Quantum Shuttle: Physics of a Numerical Challenge

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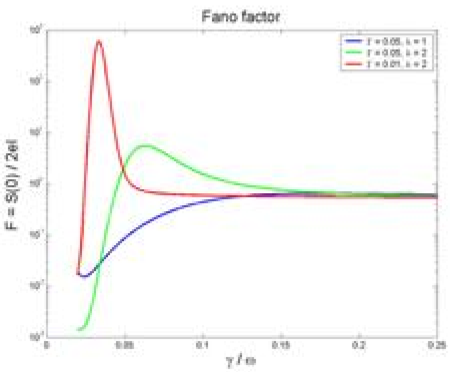
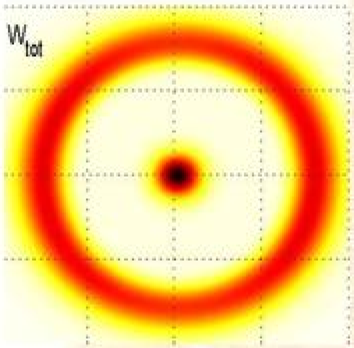
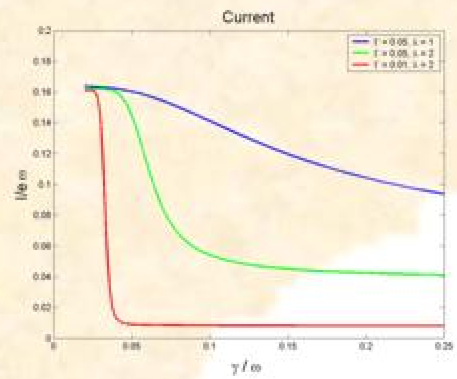


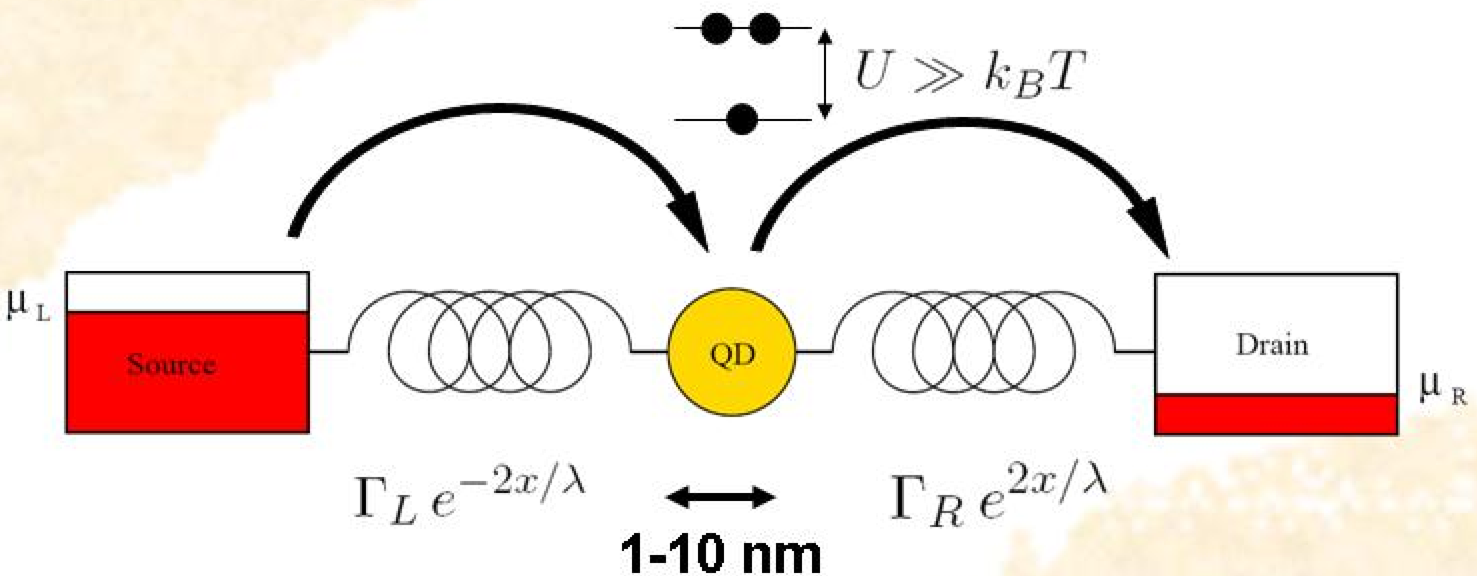




Madrid, 13.07.2006

ECMI 2006

Shuttle Device*



- 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

* L. Y. Gorelik et al., PRL. 80, 4526 (1998)

Hamiltonian

The Hamiltonian for the model reads:

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

where

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

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

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

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

Electrostatic force

Mechanical back-action

Generalized Master Equation

We express the dynamics in terms of the Generalized Master Equation:

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

Novotný et al. PRL 92 (2004)

resolved with respect to the number of electrons collected in the right lead.

