Mechanical instabilities in carbon nanotube quantum dots

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UNIVERSITÉ DE STRASBOURG

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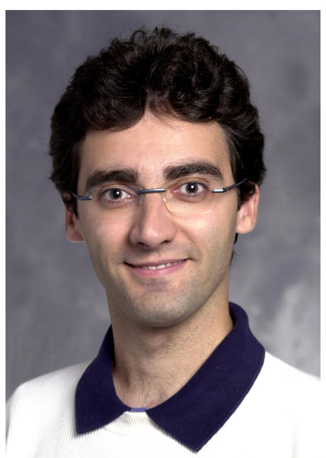
Collaborators

Fabio Pistolesi (CNRS Bordeaux/Grenoble)

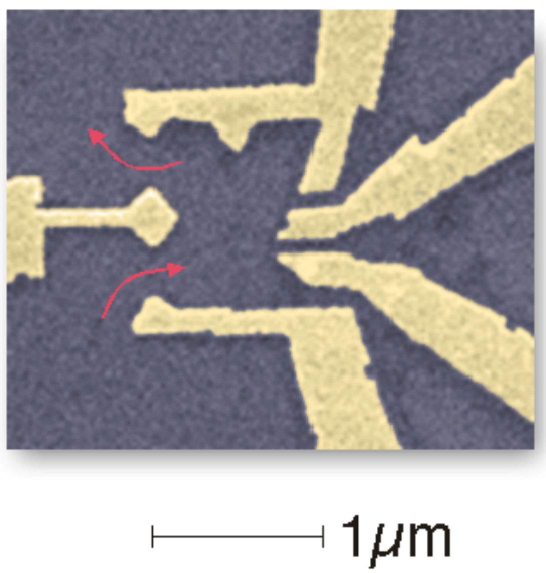


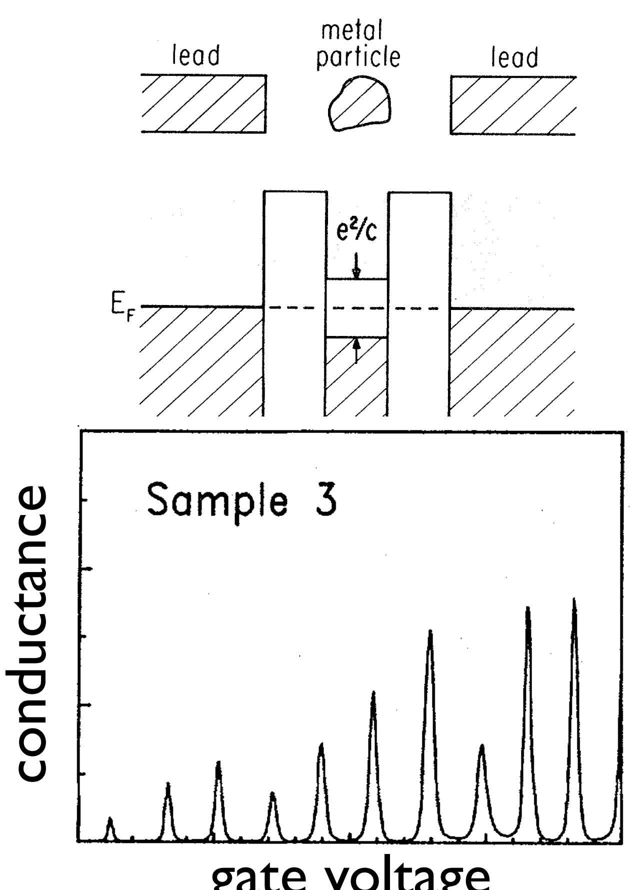
Eros Mariani (School of Physics, Exeter)

Felix von Oppen (Freie Universität Berlin)

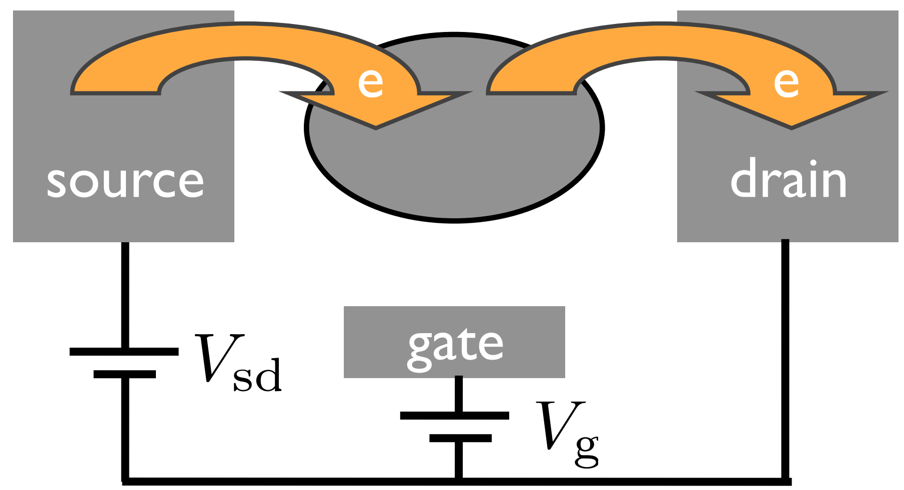
Molecular electronics

Quantum dots

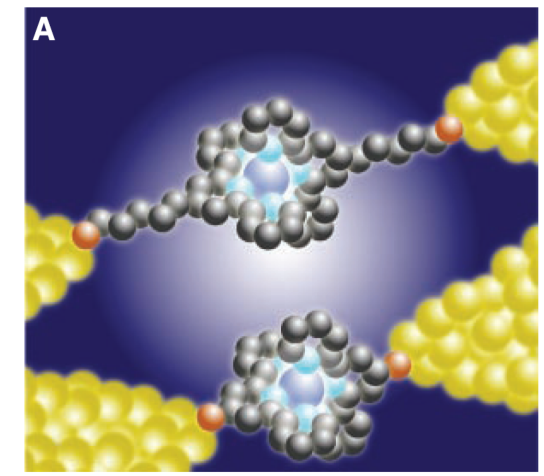


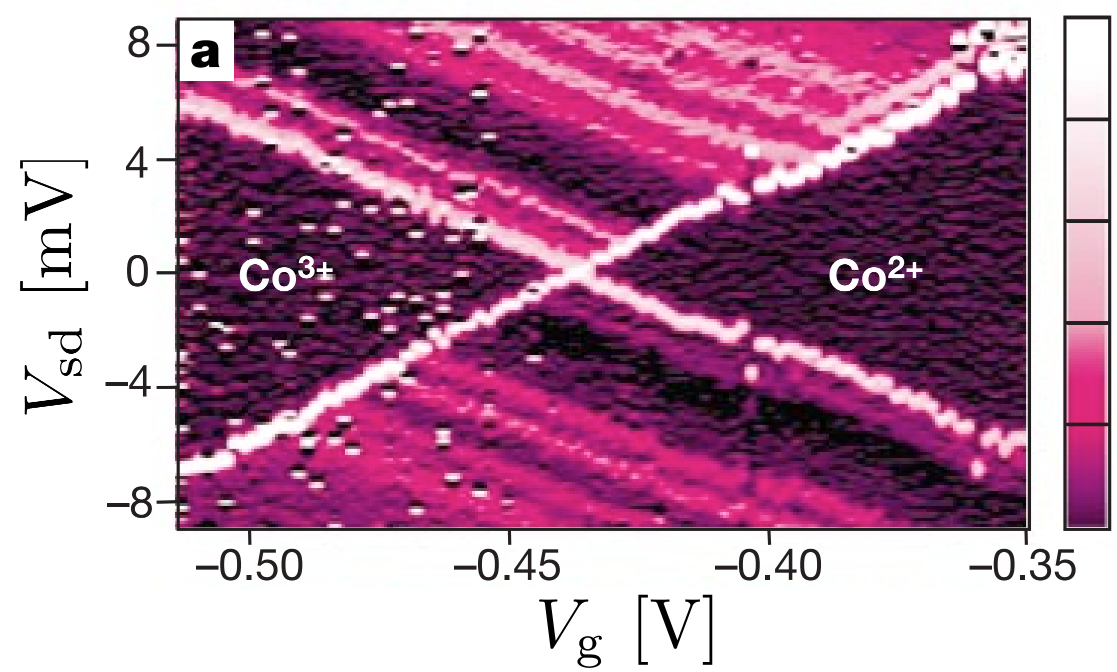


Kastner, RMP '92



Single-molecule junctions





Park *et al*, Nature '02

➡New effects due to additional degrees of freedom (vibrations, spin, conformation, ...)

