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Quantum Nanomechanics of Shuttle Systems

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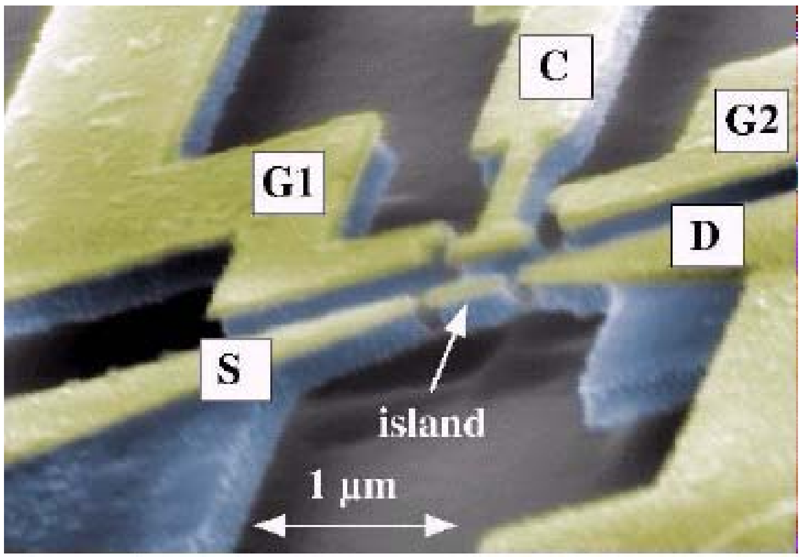
- Electromechanics of Coulomb Blockade structures
- Nanomechanical Shuttling: Quantum approach.
- Shuttling of Spin-Polarized electrons.
- Conclusions

Nanoelectromechanical Devices

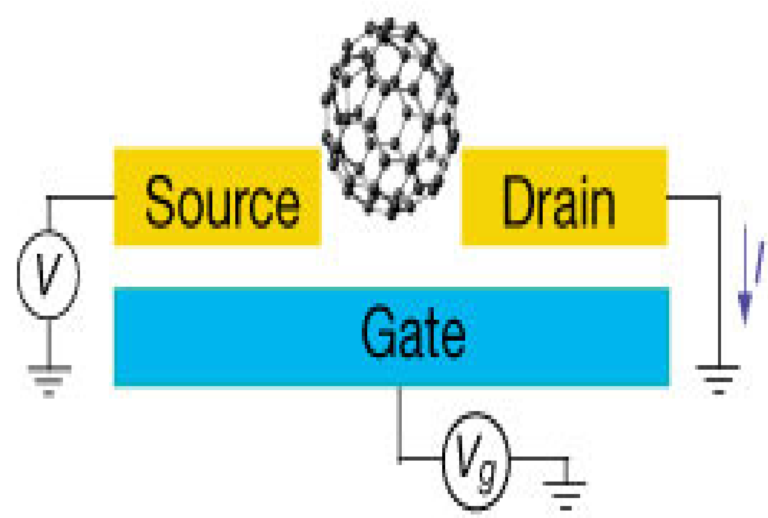
Quantum ”bell”



A. Erbe *et al.*, PRL **87**, 96106 (2001);

D. Scheible *et al.* NJP **4**, 86.1 (2002)

Single **C_{60}** Transistor

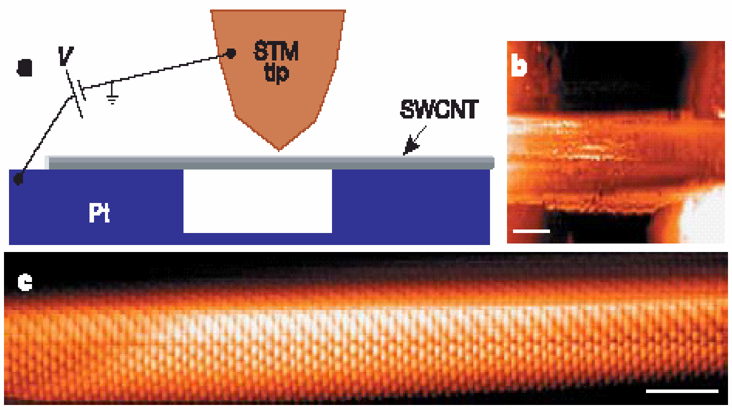


H. Park *et al.*, Nature **407**, 57 (2000)

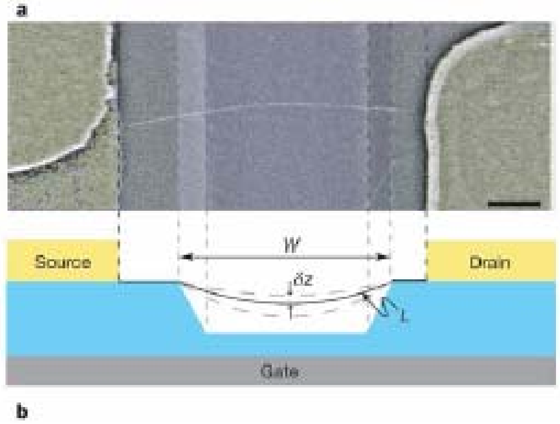
Here: Nanoelectromechanics caused by or associated with single-charge tunneling effects

CNT-Based Nanoelectromechanics

A suspended CNT has mechanical degrees of freedom => study electromechanical effects on the nanoscale.