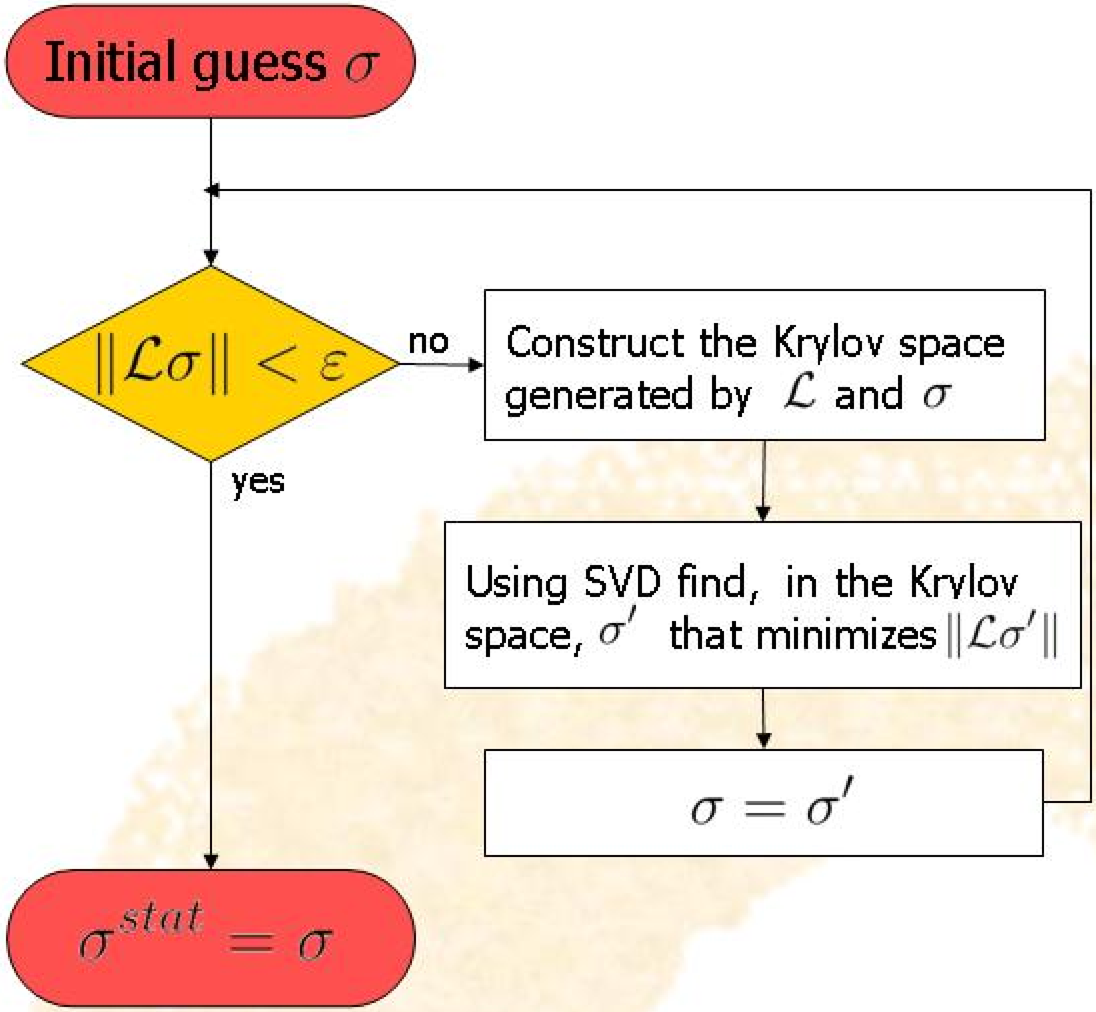
We look for the stationary solution of the GME:

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

A Matter of Sizes

- In the shuttling regime the amplitude of the oscillations reach 5-10 times the zero point uncertainty
- We are thus forced to consider up to 100 states in the mechanical Hilbert space
- The problem $\mathcal{L}\sigma^{stat} = 0$ requires the calculation of the null space of a linear operator of dimension $2 \cdot 10^4 \times 2 \cdot 10^4$
- A solution to this problem comes from the Arnoldi iteration scheme.

Arnoldi



The Krylov space

Given a vector σ and a linear operator $\mathcal{L}$, the Krylov space $\mathcal{K}_j(\mathcal{L}, \sigma)$ is defined by

$$\mathcal{K}_j(\mathcal{L}, \sigma) \equiv \mathrm{span}(\sigma, \mathcal{L}\sigma, \ldots, \mathcal{L}^{j-1}\sigma)$$

The Preconditioning Problem

- The Arnoldi iteration is very efficient to find eigenstates of well separated eigenvalues
- The Liouvillian of our problem has many eigenvalues concentrated around 0
- We mapped the problem into an easier $\mathcal{M}[\mathcal{L}[\sigma^{stat}]] = 0$ where $\mathcal{M}$ is a regular operator, inverse of the Sylvester operator.

$$\mathcal{L}_{\text{Sylv}} = \mathbf{A}\sigma + \sigma\mathbf{A}^\dagger = \begin{bmatrix} A_{00}\sigma_{00} + \sigma_{00}A_{00}^\dagger & 0 \\ 0 & A_{11}\sigma_{11} + \sigma_{11}A_{11}^\dagger \end{bmatrix}$$

where

$$A_{00} = -\frac{i}{\hbar}H_{\text{osc}} - \frac{\Gamma_L}{2}e^{-\frac{2x}{\lambda}} - \frac{i\gamma}{2\hbar}xp - \frac{\gamma m\omega}{\hbar}\left(n_B + \frac{1}{2}\right)x^2$$

$$A_{11} = -\frac{i}{\hbar}(H_{\text{osc}} - e\mathcal{E}x) - \frac{\Gamma_R}{2}e^{\frac{2x}{\lambda}} - \frac{i\gamma}{2\hbar}xp - \frac{\gamma m\omega}{\hbar}\left(n_B + \frac{1}{2}\right)x^2$$

Investigation Tools

We analyze the dynamics of the device with 3 investigation tools:

- Wigner Function distributions

$$W_{ij}^{\text{stat}}(q,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} d\xi \left\langle q - \frac{\xi}{2}\right| \sigma_{ij}^{\text{stat}} \left| q + \frac{\xi}{2}\right\rangle \exp\left(\frac{ip\xi}{\hbar}\right)$$