Molecular electronics

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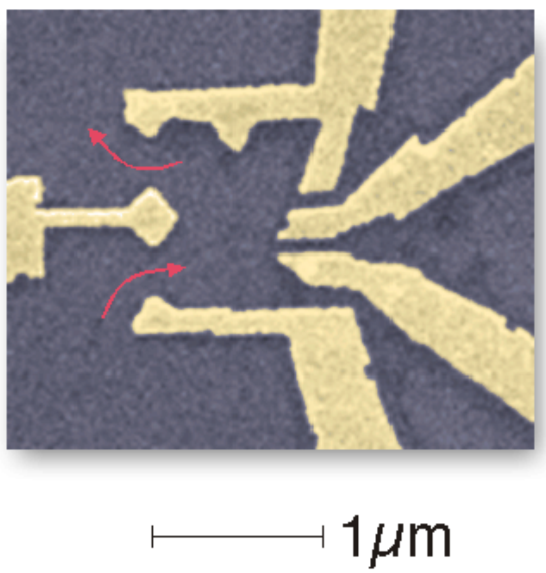

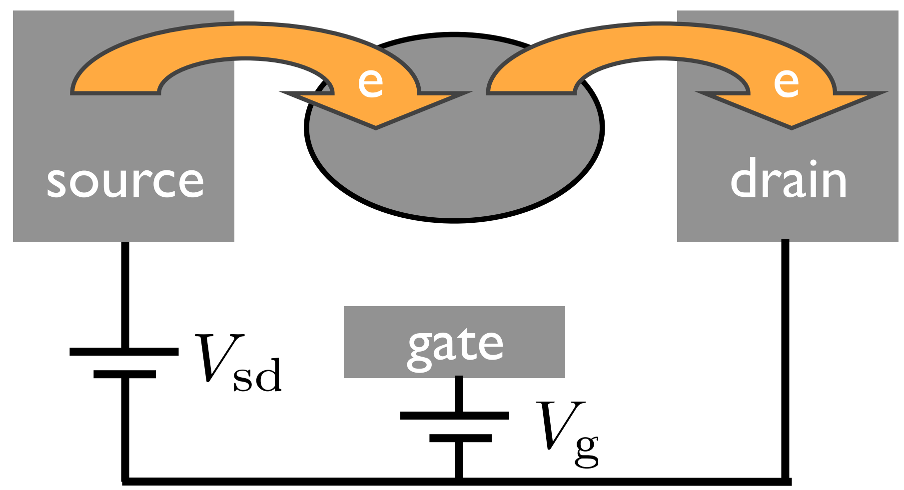

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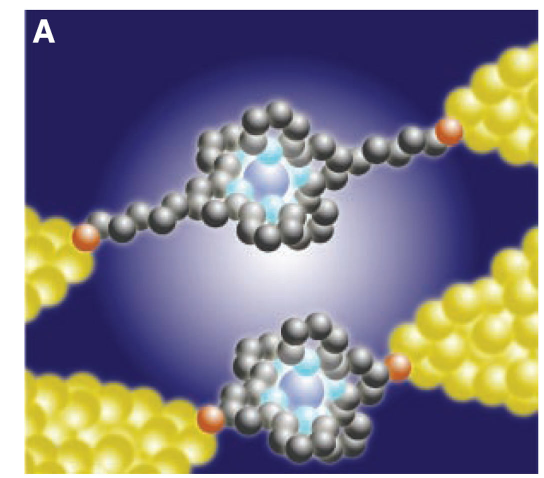
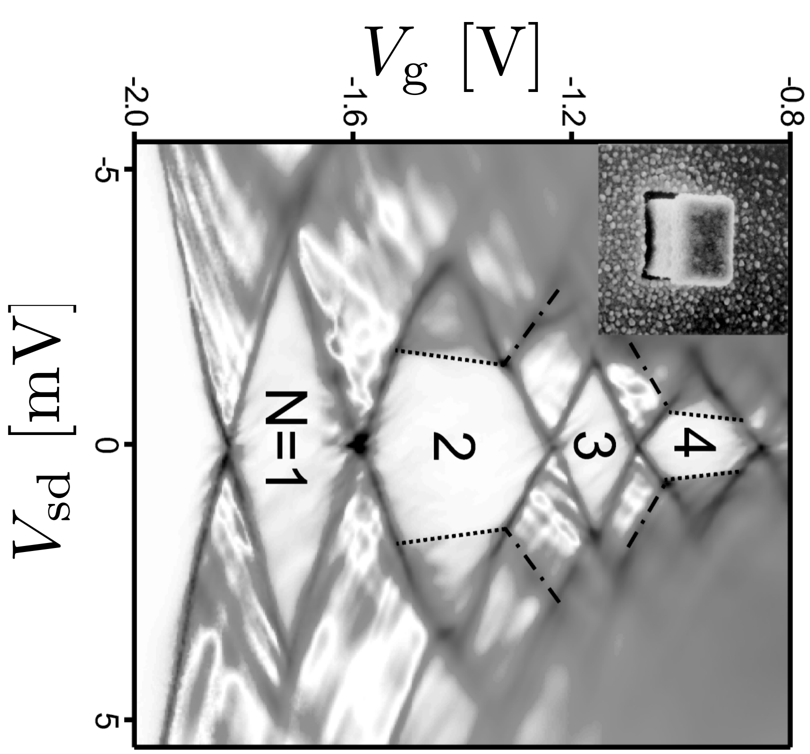
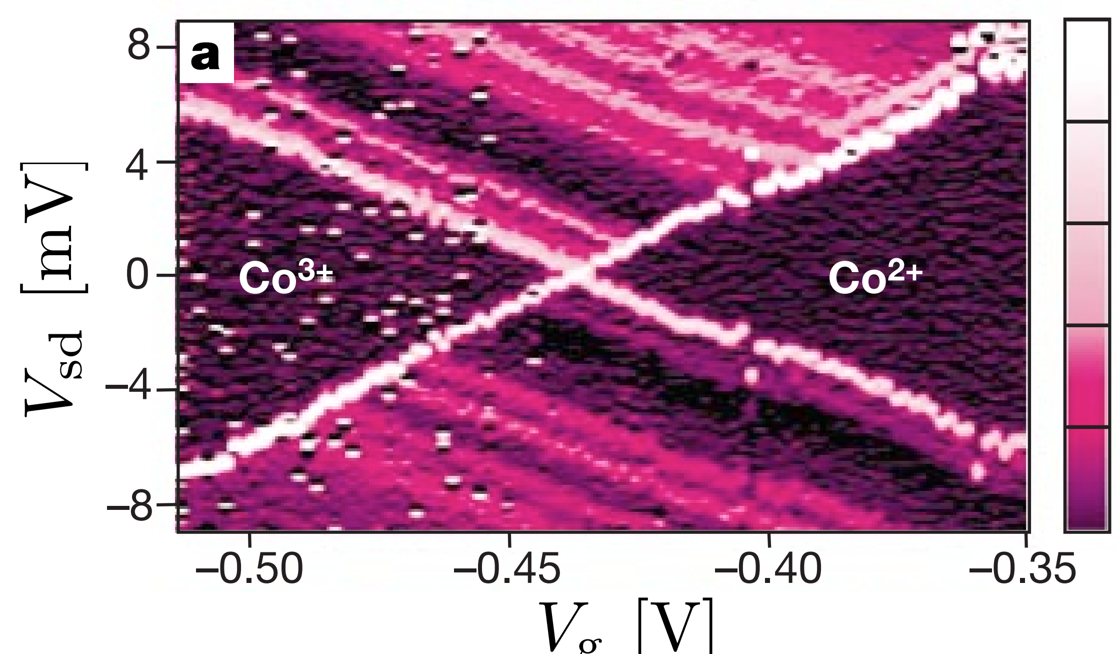