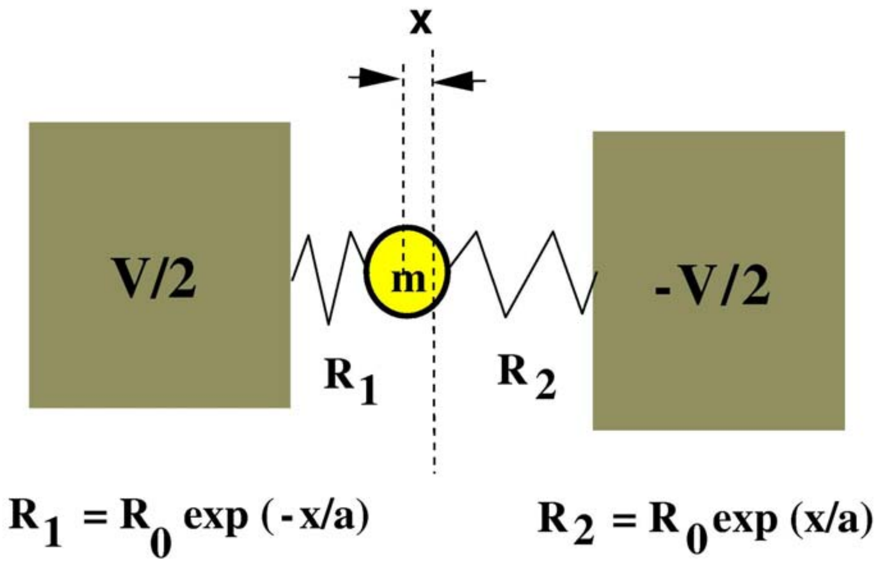


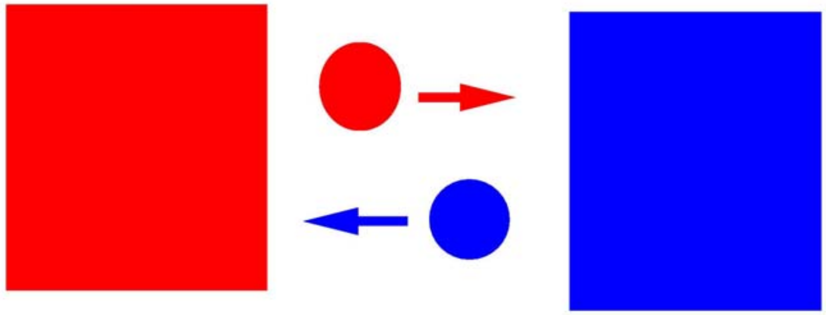
B. J. LeRoy et al., Nature **432**, 371 (2004)



V. Sazonova et al., Nature **431**, 284 (2004)

Electro-mechanical instability





Velocity direction is correlated with the charge sign

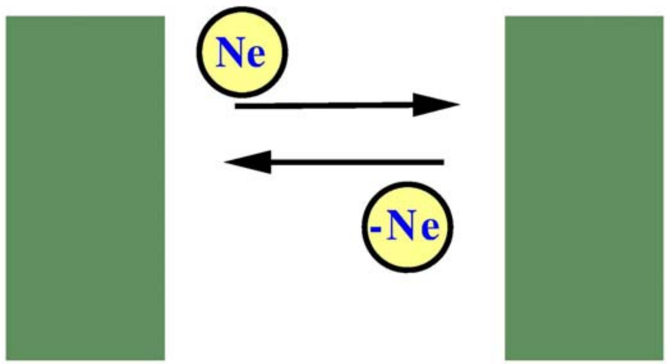
$$W = \frac{E}{T}\int_0^T dt\, Q(t)\, \dot{X}(t) > 0$$

If W exceeds the dissipated power an instability occurs

Gorelik et al., PRL 1998

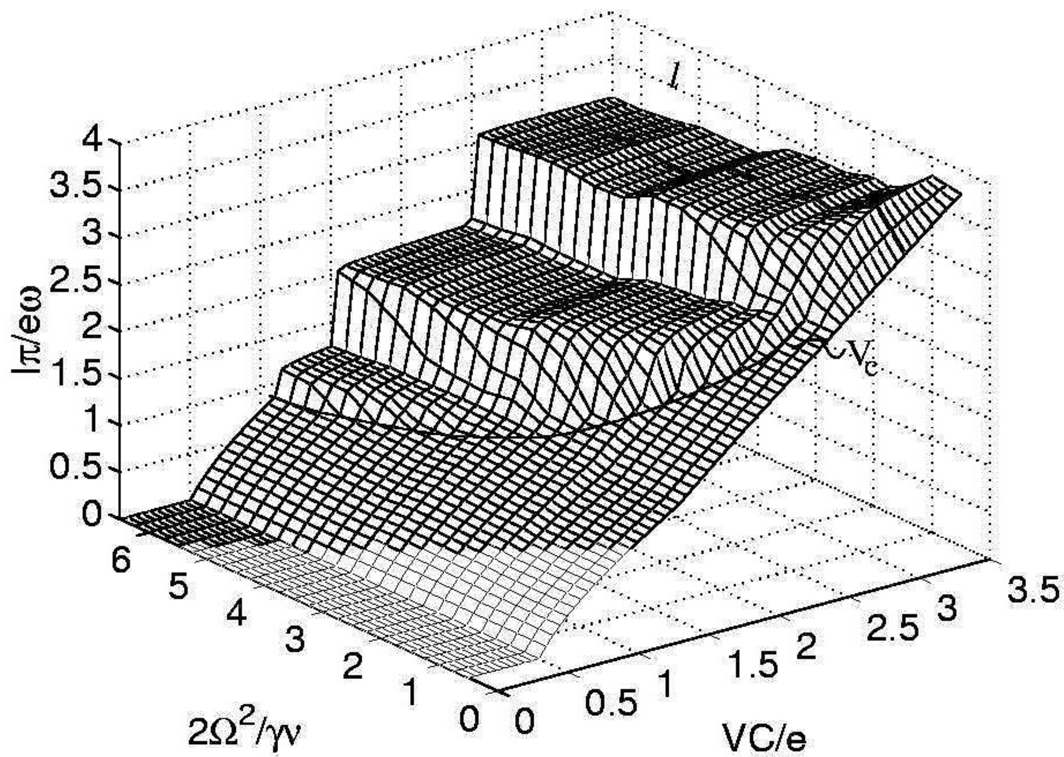
Shuttling of electronic charge

Instability occurs at $V > V_c$ and develops into a limit cycle of dot vibrations. Both V_c and vibrational amplitude are determined by dissipation.



$$I = 2eN\omega$$

$$N = \mathrm{Int}\left[\frac{VC}{2e}\right]$$



Quantum Nanoelectromechanics of Shuttle Systems

$$\delta X \, \delta P \cong \eta$$

$$\delta X \cong 2X_0 \equiv \sqrt{\frac{2\eta}{M\omega}}$$

If $\dfrac{R(X+\delta X)}{R(X)} >> 1$ then quantum fluctuations of the grain significantly affect nanoelectromechanics.

