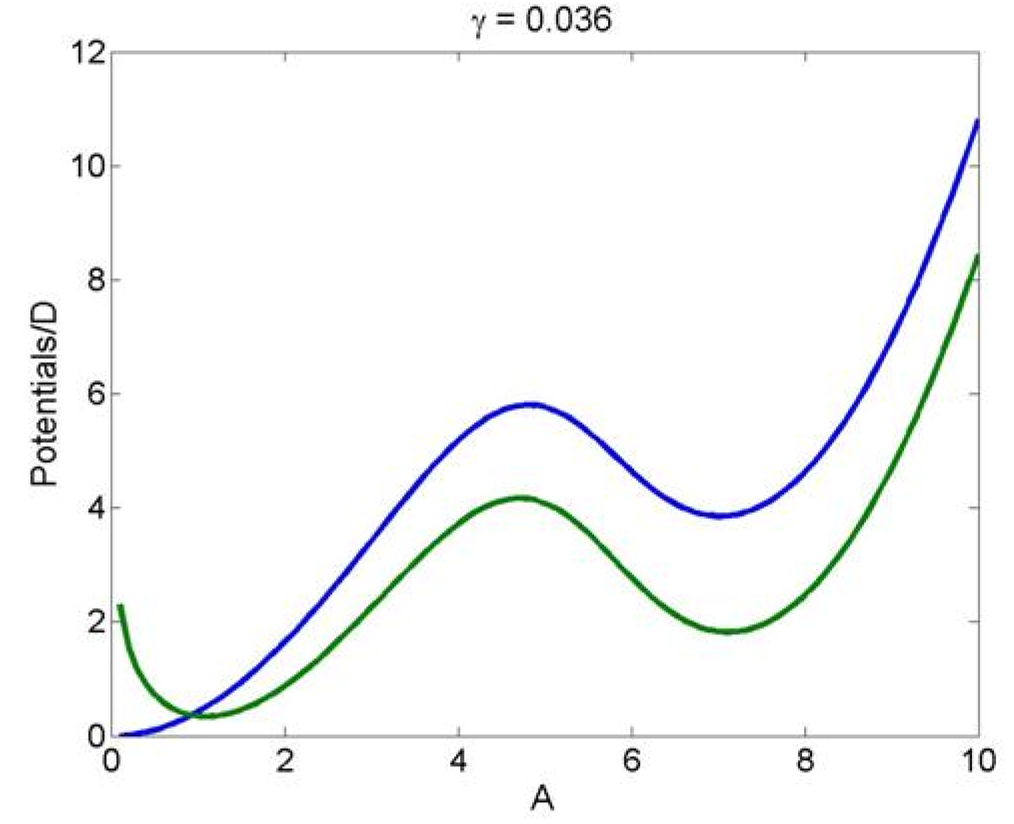
$$\frac{\partial \mathcal{W}(A,t)}{\partial t} = \frac{\partial}{\partial A}\left[\mathcal{V}'(A) + D\frac{\partial}{\partial A}\right]\mathcal{W}(A,t)$$