De Franceschi *et al.*, PRL '01



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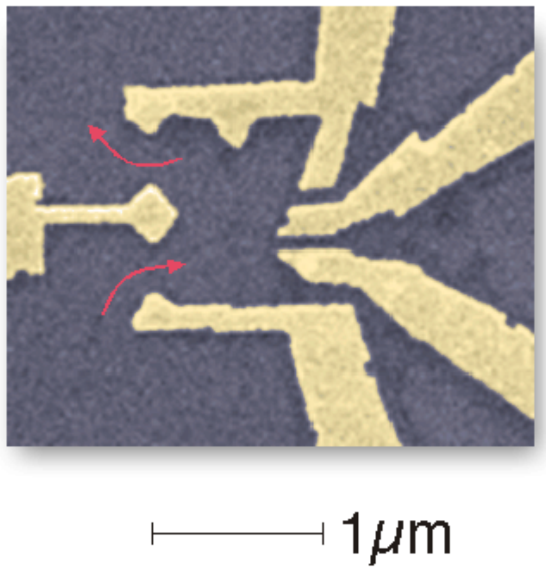
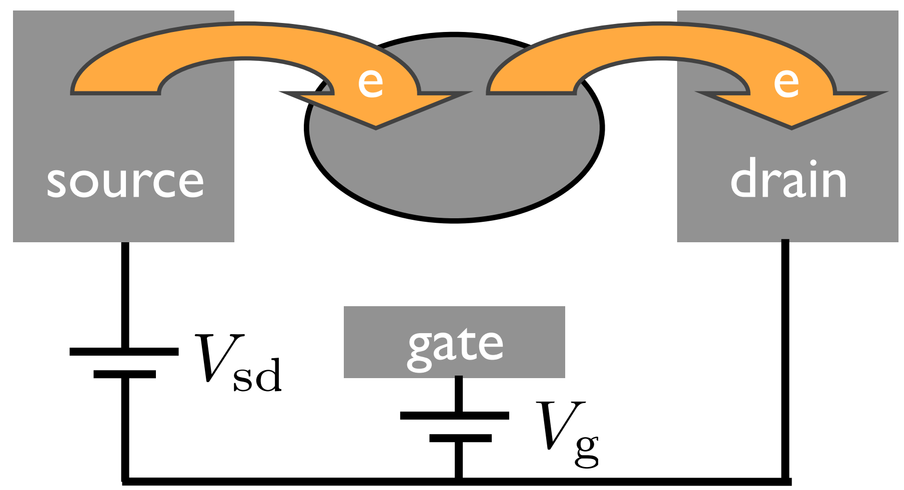
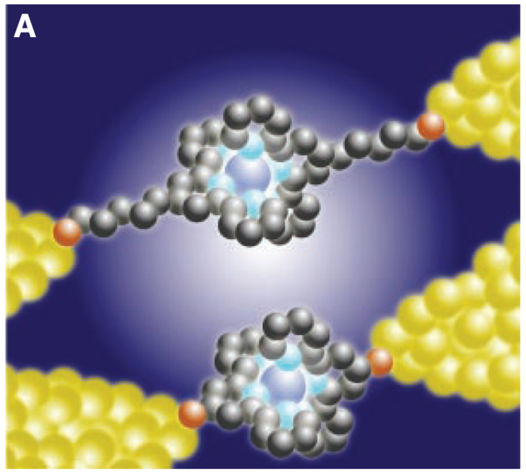
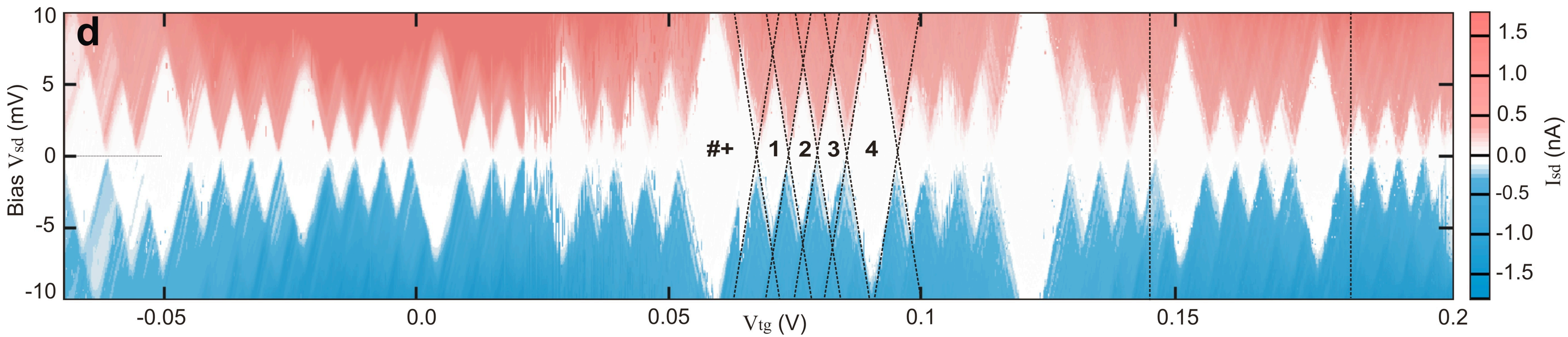