<u>Do we have a shuttle instability in this case?</u>

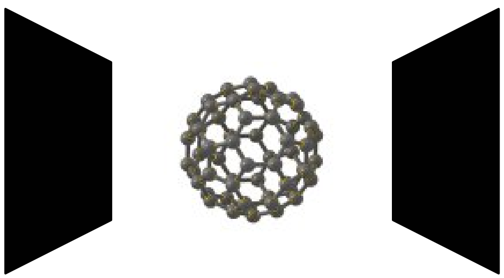
We will give a positive answer to this question

Conditions for Quantum Shuttling

$$\frac{2X_0}{\lambda} \gtrsim 1$$

λ – Tunneling length

1. Fullerene based SET

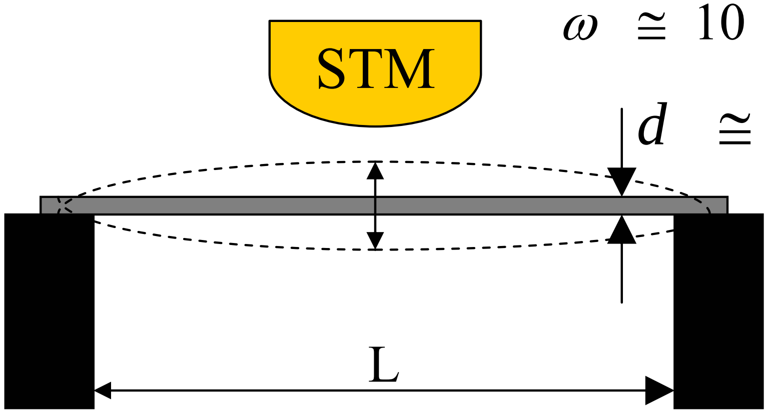


$$\omega \cong 1\ \text{THz}$$

$$\frac{X_0}{\lambda} \cong 0.1$$

→ Quasiclassical shuttle vibrations.

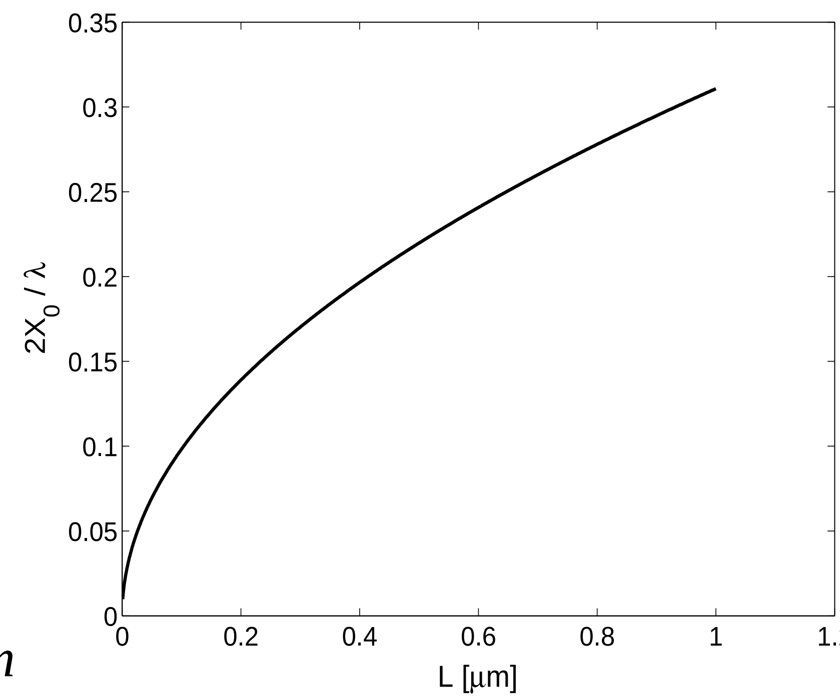
2. Suspended CNT



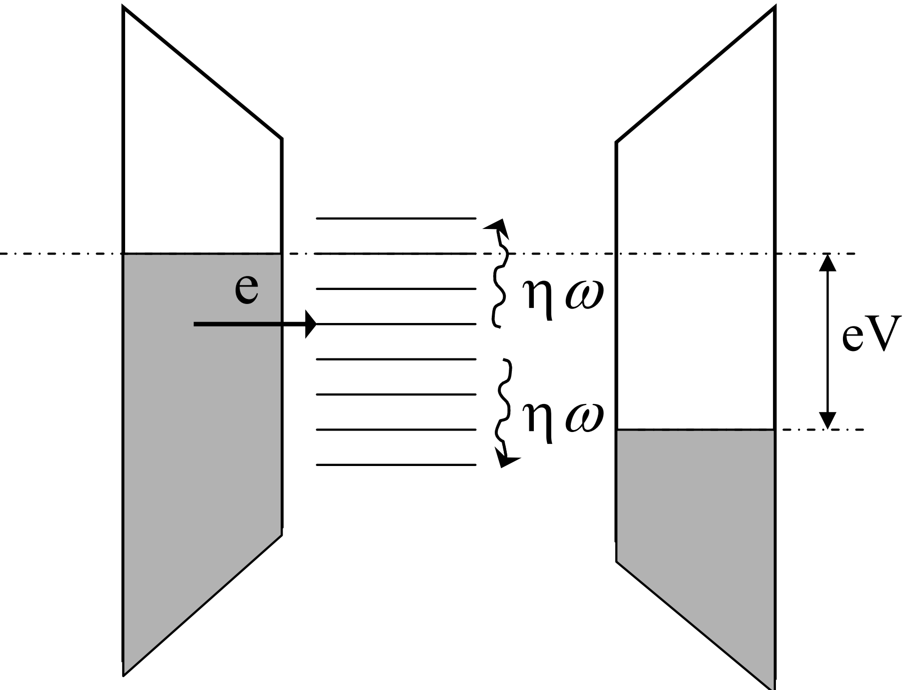
$$\omega \cong 10^{14}\ \text{Hz} \left(\frac{d}{L}\right)^2$$