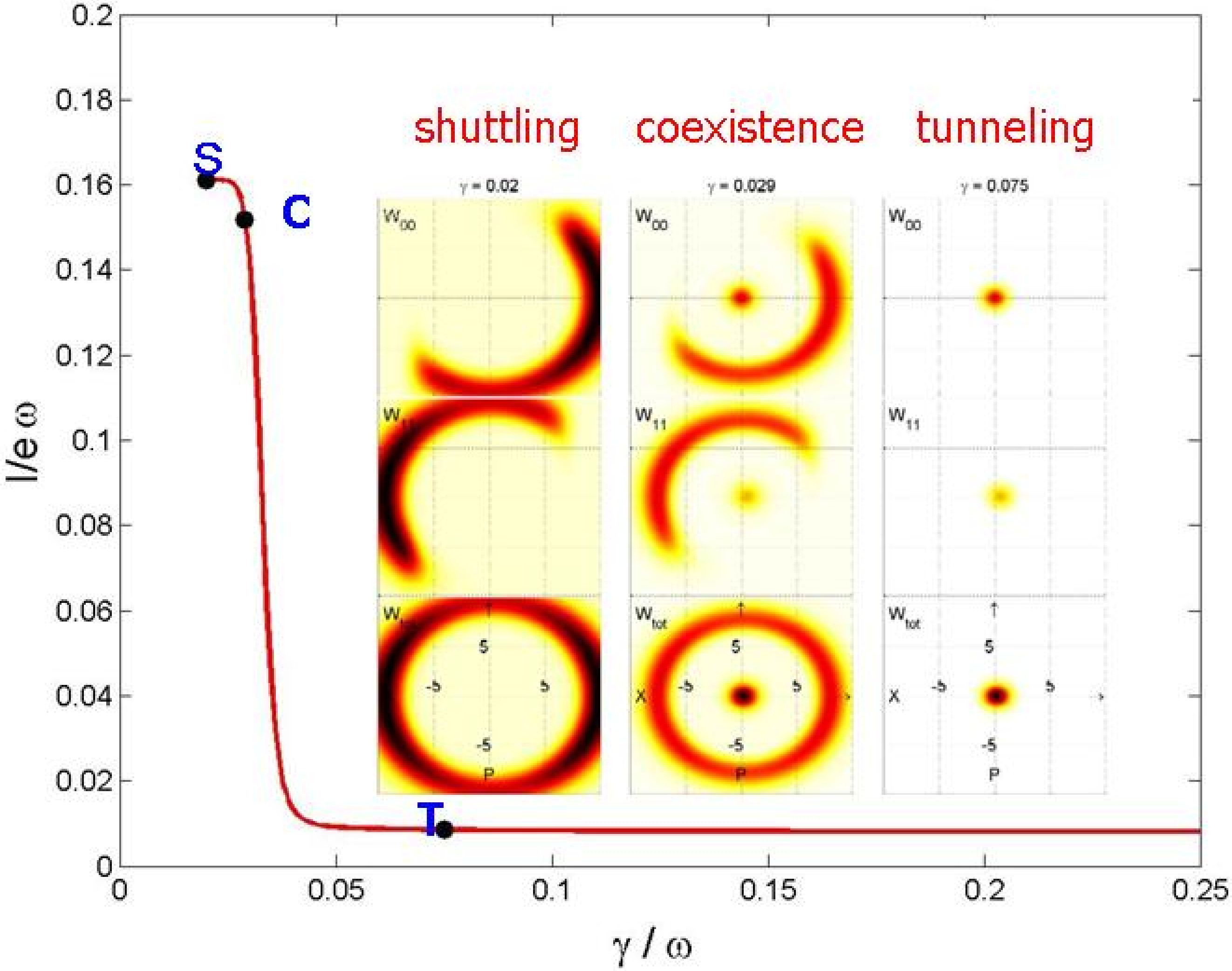
- Current

$$I^{\text{stat}} = \text{Tr}_{\text{sys}}\{\Gamma_L(x)|0\rangle\langle 0|\sigma^{\text{stat}}\}$$

- Current noise (Fano factor)

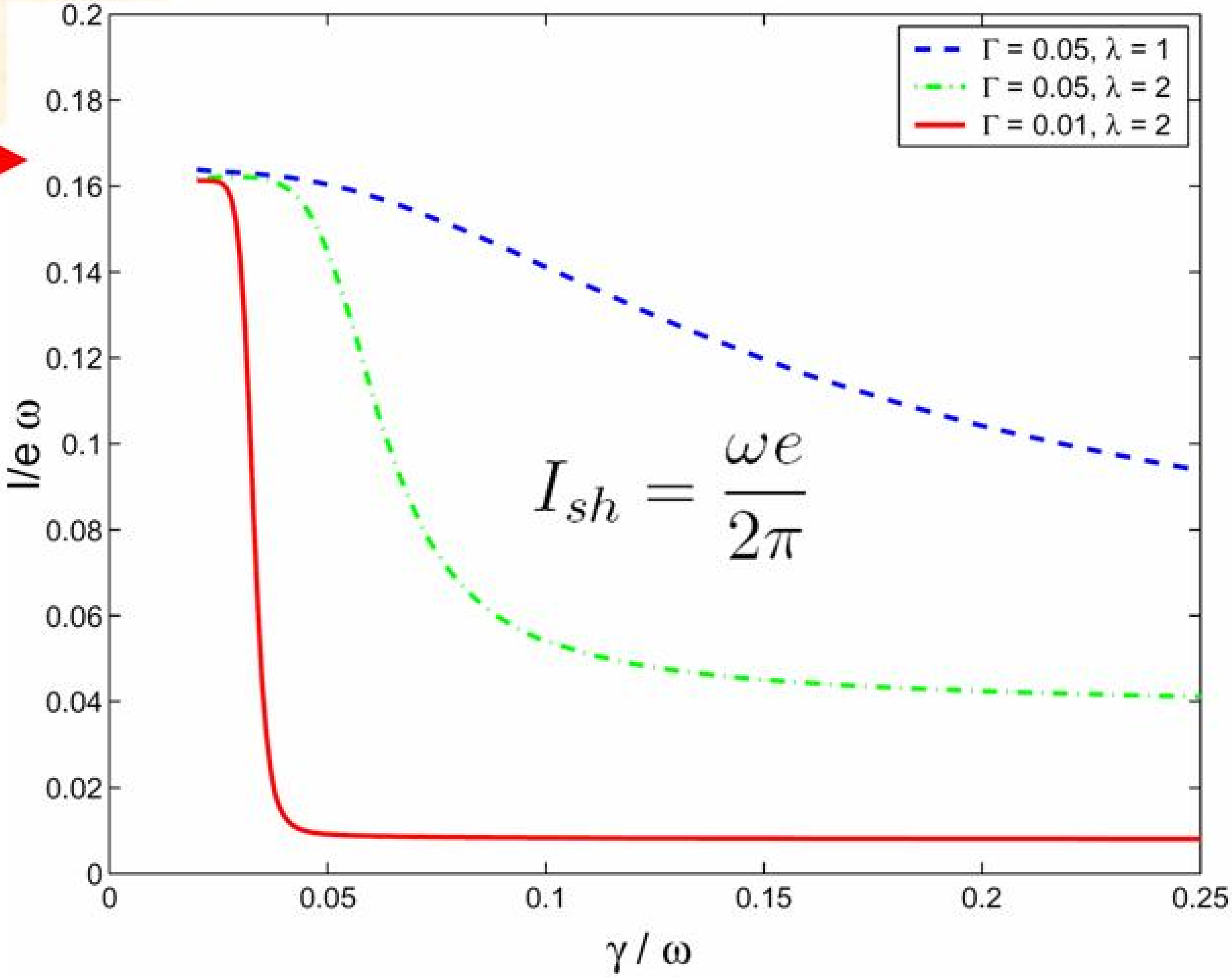
$$F = \frac{S(0)}{2eI} = 1 - \frac{2e\Gamma_R}{I}\text{Tr}_{osc}\left(e^{\frac{2x}{\lambda}}\left[\mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}\left(\begin{array}{c}\Gamma_R e^{\frac{x}{\lambda}}\,\sigma_{11}^{stat}\,e^{\frac{x}{\lambda}}\\ 0\end{array}\right)\right]_{11}\right)$$