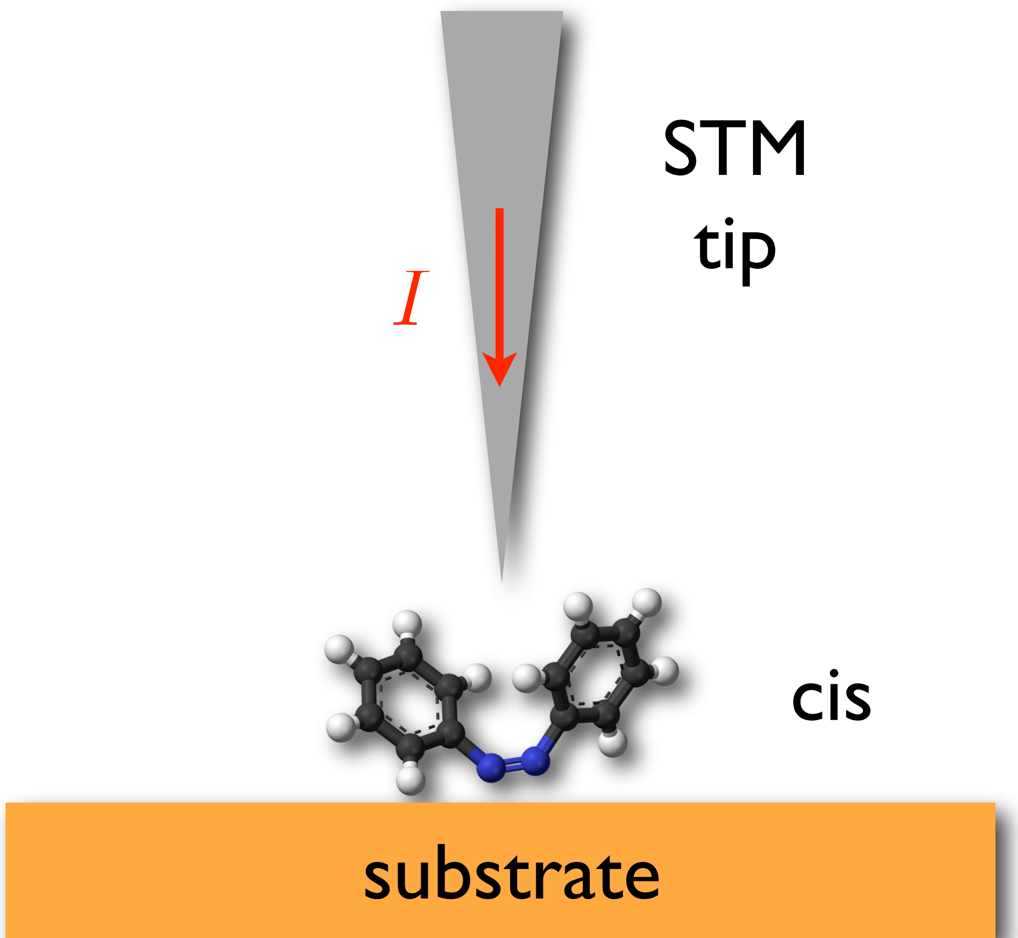


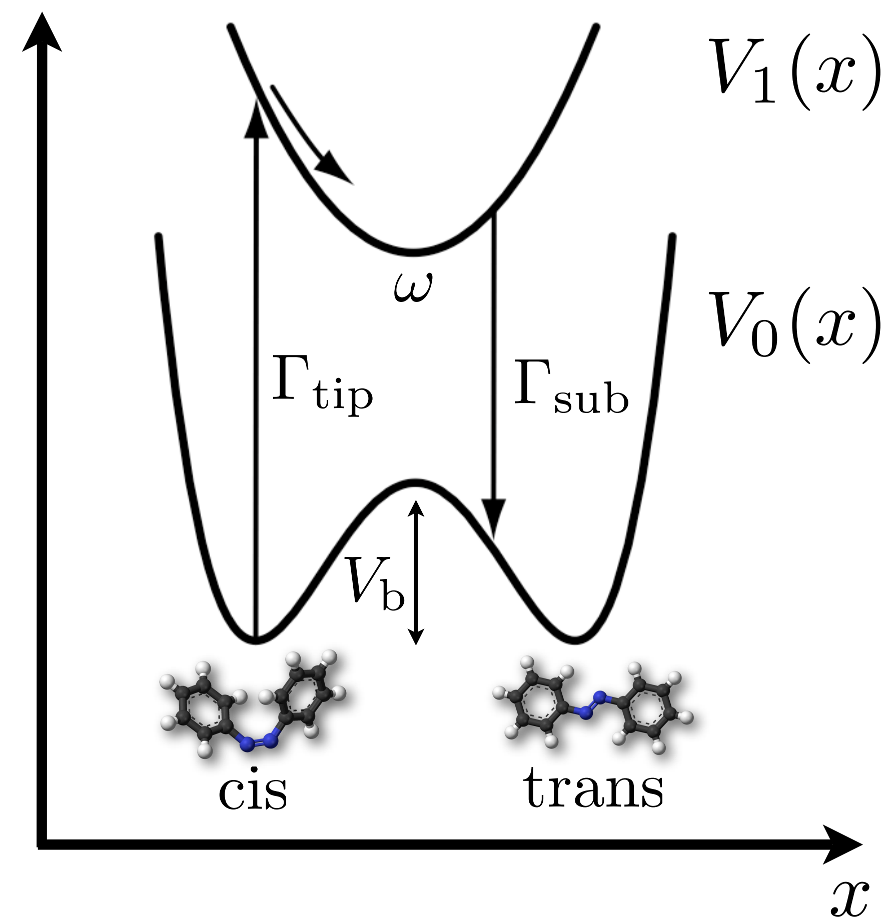
Franck-Condon blockade in suspended CNT quantum dots

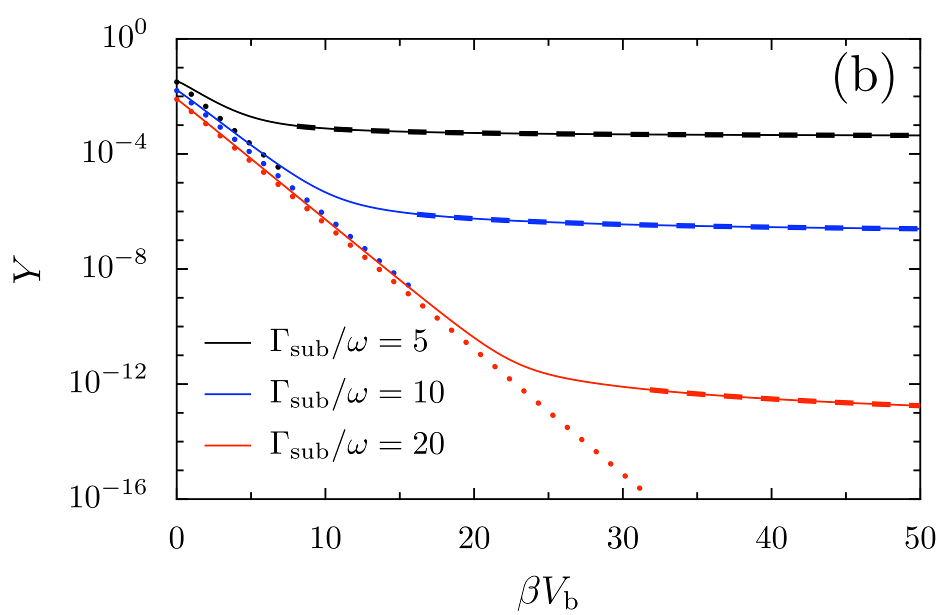


[Koch, von Oppen, PRL '05]
[Leturcq *et al.*, Nature Physics '09]

Current-induced conformational switching







$$\Gamma_{\mathrm{tip}} \ll \omega \ll \Gamma_{\mathrm{sub}}$$

$\Downarrow$

Quantum yield $\simeq 10^{-10}$

[F. Elste, GW, C. Timm, F. von Oppen, Appl. Phys. A **93**, 345 (2008)]

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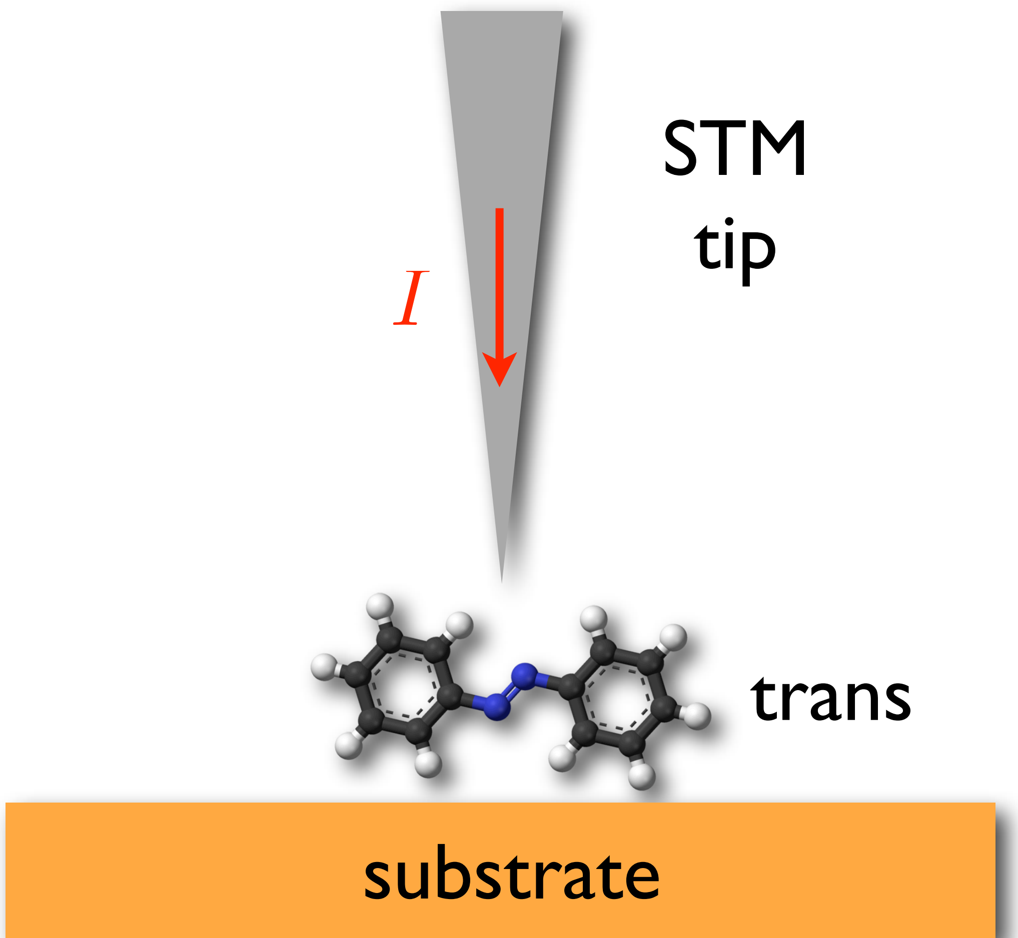