$$d \cong 1\ \text{nm}$$

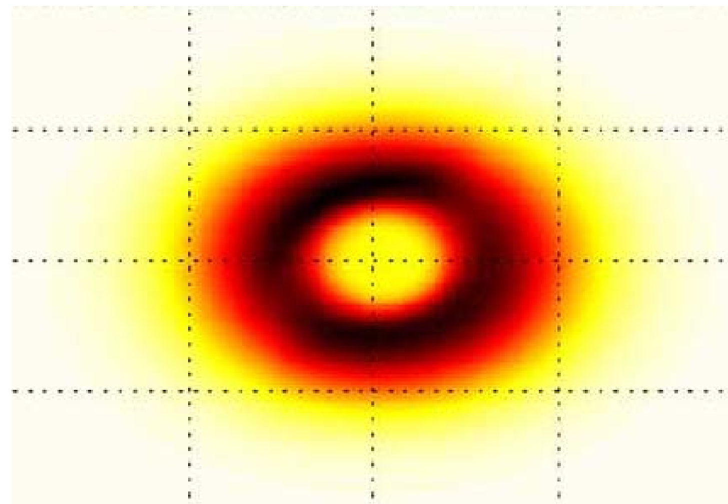
$$\omega \cong 10^8 - 10^9\ \text{Hz} \quad \text{for SWNT} \quad \text{with} \quad L \cong 1\ \mu m$$



Quantum Shuttle Instability



Quantum vibrations, generated by tunneling electrons, remain undamped and accumulate in a **coherent "condensate"** of phonons, which is classical shuttle oscillations.



Phase space trajectory of shuttling.
From Ref. (3)

$$\gamma < \gamma_{\mathrm{thr}} \equiv \Gamma \frac{d}{\lambda}$$

$$d = \frac{eE}{2k}$$

Shift in oscillator position caused by charging it by a single electron charge

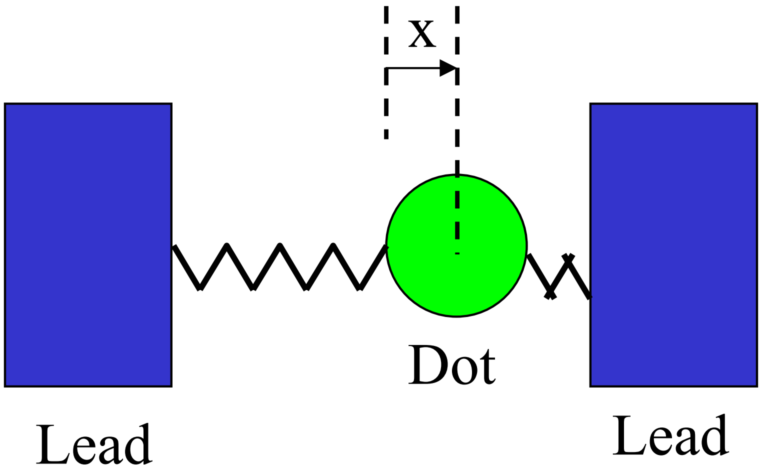
References:

(1) D. Fedorets *et al*. Phys. Rev. Lett. 92, 166801 (2004)

(2) D. Fedorets, Phys. Rev. B **68**, 033106 (2003)

(3) T. Novotny *et al*. Phys. Rev. Lett. **90** 256801 (2003)

Theory of Quantum Shuttle



The Hamiltonian:

$$H = H_{Leads} + H_{Dot} + H_T$$

$$H_{Leads} = \sum_{\alpha,k} (\varepsilon_{\alpha k} - \mu_\alpha) a^+_{\alpha k} a_{\alpha k}$$

$$H_{Dot} = [\varepsilon_0 - eE\hat{x}] c^+ c + H_v,$$

$$H_T = \sum_{\alpha,k} T_\alpha(\hat{x})(a^+_{\alpha k} c + c^+ a_{\alpha k})$$

$$H_v = \left[\hat{p}^2 + \hat{x}^2\right]/2$$

$$T_{L,R}(x) = T_0 e^{\mu x/\lambda}, \mu_{L,R} = \mu \pm eV/2$$

Time evolution in Schrödinger picture:

$$\partial_t \hat{\sigma}(t) = -i[H, \hat{\sigma}(t)]$$

Total density operator

Reduced density operator

$$\hat{\rho}(t) \equiv Tr_{leads} \hat{\sigma}(t) \equiv \begin{pmatrix} \hat{\rho}_0(t) & \hat{\rho}_{01}(t) \\ \hat{\rho}_{10}(t) & \hat{\rho}_1(t) \end{pmatrix}$$

Generelized Master Equation

$\hat{\rho}_0$: density matrix operator of the *uncharged* shuttle
$\hat{\rho}_1$: density matrix operator of the *charged* shuttle