Wigner Function

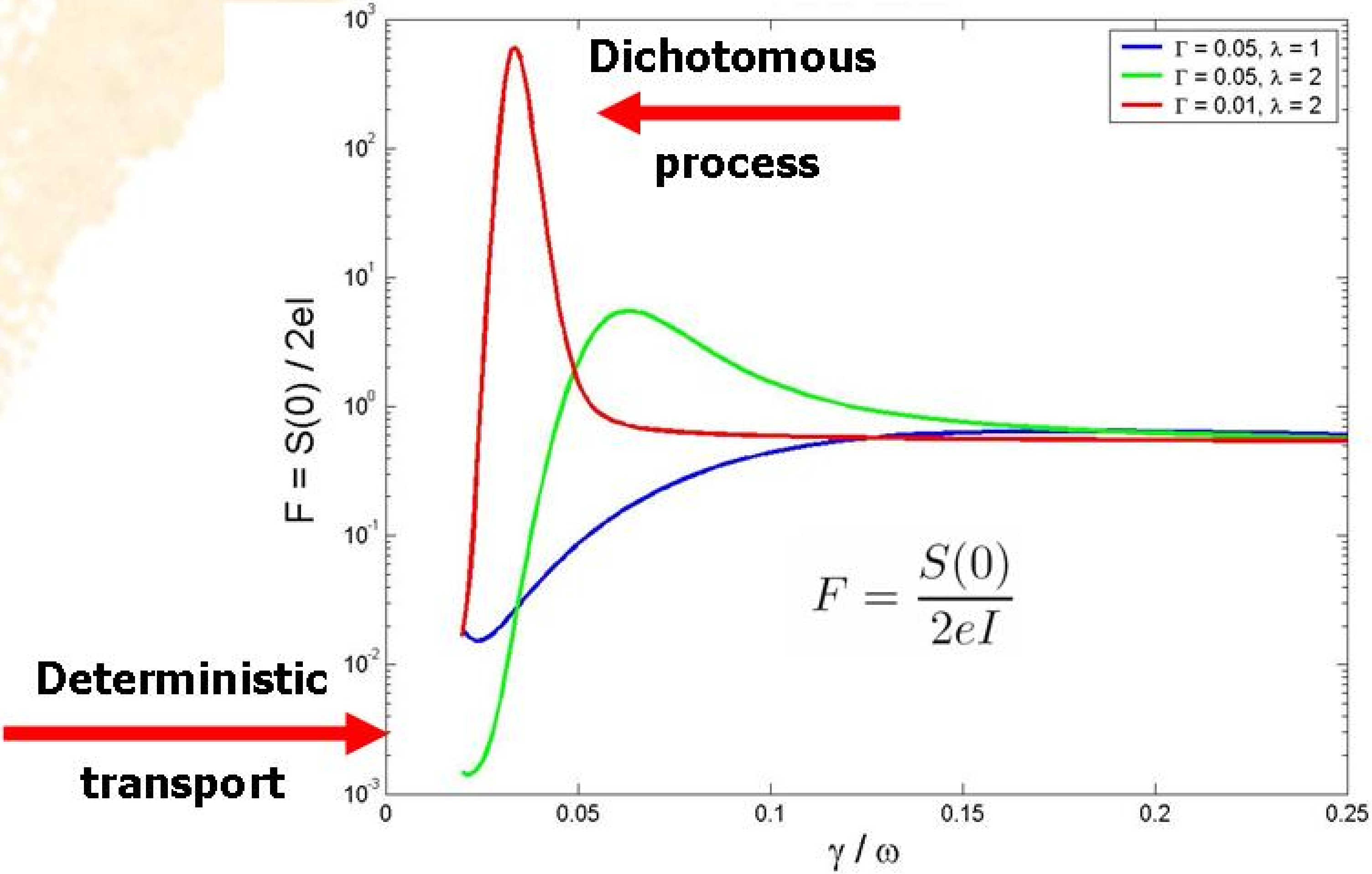


Current

Shuttling current



Current Noise



$$F = \frac{S(0)}{2eI}$$

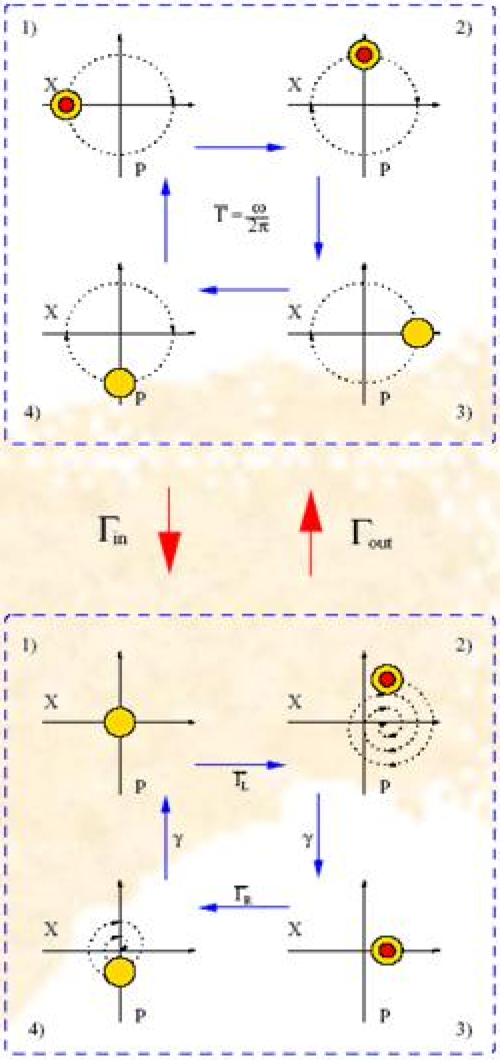
The three regimes

γ

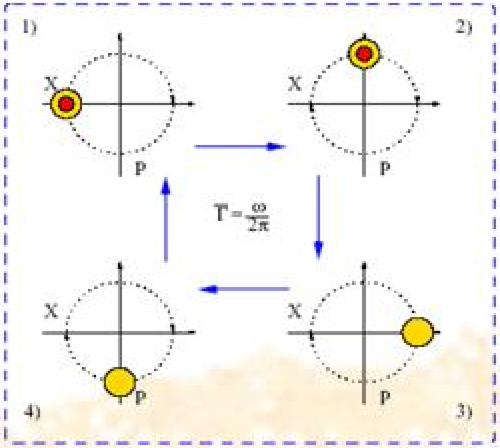
Shuttling $\left\langle \Gamma_{L,R} \exp\left(\mp\frac{2x}{\lambda}\right)\right\rangle_{stat} \approx \omega \gg \gamma$