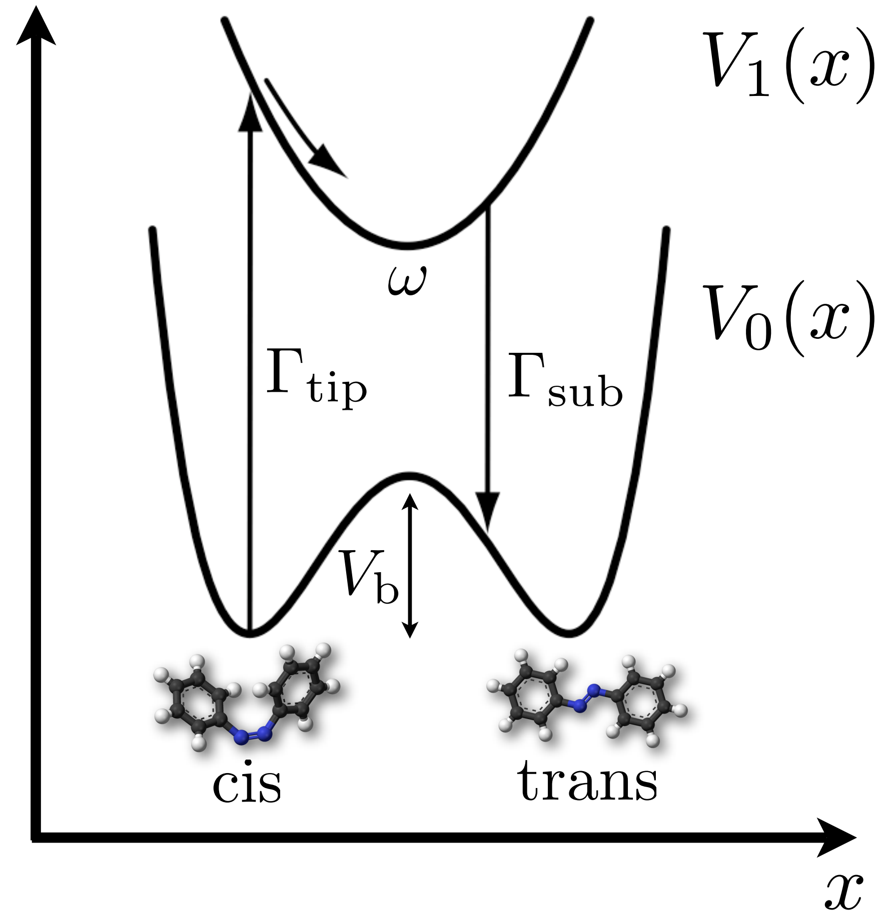

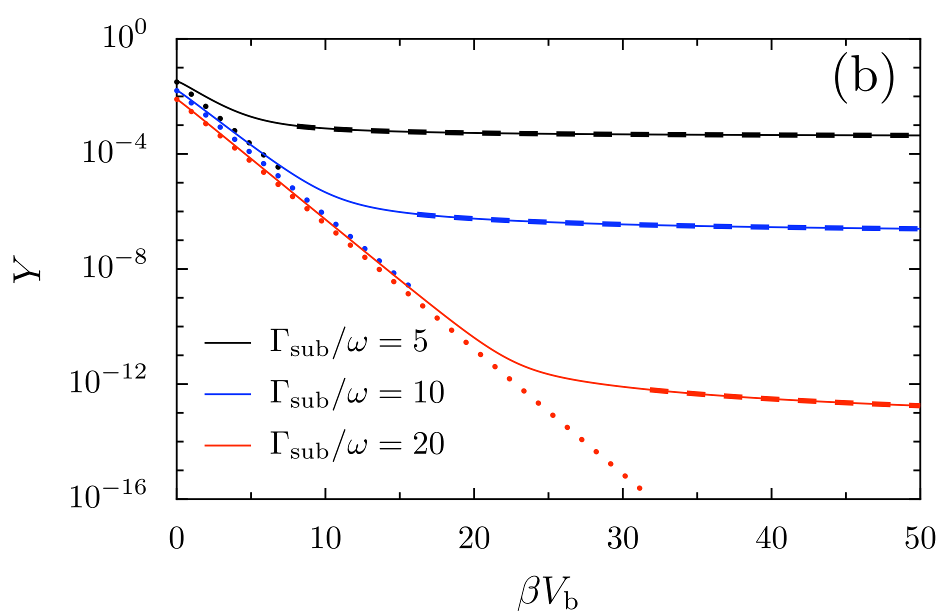

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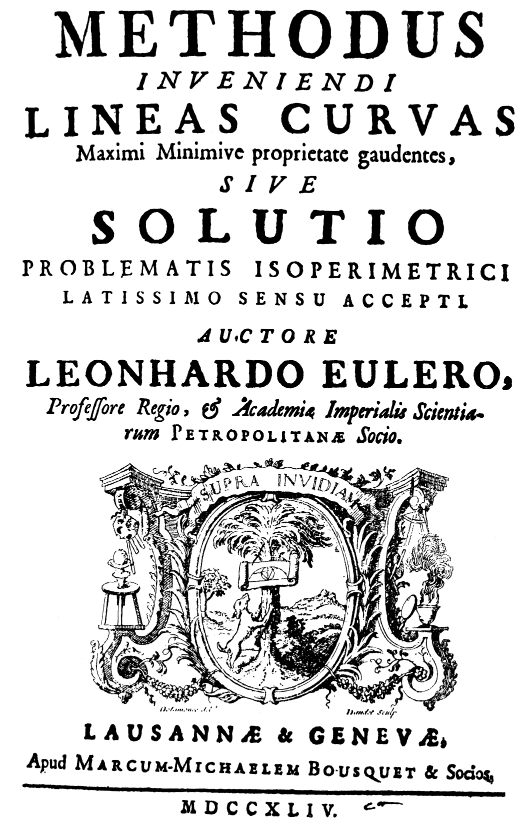
Euler buckling instability

Paradigm of (continuous) mechanical instability:

[L. Euler, 1744]


METHODUS
INVENIENDI
LINEAS CURVAS
Maximi Minimive proprietate gaudentes,
SIVE
SOLUTIO
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LATISSIMO SENSU ACCEPTI
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LEONHARDO EULERO,
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SUPRA INVIDIAM
LAUSANNÆ & GENEVÆ,
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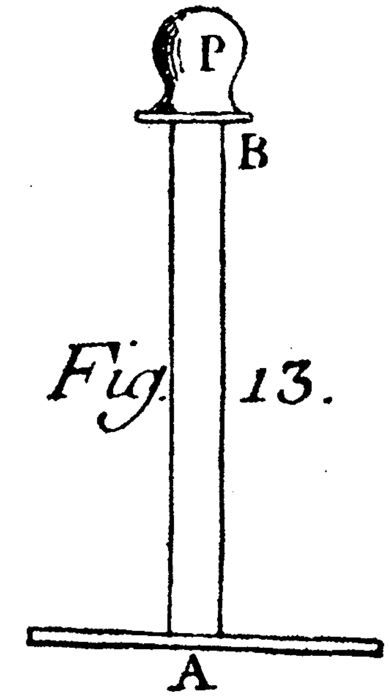
MDCCXLIV.