At large voltages equations for $\hat{\rho}_0, \hat{\rho}_1$ are local in time:

$$\partial_t \hat{\rho}_0 = -i[H_v + eE\hat{x}, \hat{\rho}_0]_- - \{\Gamma_L(\hat{x}), \hat{\rho}_0\}_+ + \sqrt{\Gamma_R(\hat{x})}\hat{\rho}_1\sqrt{\Gamma_R(\hat{x})} + L_\gamma \hat{\rho}_0$$

Free oscillator dynamics — Electron tunnelling — Dissipation

$$\partial_t \hat{\rho}_1 = -i[H_v - eE\hat{x}, \hat{\rho}_1]_- - \{\Gamma_R(\hat{x}), \hat{\rho}_1\}_+ + \sqrt{\Gamma_L(\hat{x})}\rho_0\sqrt{\Gamma_L(\hat{x})} + L_\gamma \hat{\rho}_1$$

$$L_\gamma \hat{\rho}_\alpha \equiv -\frac{i\gamma}{2}\left[\hat{x},\{\hat{p},\hat{\rho}_\alpha\}\right] - \frac{\gamma}{2}\left[\hat{x},\left[\hat{x},\hat{\rho}_\alpha\right]\right]$$

$\hat{\rho}_- \equiv \hat{\rho}_0 - \hat{\rho}_1$: describes shuttling of electrons
$\hat{\rho}_+ \equiv \hat{\rho}_0 + \hat{\rho}_1$: describes vibrational space.

Approximation: $x_0/\lambda << 1, \quad eE/k\lambda << 1, \quad \gamma << 1$

Shuttle instability

After linearisation in *x* (using the small parameter x_o/λ) one finds:

$$\dot{x} = p$$

$$\dot{p} = -x - \gamma p - \frac{d}{2x_0} n_-$$

$$\dot{n}_- = -\frac{\Gamma}{\eta} n_- + \frac{2\Gamma x_0}{\eta\lambda} x$$

$$x(t) \equiv x_0^{-1} Tr\left[\hat{\rho}_+(t)\hat{x}\right]$$

$$p(t) \equiv \frac{x_0}{\eta} Tr\left[\hat{\rho}_+(t)\hat{p}\right]$$

$$n_-(t) = 1 - Tr\left[\hat{\rho}_1(t)\right]$$

Result: *an initial deviation from the equilibrium position grows exponentially if the dissipation is small enough*:

$$x(t) \propto \exp(\alpha t);$$

$$\alpha = (\gamma_{thr} - \gamma)/2; \quad \gamma < \gamma_{thr} \equiv \frac{\Gamma}{\eta}\frac{d}{\lambda}$$

Semiclassical and Quantum Regimes of Shuttling

Pumping of the energy

$$W_{cl}(E) \approx \frac{eE\lambda\Gamma(x)}{\eta},$$

$$\delta x_q \approx \eta / \sqrt{2m\omega}$$

$\delta\Gamma_q \approx$ Quantum correction to the pumping results in quantum part of the shuttling energy δW_q