Coexistence

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



Classical shuttling



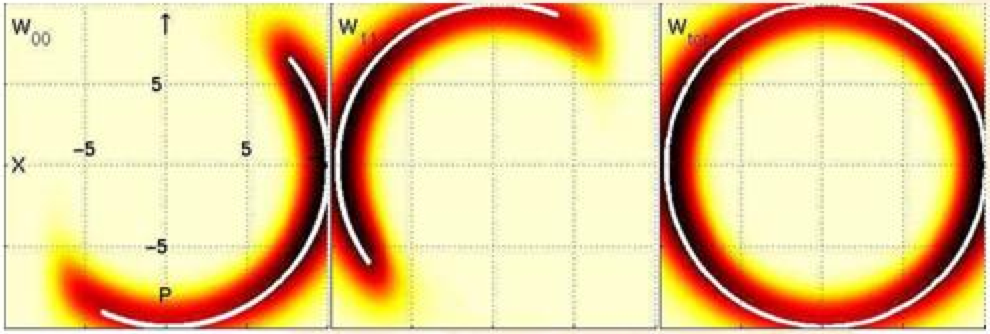
This regime is characterized by the low noise

We assume no noise and we reduce the GME to a set of coupled ordinary differential equations:

$$\dot{X} = P$$

$$\dot{P} = -X + d^* Q - \gamma^* P$$

$$\dot{Q} = \Gamma_L^* e^{-2X}(1 - Q) - \Gamma_R^* e^{2X} Q$$



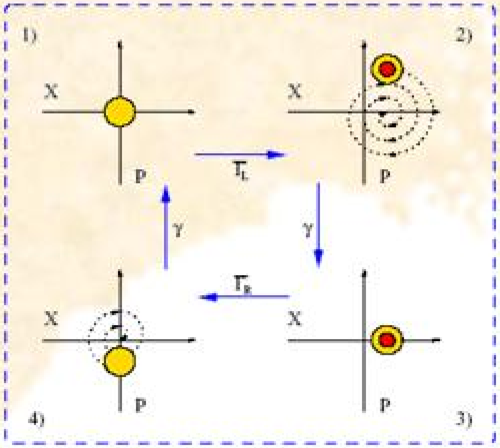
Renormalized resonant tunnelling

Due to time scale separation only two states are relevant for the transport properties:

Neutral (at rest) Charged (displaced)

We can describe the dynamics of the system using a two state model with renormalized tunnelling rates:

$$\frac{d}{dt}\begin{pmatrix} p_{00} \\ p_{11} \end{pmatrix} = \begin{pmatrix} \tilde{\Gamma}_R\, p_{11} - \tilde{\Gamma}_L\, p_{00} \\ \tilde{\Gamma}_L\, p_{00} - \tilde{\Gamma}_R\, p_{11} \end{pmatrix} \equiv \mathcal{L}\begin{pmatrix} p_{00} \\ p_{11} \end{pmatrix}$$



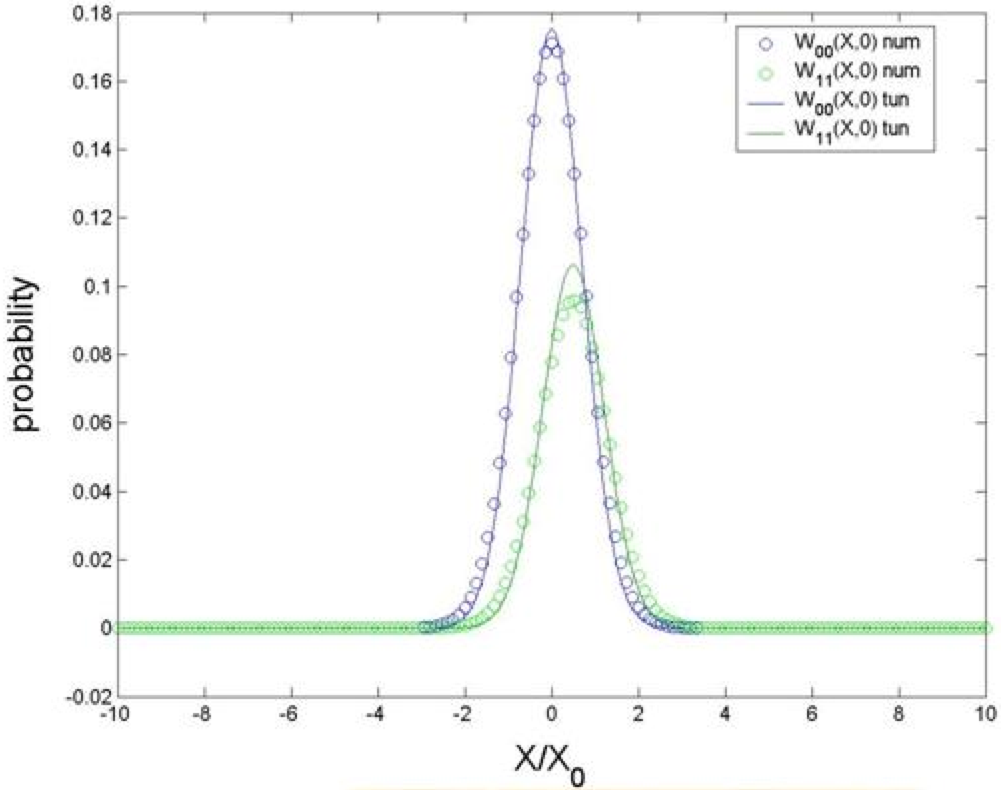
where

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

$$\tilde{\Gamma}_R = \Gamma_R\, \mathrm{Tr}_{\mathrm{mech}}\left\{\sigma_{\mathrm{th}}(e\mathcal{E}) e^{\frac{2\hat{x}}{\lambda}}\right\}$$