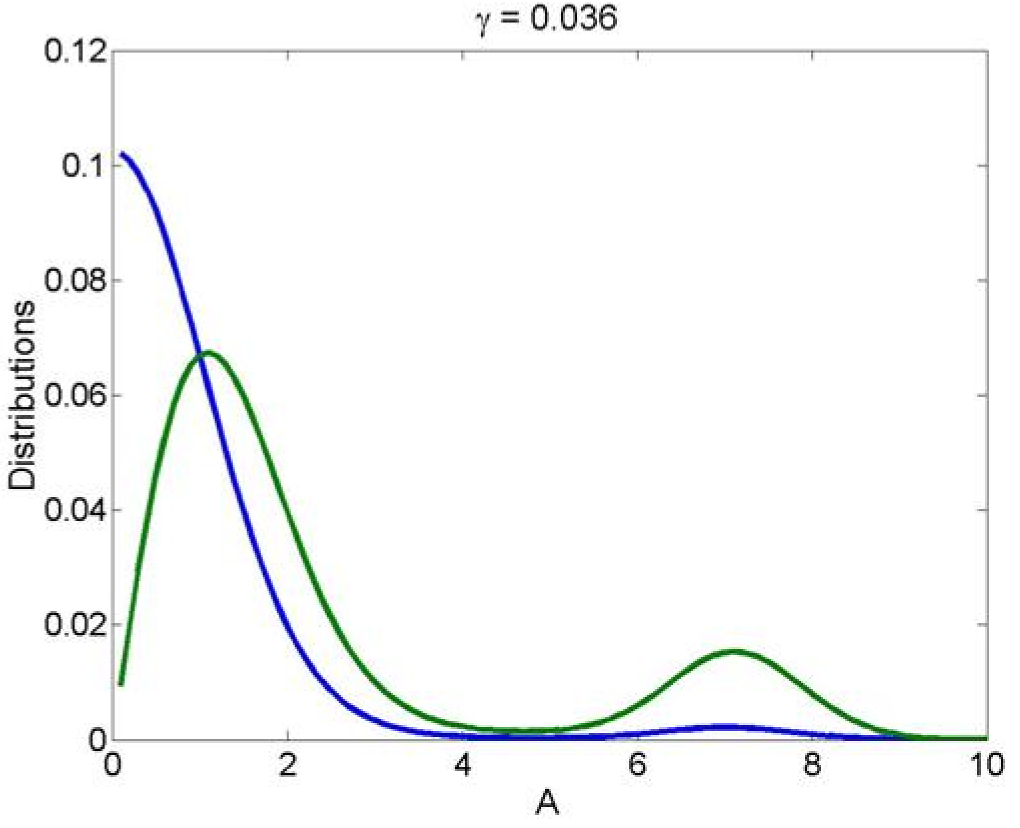
where

$$\mathcal{V}(A) = V(A) - D\ln(A)$$

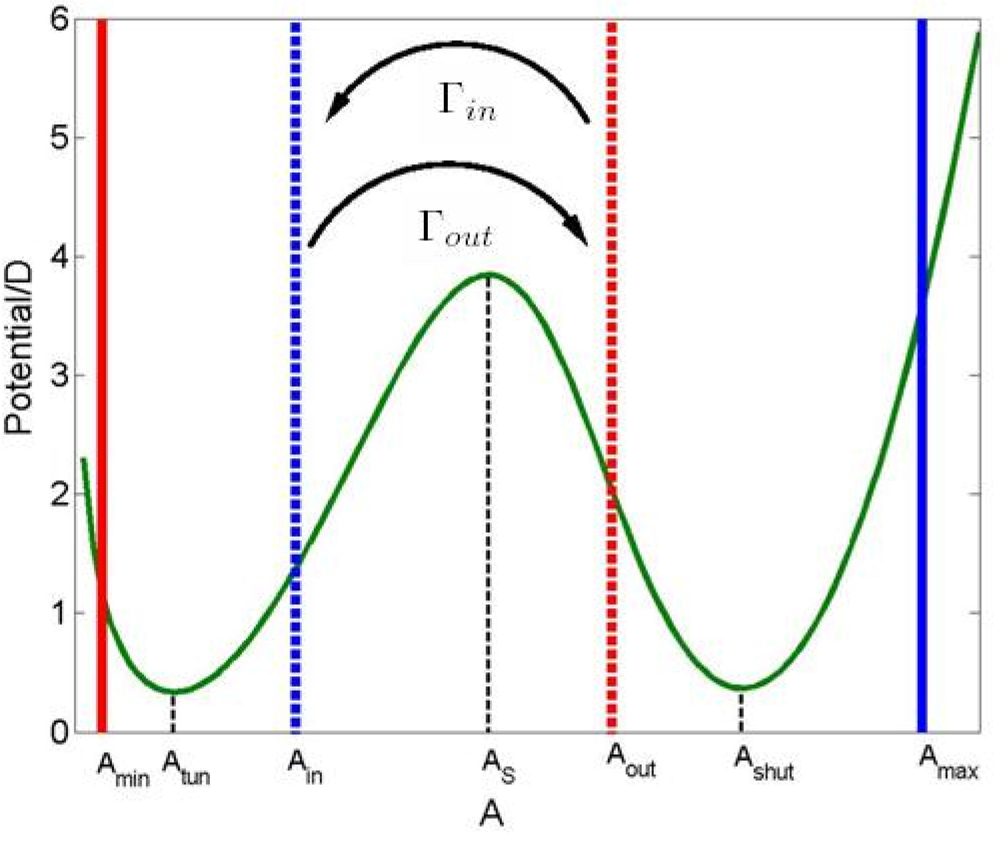
* D. Fedorets, L. Y. Gorelik, R. I. Shekhter, and M. Jonson,cond-mat/0311105.