$$\delta W_q = \frac{E_c}{E} W_{cl}$$

$$\delta W_q = W_{cl}(E_c)$$

$$E_c \equiv \Gamma\eta / eM\omega\lambda^3 \propto \eta$$

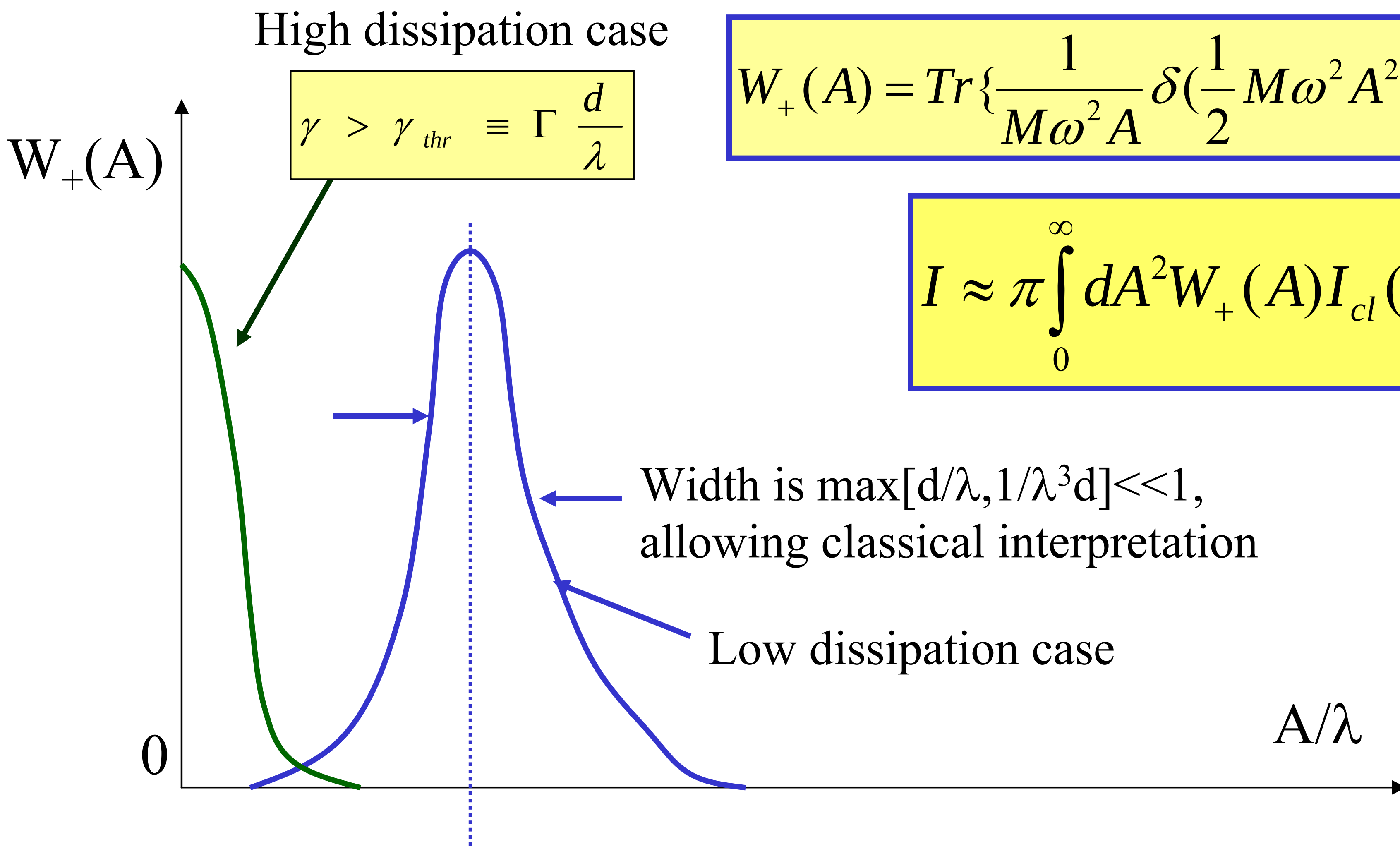
1). $E >> E_c -$ Semiclassical limit

1). $E \leq E_c -$ Quantum limit

Results for Semiclassical Shuttling

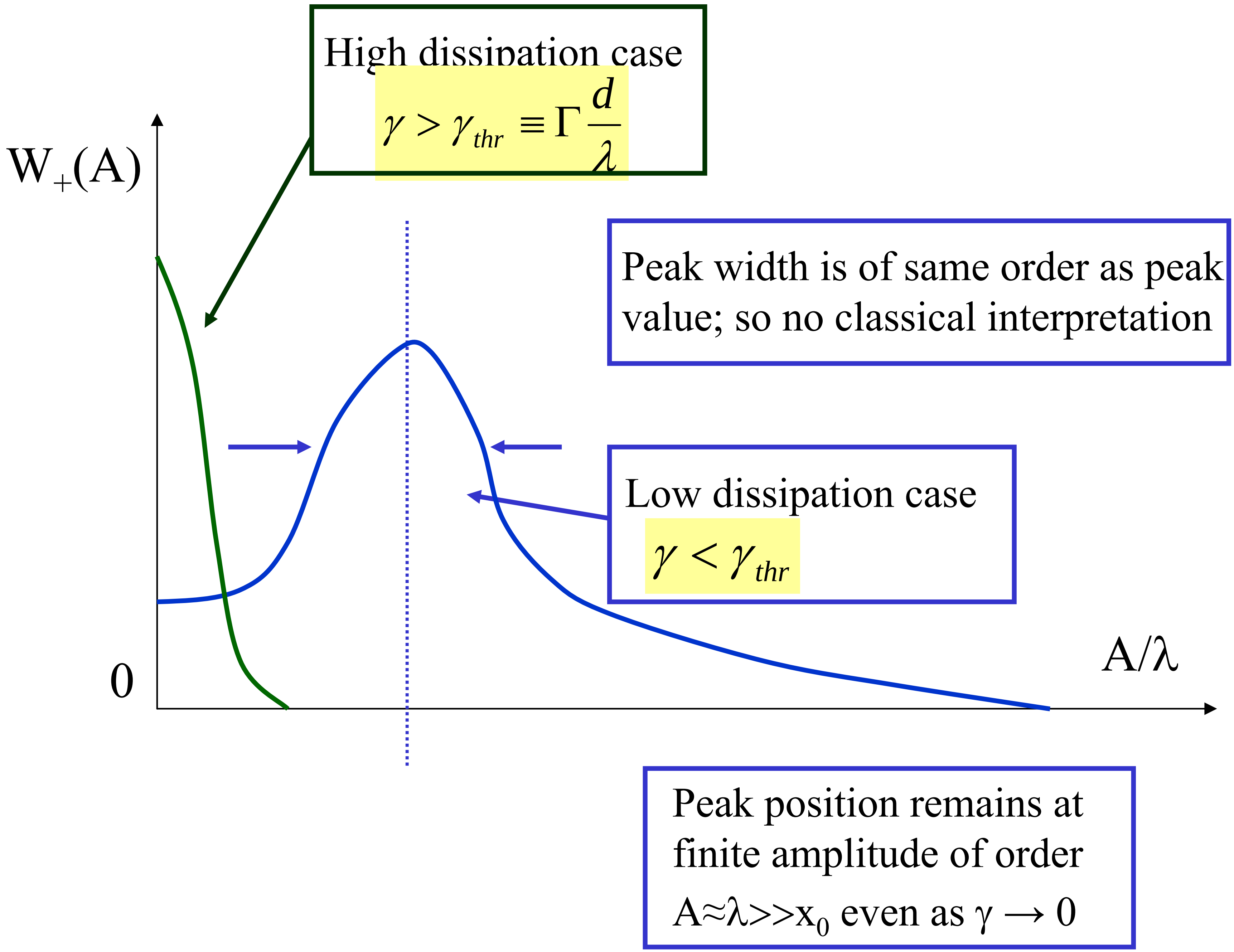
$$W_+(A) = Tr\{\frac{1}{M\omega^2 A}\delta(\frac{1}{2}M\omega^2 A^2 - \hat{H}_\omega)\hat{\rho}_+\}$$

$$I \approx \pi \int_0^\infty dA^2 W_+(A) I_{cl}(A)$$

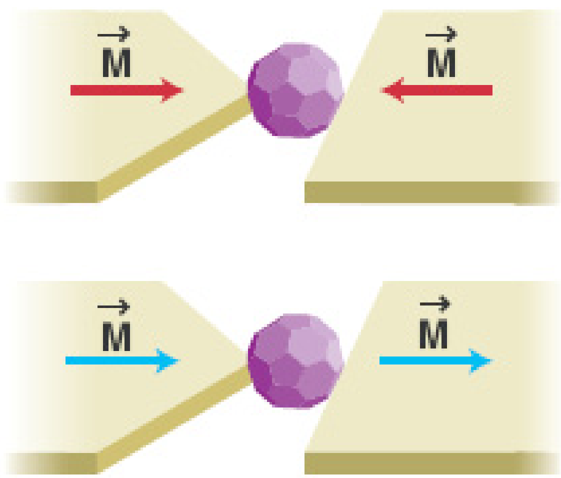


Peak position same
as obtained in classical
description of shuttle
motion, EPL 2002