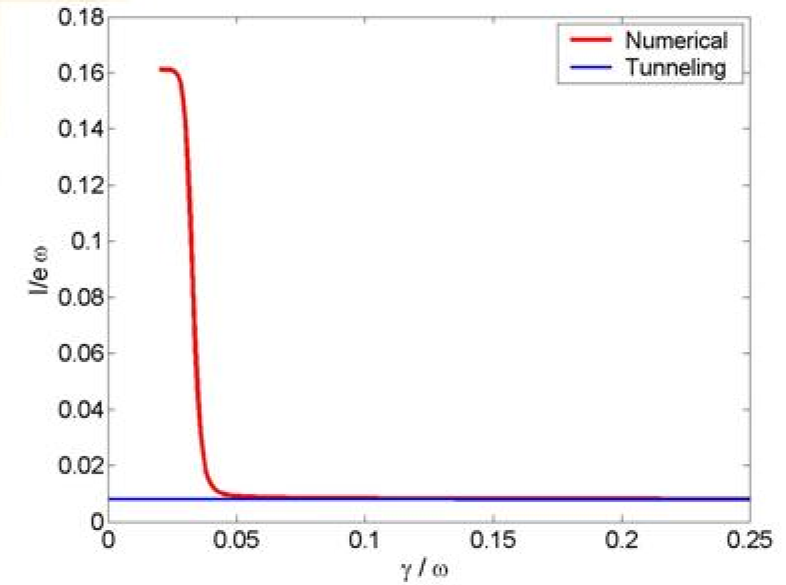
Comparison (i)

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.

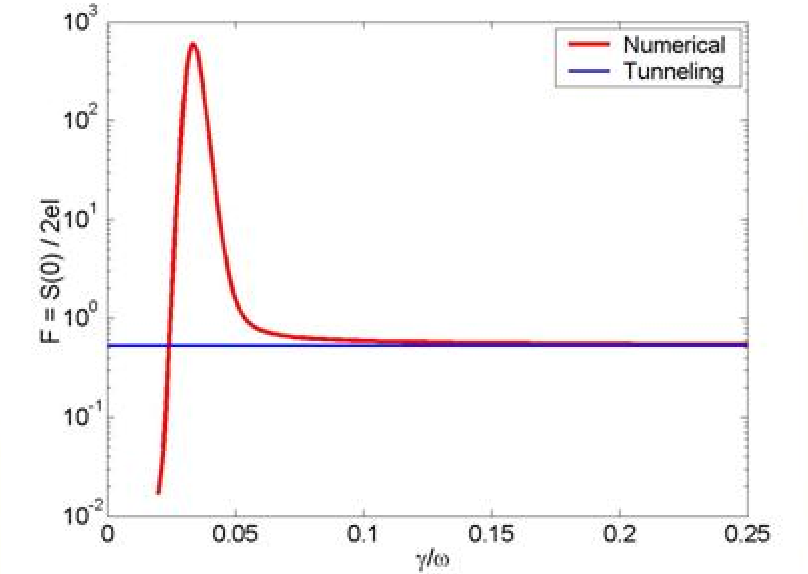


Comparison (ii)

Current



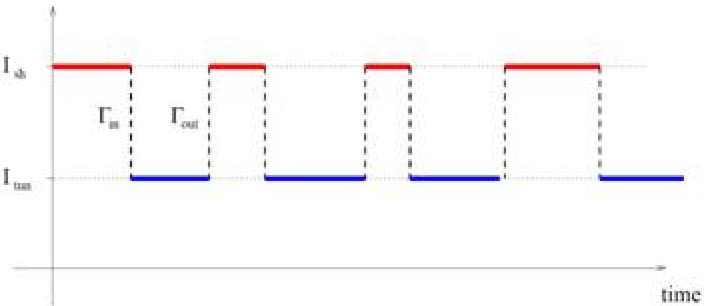
Fano factor



Dichotomous Process

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

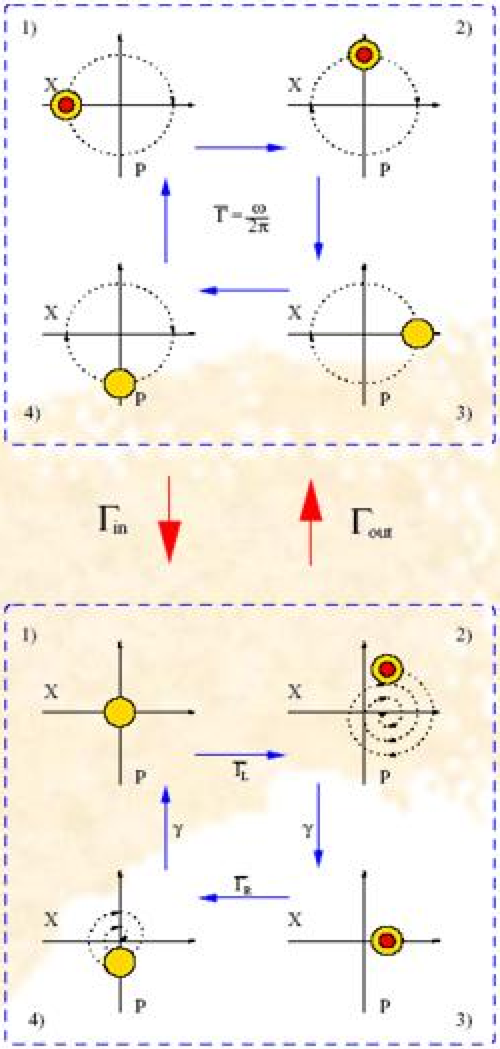
THEN the dynamics resembles:
Dichotomous process between current channels



In this limit **current** and **Fano factor** read:

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

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



Effective Potential

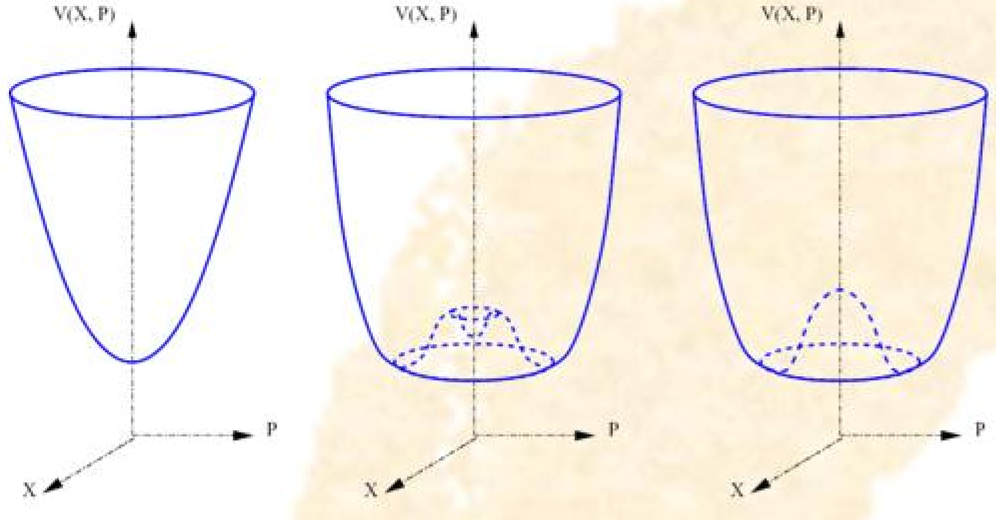
The GME is reduced to the radial Kramers´ equation