$F < F_c$

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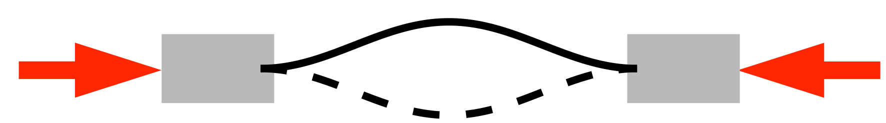


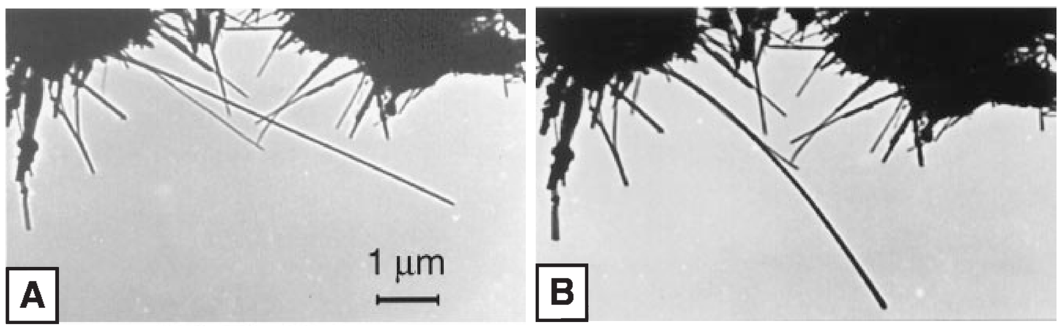
➡ Elastic rod buckles when compression exceeds critical force F_c

Euler buckling instability

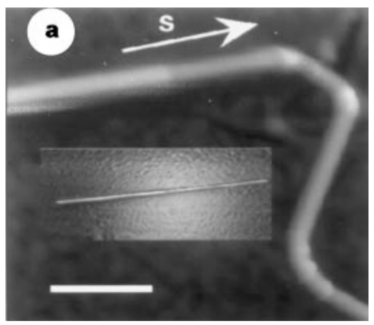
Euler buckling instability

Nanomechanical instabilities:

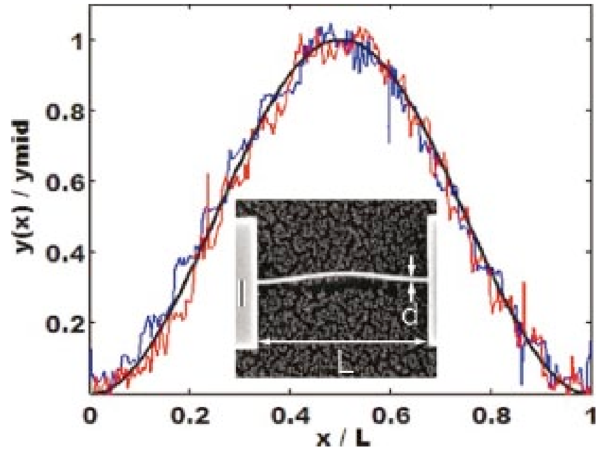
electrostatic deflection of CNT
[de Heer group, Nature '99]



wrinkling by compression
[Falvo *et al.*, Nature '97]



mechanical bending
of SiO_2 nanobeam
[Carr, Wybourne, APL '03]



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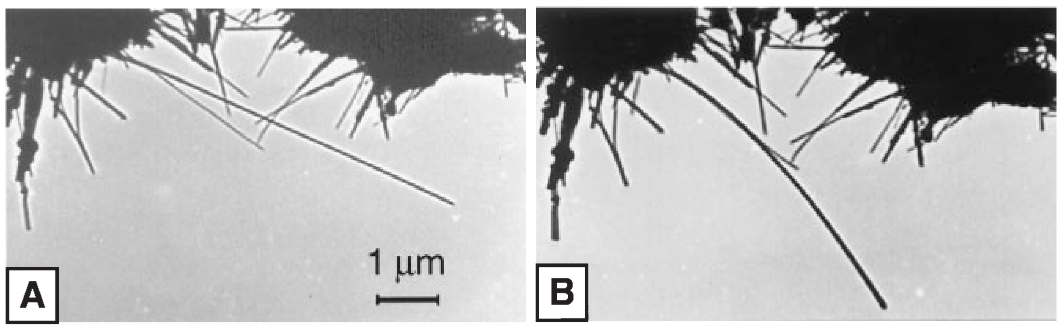

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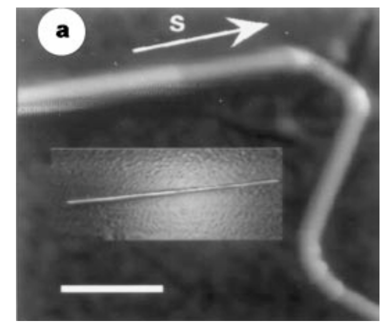

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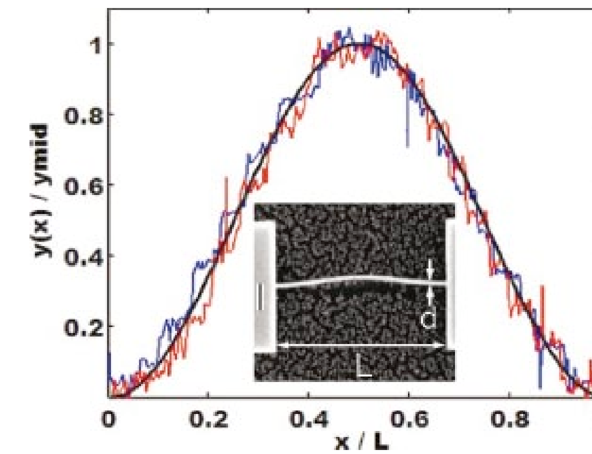
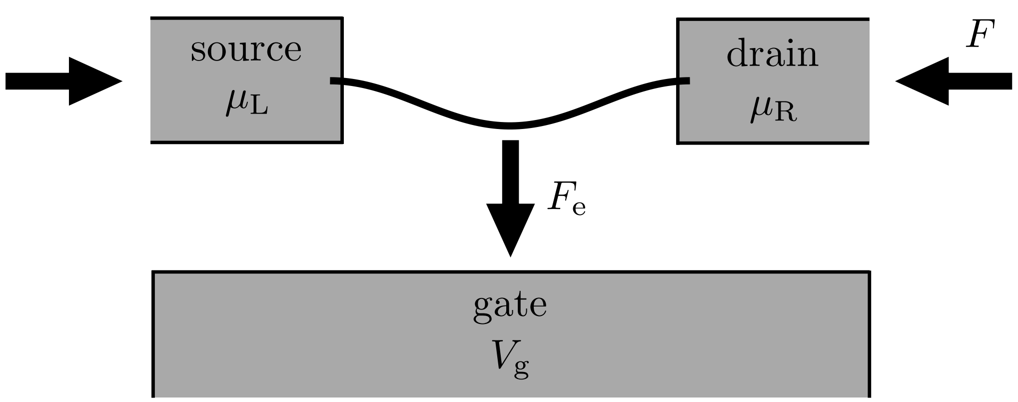


Euler instability in nano**electro**mechanical systems?



e.g.:
- nanobeam
- carbon nanotube

Question:

interplay between mechanical & electronic degrees of freedom

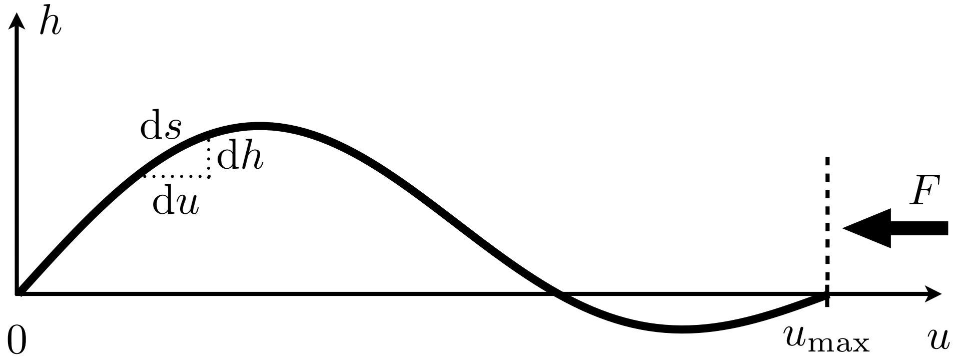
- how Euler instability affects transport characteristics?
- how current flow affects back Euler instability?