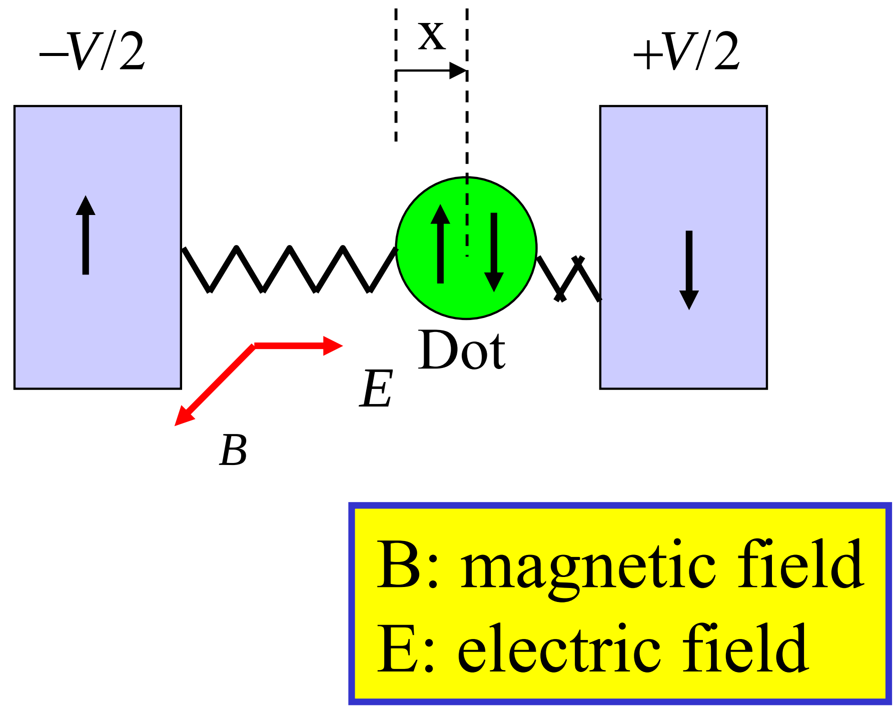
Sketch of results in "quantum" regime: $E \ll E_C$



Spintronics of Nanomechanical Shuttle



A. Pasupathy et al., Science **306**,86 (2004)



D.Fedorets et al., PRL, **95**, 057203-1, 2005

Formulation of the problem

$$H = H_{Leads} + H_T + H_{Dot} + H_{bath} + H_{bath-osc}$$

$$H_{Leads} = \sum_{\alpha,k} \varepsilon_{\alpha k} a^{+}_{\alpha k} a_{\alpha k}, \quad H_T = \sum_{\alpha,k} T_\alpha(x)\left[a^{+}_{\alpha k} c_\alpha + c^{+}_{\alpha} a_{\alpha k}\right]$$

$$H_{Dot} = (\varepsilon_0 - xd)\left[c^{+}_{\uparrow} c_{\uparrow} + c^{+}_{\downarrow} c_{\downarrow}\right] + U c^{+}_{\uparrow} c_{\uparrow} c^{+}_{\downarrow} c_{\downarrow} - \frac{h}{2}\left[c^{+}_{\uparrow} c_{\downarrow} + c^{+}_{\downarrow} c_{\uparrow}\right] +$$

$$\frac{1}{2}\left[p^2 + x^2\right]$$

Density matrix for the "spin-polarized" shuttle

Four basic vector for the electronic space

$$|0\rangle \quad |\uparrow\rangle \equiv c_{\uparrow}^{+}|0\rangle \quad |\downarrow\rangle \equiv c_{\downarrow}^{+}|0\rangle \quad |2\rangle \equiv c_{\downarrow}^{+}c_{\uparrow}^{+}|0\rangle$$

Density matrix

$$\hat{\rho}_0 = \langle 0|\hat{\rho}|0\rangle$$

$$\hat{\rho}_2 = \langle 2|\hat{\rho}|2\rangle$$

$$\hat{\rho}_1 = \begin{Bmatrix} \hat{\rho}_{\uparrow} & \hat{\rho}_{\uparrow\downarrow} \\ \hat{\rho}_{\downarrow\uparrow} & \hat{\rho}_{\downarrow} \end{Bmatrix}$$

$$\hat{\rho}_{\uparrow} = \langle\uparrow|\hat{\rho}|\uparrow\rangle$$

$$\hat{\rho}_{\uparrow\downarrow} = \langle\uparrow|\hat{\rho}|\downarrow\rangle$$

Spin-vibrational dynamics

$$\partial_t \hat{\rho}_0 = -i[H_v + eE\hat{x}, \hat{\rho}_0] - \frac{1}{2}\{\Gamma_L(\hat{x}), \hat{\rho}_0\} + \sqrt{\Gamma_R(\hat{x})}\hat{\rho}_1\sqrt{\Gamma_R(\hat{x})} + \Lambda_\gamma \hat{\rho}_0$$

$$\partial_t \hat{\rho}_2 = -i[H_v - eE\hat{x}, \hat{\rho}_2] - \frac{1}{2}\{\Gamma_L(\hat{x}), \hat{\rho}_2\} + \sqrt{\Gamma_L(\hat{x})}\hat{\rho}_\downarrow\sqrt{\Gamma_L(\hat{x})} + \Lambda_\gamma \hat{\rho}_2$$