Potentials and distributions





Switching rates



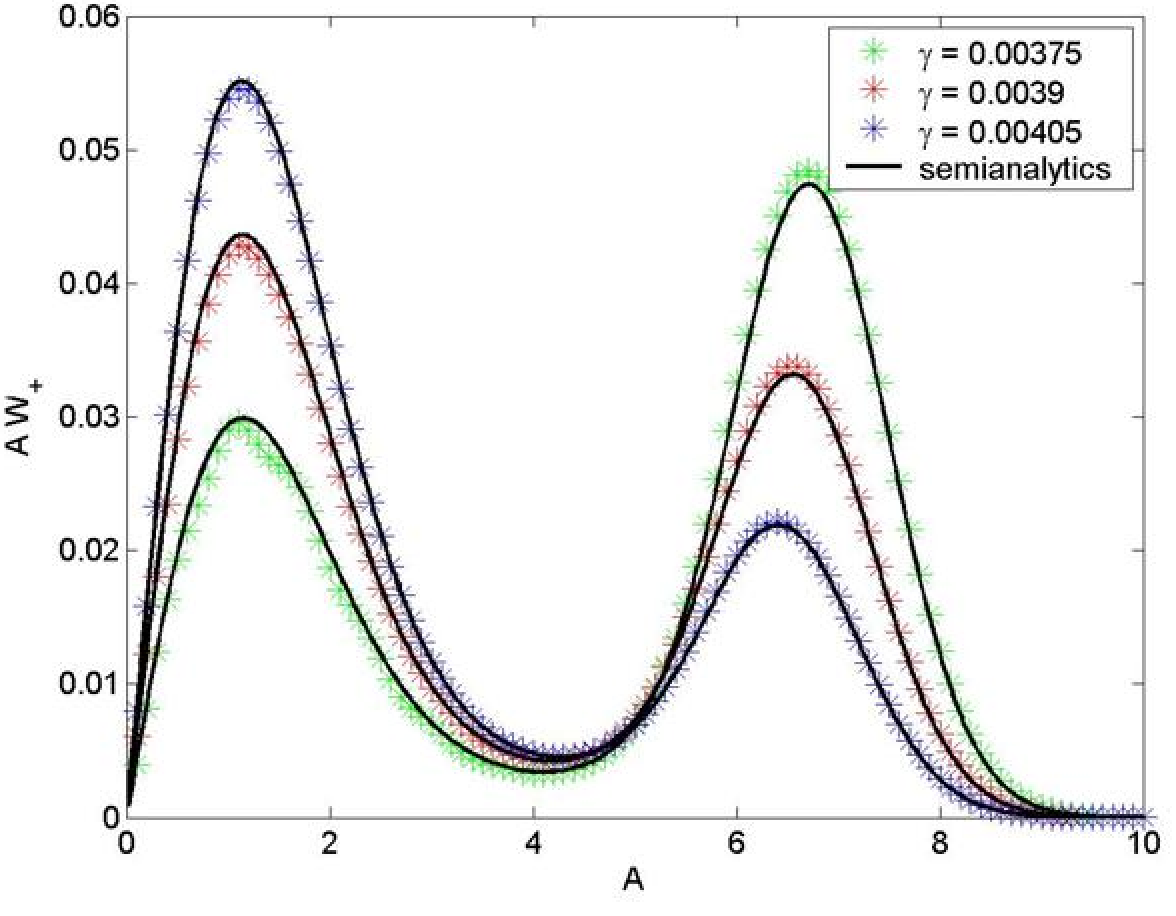
$$\Gamma_{\rm out} = D\left(\int_{A_{\rm tun}}^{A_{\rm out}} dA\, e^{-\frac{\mathcal{V}(A)}{D}} \int_{A}^{A_{\rm out}} dB\, e^{\frac{\mathcal{V}(B)}{D}}\right)^{-1}$$

$$\Gamma_{\rm in} = D\left(\int_{A_{\rm shut}}^{A_{\rm in}} dA\, e^{-\frac{\mathcal{V}(A)}{D}} \int_{A}^{A_{\rm in}} dB\, e^{\frac{\mathcal{V}(B)}{D}}\right)^{-1}$$