Motivation:

strong electromechanical coupling close to instability

Euler buckling instability

Classical elasticity theory:



bending energy

work done by applied force

$$\mathcal{L} = \int_0^L \mathrm{d}s \left[\frac{\sigma}{2}\dot{h}^2 - \frac{\kappa}{2}\frac{h''^2}{1-h'^2} - F\left(\sqrt{1-h'^2} - 1\right) \right]$$

harmonic approximation:

$$\mathcal{L} \simeq \int_0^L \mathrm{d}s \left(\frac{\sigma}{2}\dot{h}^2 - \frac{\kappa}{2}h''^2 + \frac{F}{2}h'^2 \right)$$

Euler buckling instability

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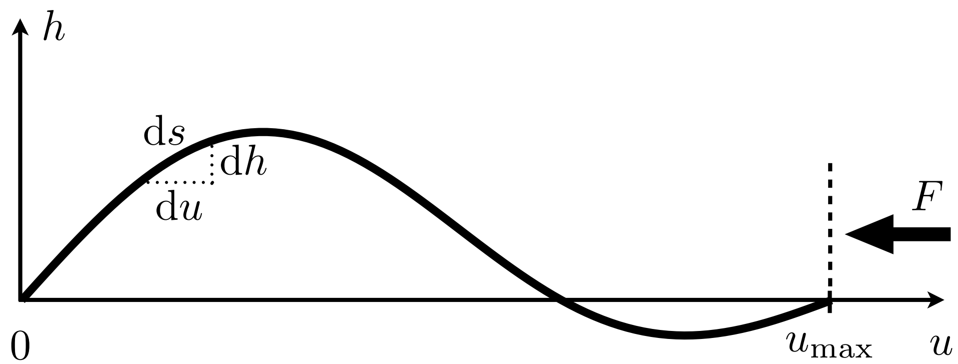

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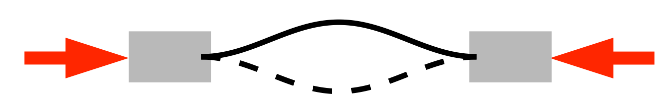
- restrict to low-energy unstable mode with mode amplitude X:



- include anharmonic corrections:

$$\boxed{H_{\mathrm{vib}} = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2 + \frac{\alpha}{4}X^4}$$

critical force: $F_c = \kappa \left(\frac{2\pi}{L}\right)^2$

anharmonicity: $\alpha = F_c L \left(\frac{\pi}{2L}\right)^4$

$$\omega^2 = \omega_0^2 \left(1 - \frac{F}{F_c}\right)$$

frequency for $F = 0$: $\omega_0 = \sqrt{\frac{\kappa}{\sigma}}\left(\frac{2\pi}{L}\right)^2$

Euler buckling instability

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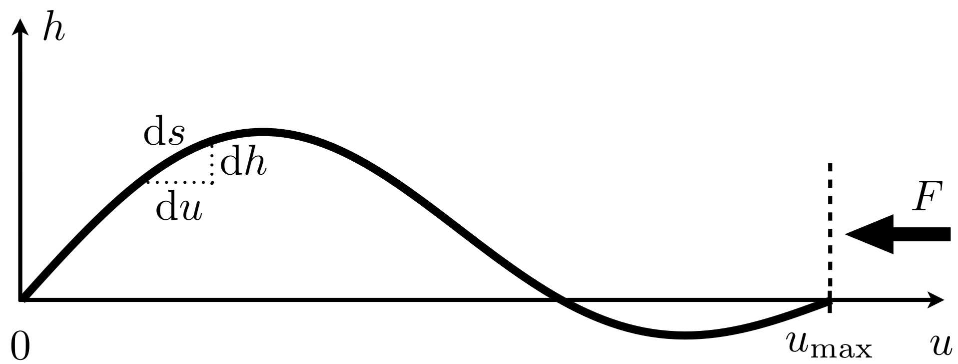

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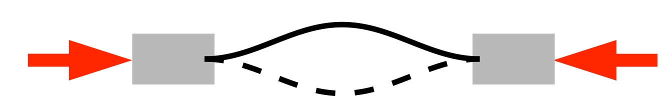

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➡ Euler instability

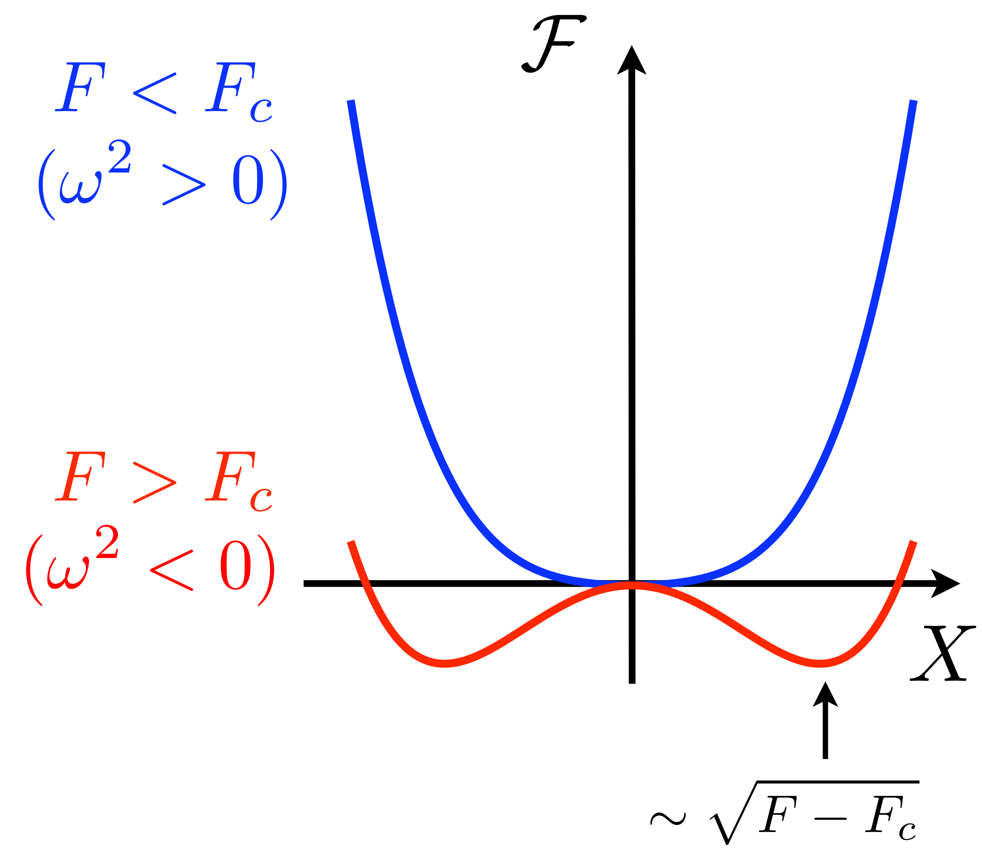
➡ "critical slowing down"

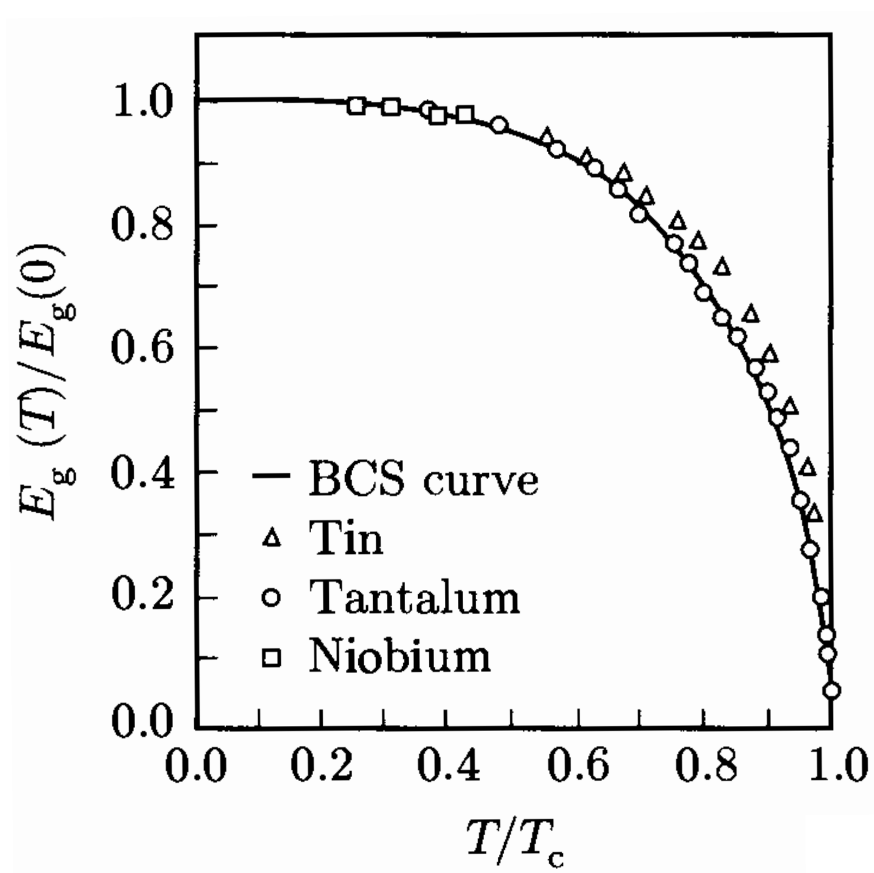
Euler buckling instability

Template for Landau theory of continuous phase transitions:

$$\boxed{H_{\text{vib}} = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2 + \frac{\alpha}{4}X^4}$$