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

where

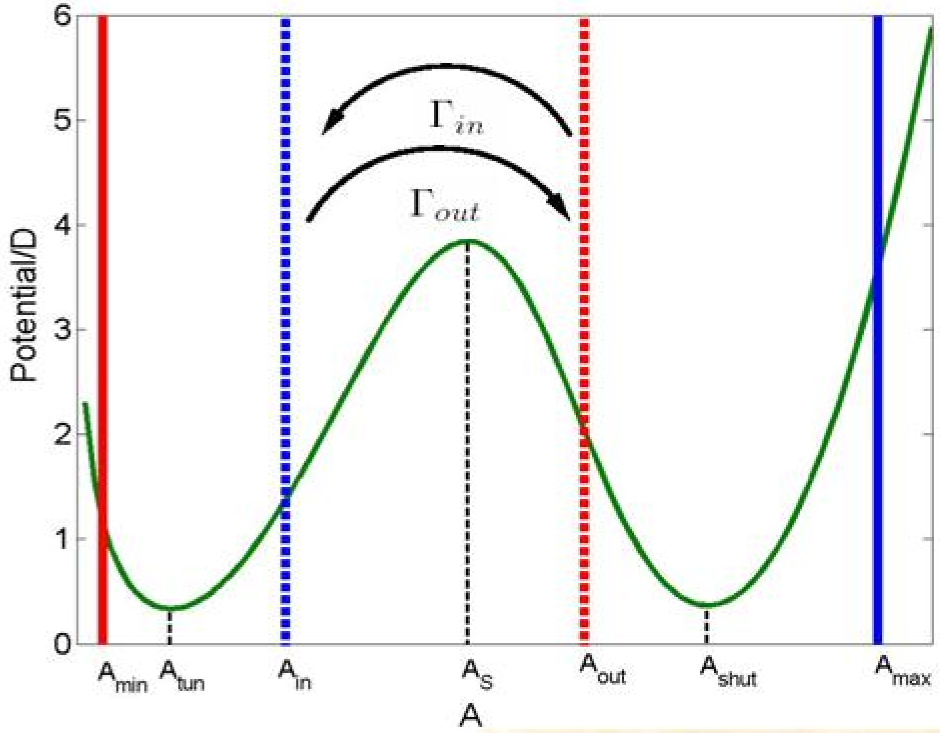
$$\bar{W}_+(A,t) \equiv \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\varphi \, [W_{00}(A,\varphi) + W_{11}(A,\varphi)]$$

while the effective potential is:



TUNNELING COEXISTENCE SHUTTLING

Switching Rates



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

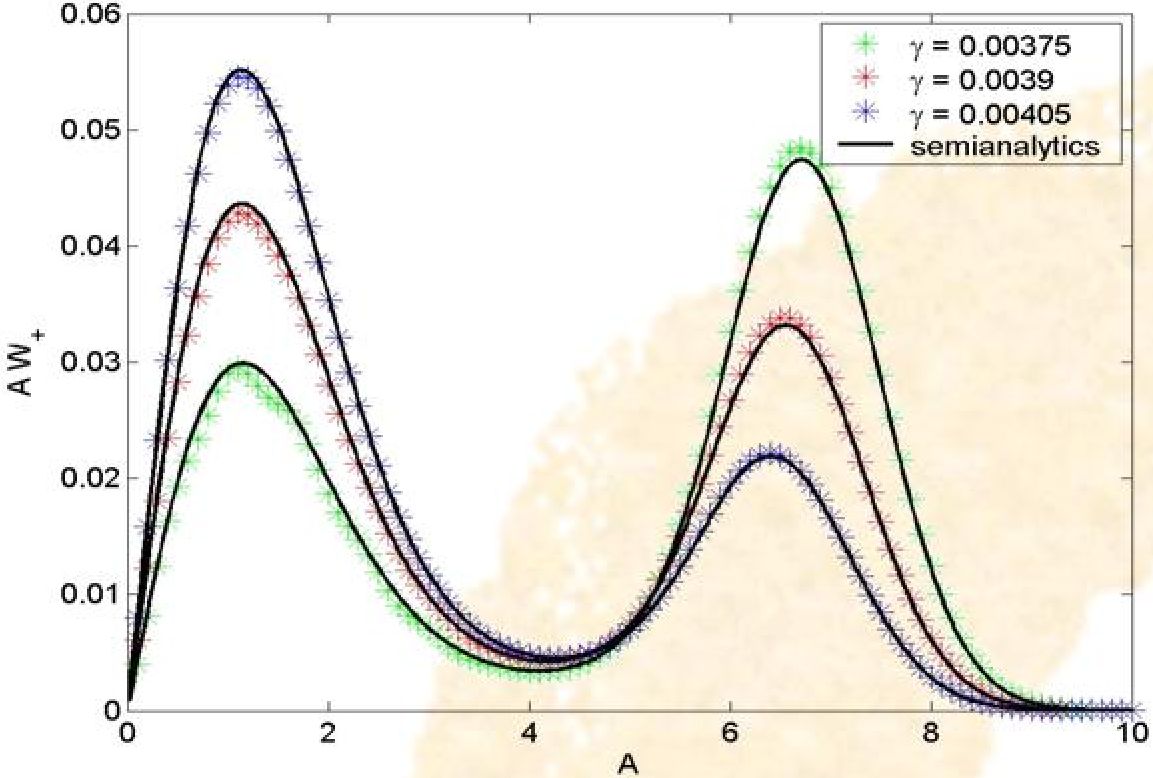
$$\Gamma_{\text{in}} = D \left(\int_{A_{\text{in}}}^{A_{\text{shut}}} dB \, e^{\frac{\mathcal{V}(B)}{D}} \int_{B}^{A_{\text{max}}} dA \, e^{-\frac{\mathcal{V}(A)}{D}} \right)^{-1}$$