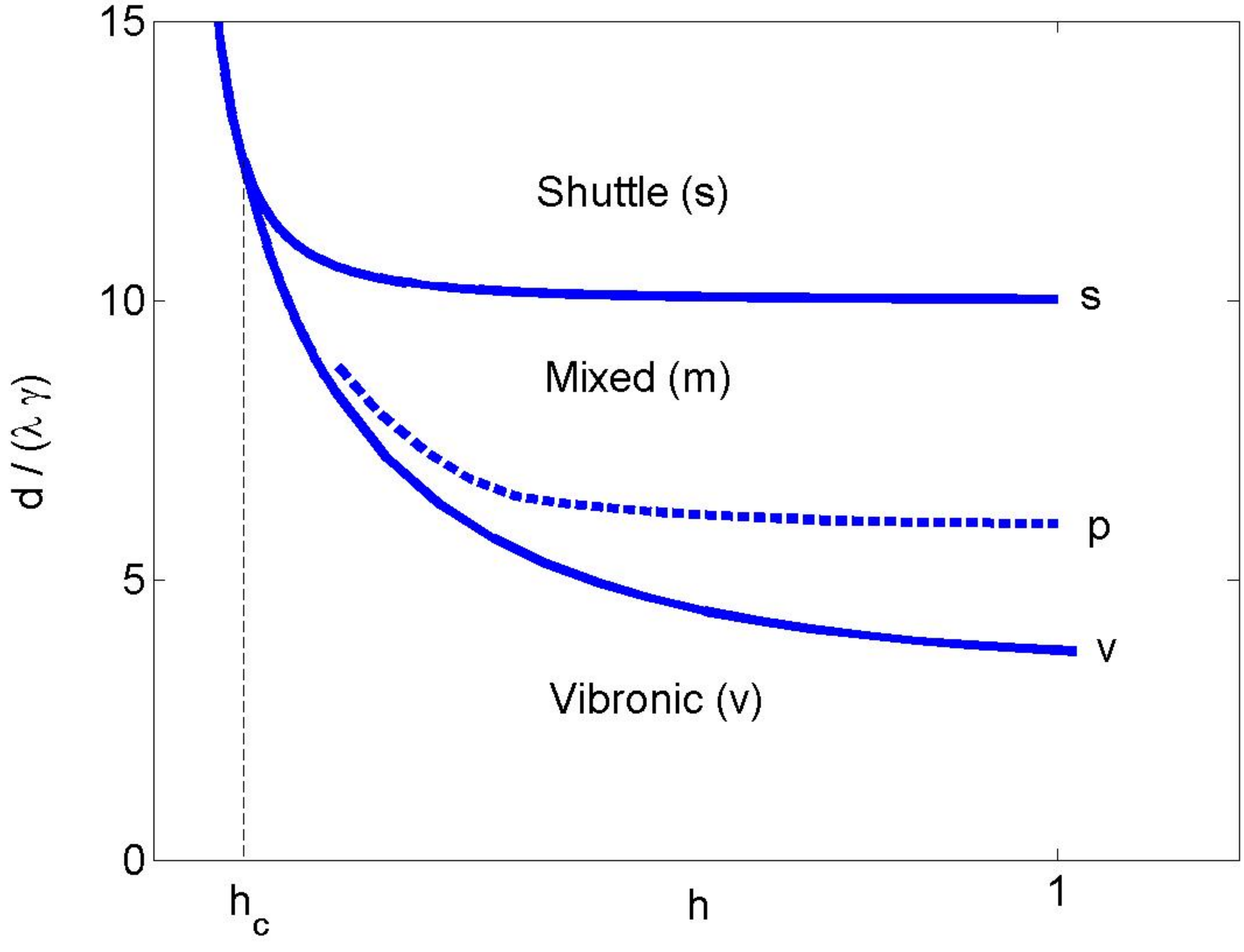
$$\partial_t \hat{\rho}_\downarrow = -i[H_v, \hat{\rho}_\downarrow] + ih(\hat{\rho}_{\uparrow\downarrow} - \hat{\rho}_{\downarrow\uparrow}) - \frac{1}{2}\{\Gamma_+(\hat{x}), \hat{\rho}_\downarrow\} + \Lambda_\gamma \hat{\rho}_\downarrow$$

$$\partial_t \hat{\rho}_\uparrow = -i[H_v, \hat{\rho}_\uparrow] - ih(\hat{\rho}_{\uparrow\downarrow} - \hat{\rho}_{\downarrow\uparrow}) + \sqrt{\Gamma_L(\hat{x})}\hat{\rho}_0\sqrt{\Gamma_L(\hat{x})} + \sqrt{\Gamma_R(\hat{x})}\hat{\rho}_2\sqrt{\Gamma_R(\hat{x})} + \Lambda_\gamma \hat{\rho}_\downarrow$$

$$\partial_t \hat{\rho}_{\downarrow\uparrow} = -i[H_v, \hat{\rho}_{\downarrow\uparrow}] - ih(\hat{\rho}_\downarrow - \hat{\rho}_\uparrow) - \frac{1}{2}\Gamma_+(\hat{x})\rho_{\downarrow\uparrow} + \Lambda_\gamma \hat{\rho}_{\downarrow\uparrow}$$

$$\partial_t \hat{\rho}_{\uparrow\downarrow} = -i[H_v, \hat{\rho}_{\uparrow\downarrow}] + ih(\hat{\rho}_\downarrow - \hat{\rho}_\uparrow) - \frac{1}{2}\Gamma_+(\hat{x})\hat{\rho}_{\uparrow\downarrow} + \Lambda_\gamma \hat{\rho}_{\uparrow\downarrow}$$

"*Phase Diagram*"



Conclusions

- Electro-mechanical coupling may result in a vibrational instability and "quantum shuttling" of electric charge

2. In the magnetic NEM-SET the shuttle effects can be controlled via external magnetic field.

3. Different stable regimes of the spintronic NEM-SET operation are found and analyzed.