Comparison (iv)

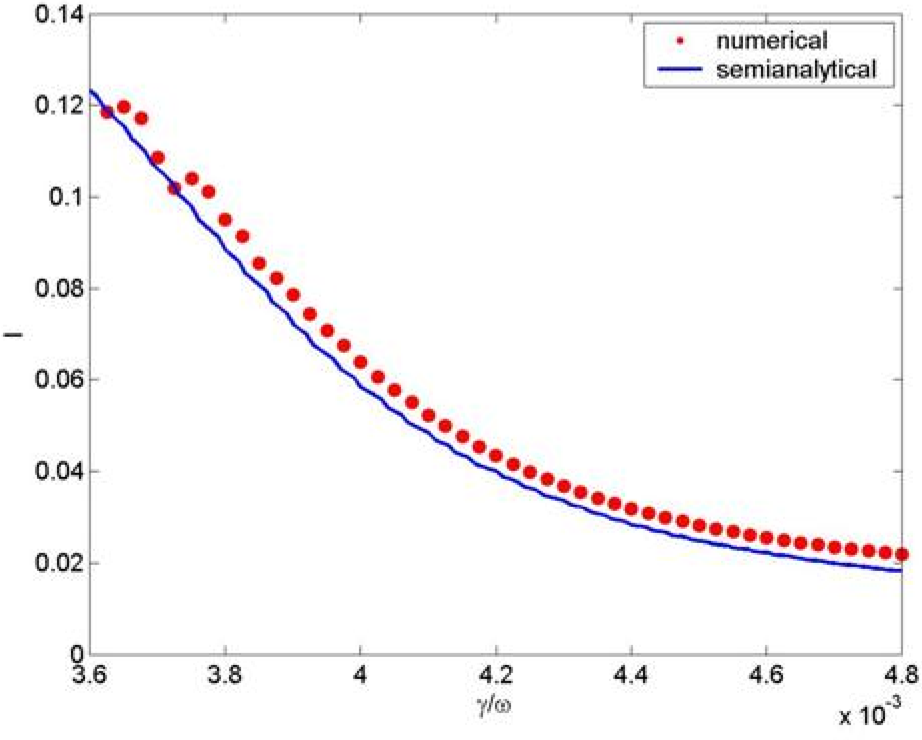
Classical limit

Phase space distribution

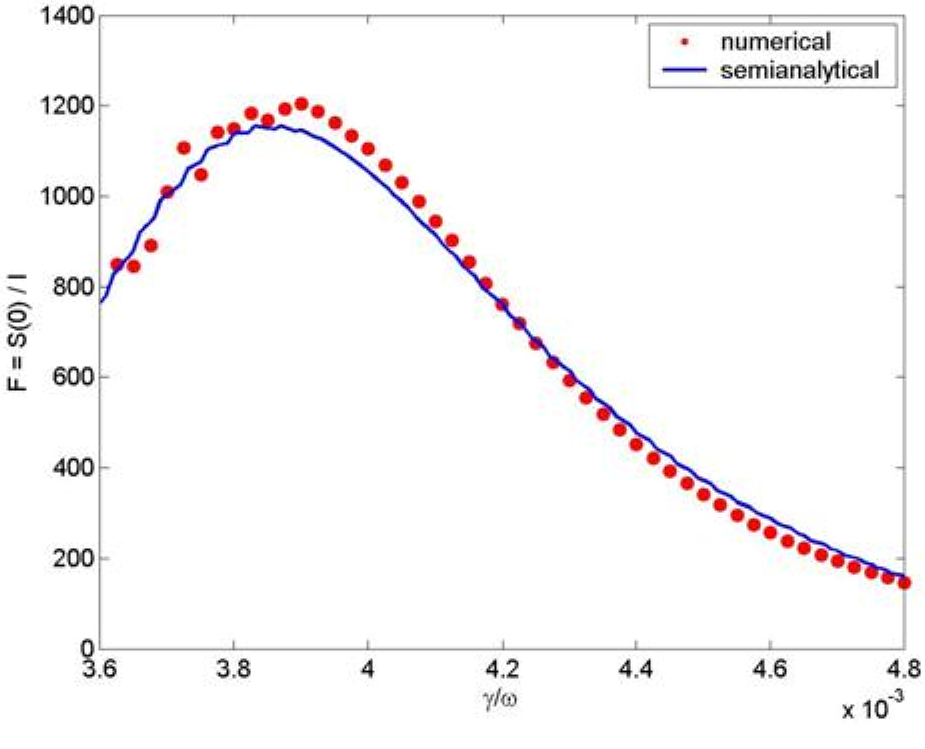


Still Classical (but noisy) limit

Current

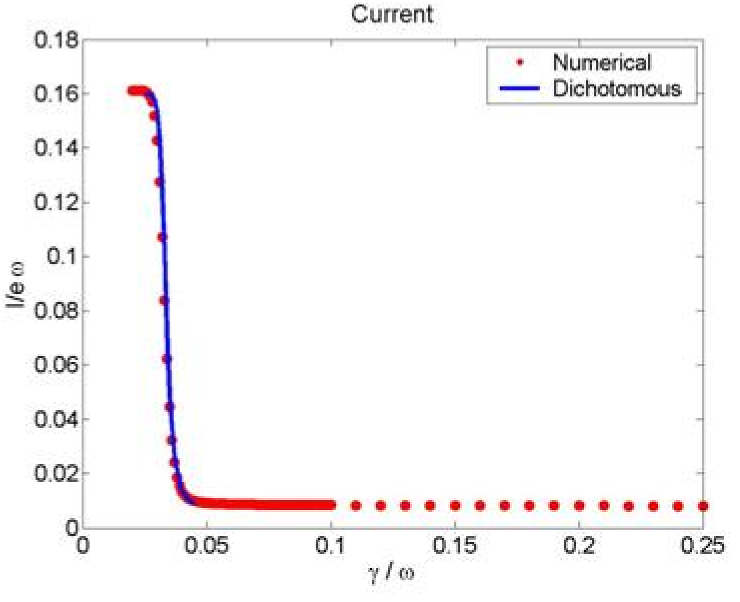


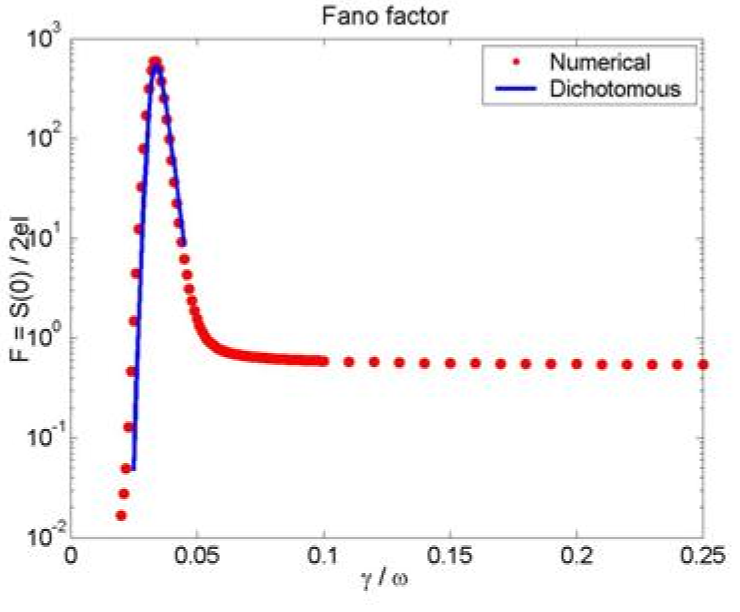
Fano factor



Comparison (v)

Fitted Quantum Limit





The diffusion coefficient is used as a fitting parameter

EFFECTIVE TEMPERATURE?

Conclusions

- We have studied the simplest model of single dot shuttling device using three investigation tools:

  PHASE SPACE, CURRENT, NOISE

- We have calculated the numerical solution in the full quantum description. The NEMS that we have studied exhibits three dynamical regimes:

  TUNNELING, SHUTTLING, COEXISTENCE REGIME

- For each regime we have reduced the original description in order to detect the simpler underlying dynamics and give a more transparent physical picture.