Comparison (i)

classical limit

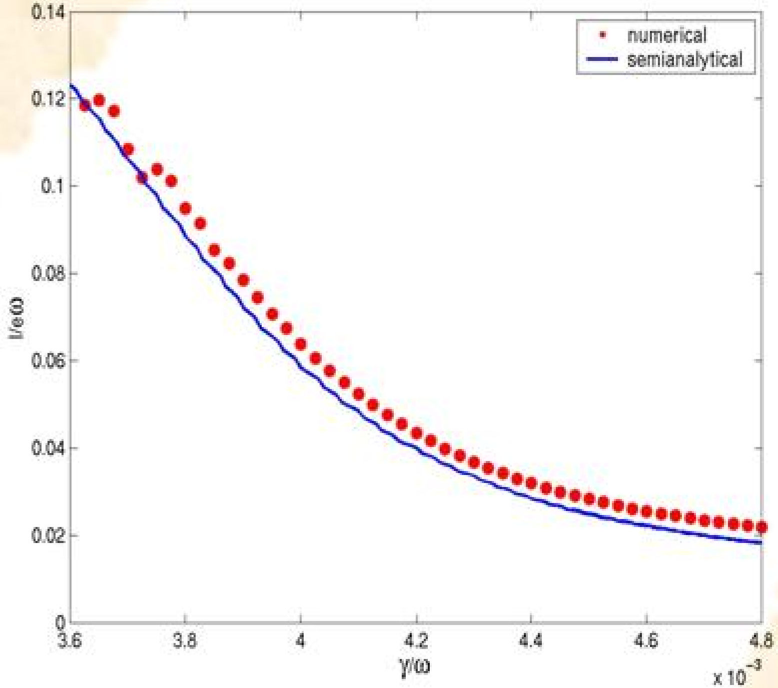
$\lambda \gg x_0$ where x_0 is the zero point uncertainty length

Wigner Function

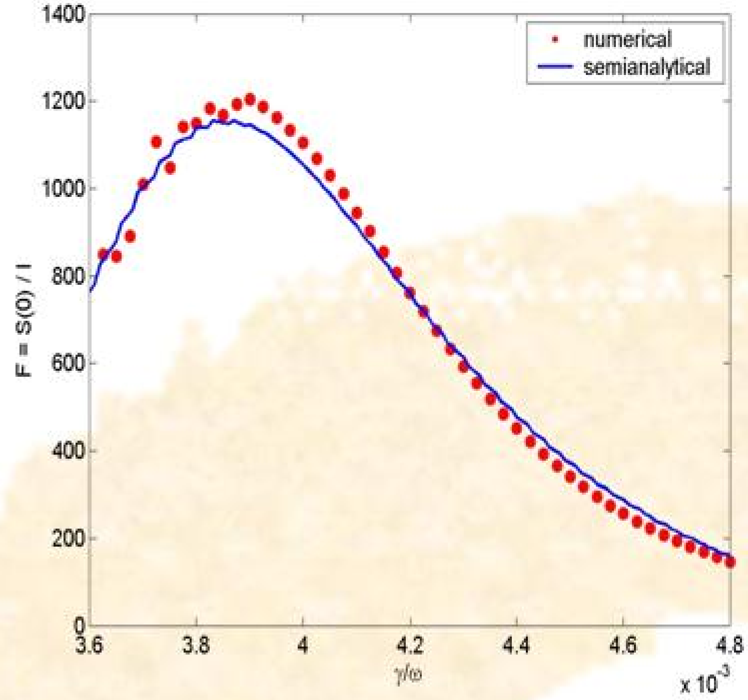


still classical (but noisy) limit

Current



Fano factor

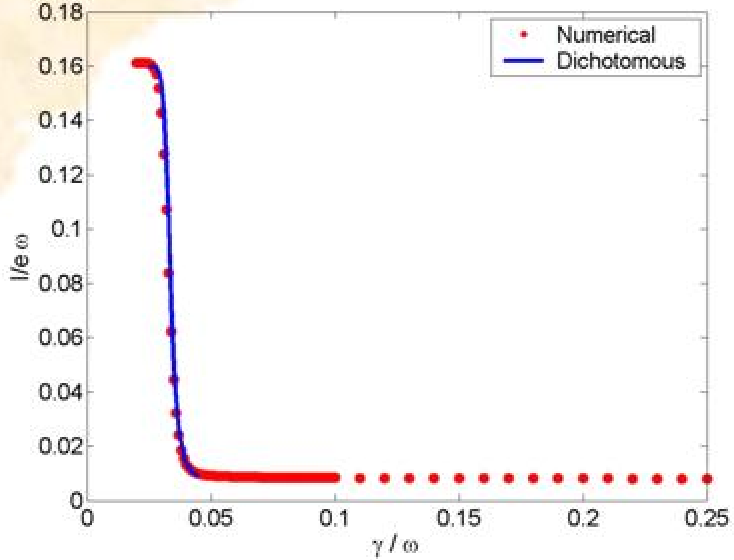


Donarini, PhD thesis, cond-mat/0501242

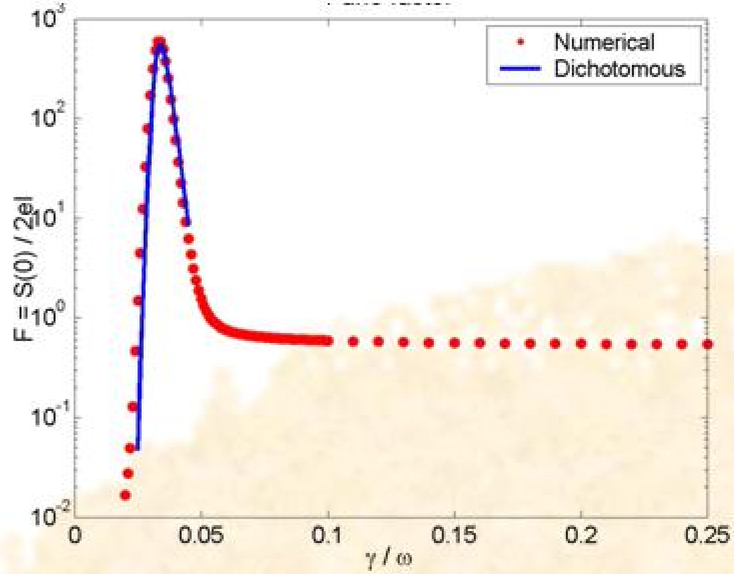
Comparison (ii)

fitted Quantum limit

Current



Fano factor



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.