- buckling is a **continuous** instability
- buckled state for $F > F_c: \ X \sim \sqrt{F - F_c}$





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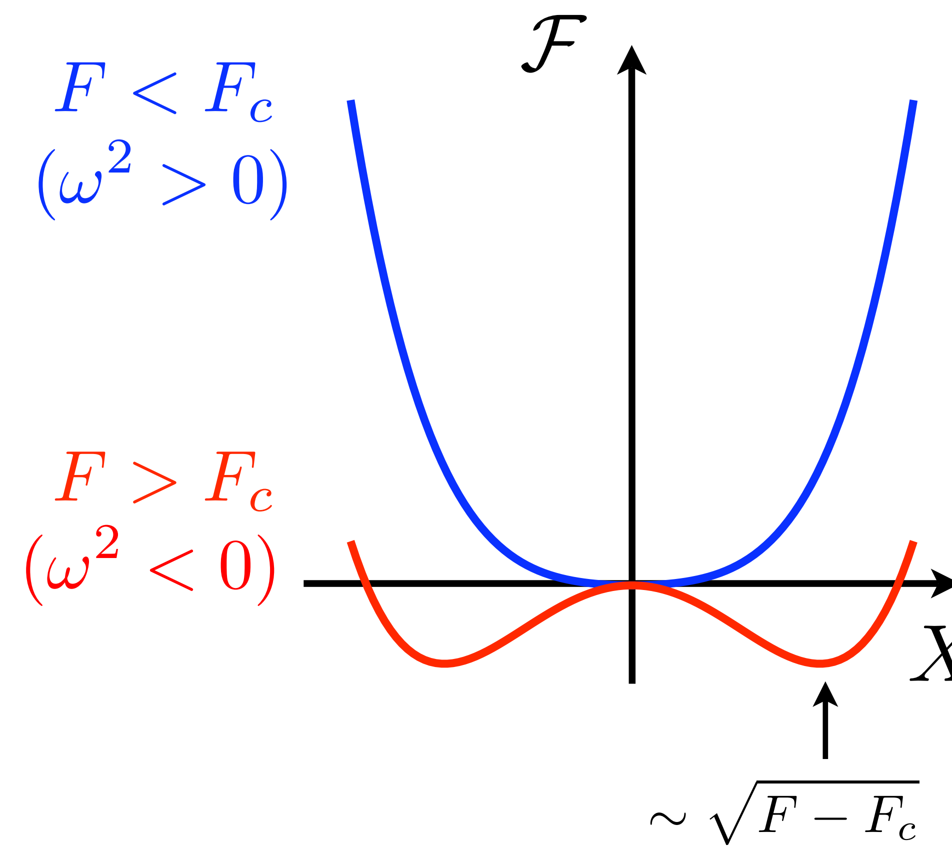
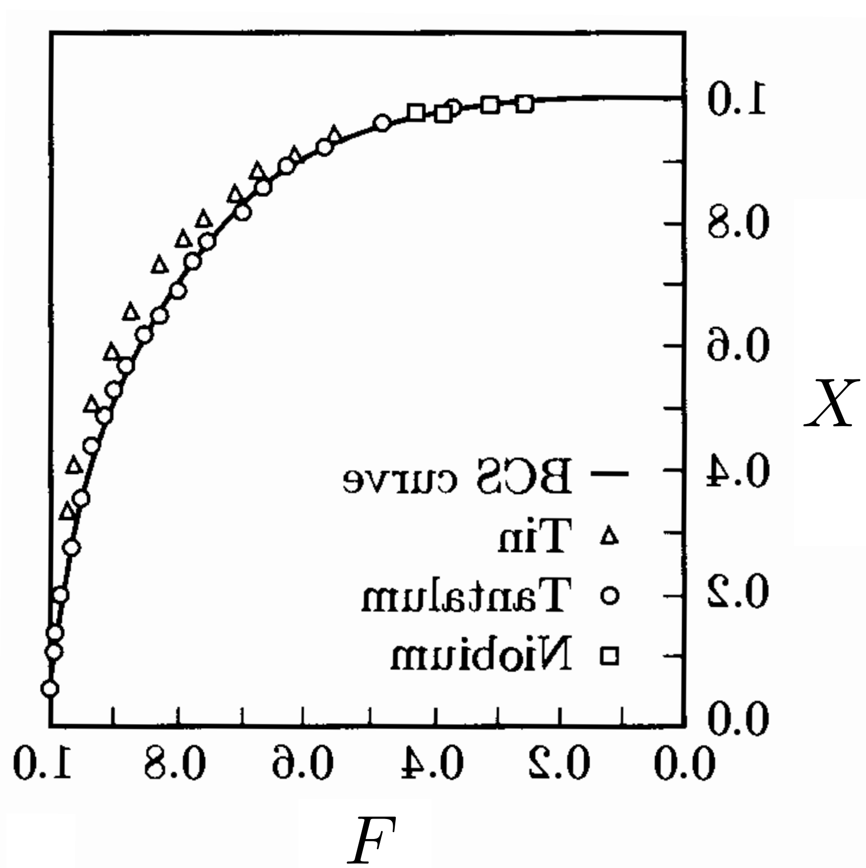
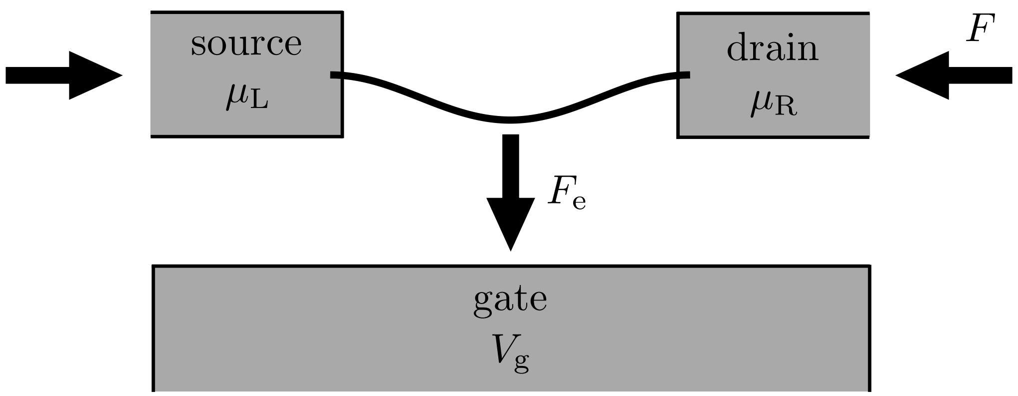




	Landau	Euler
order parameter	$\langle \phi \rangle$	X
"temperature"	T	F

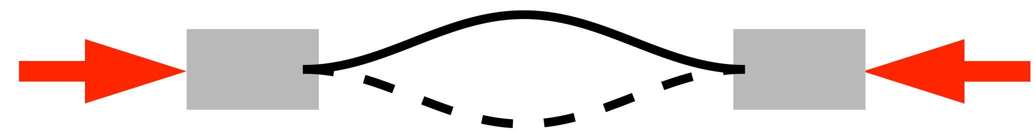
Electromechanical coupling

Capacitive coupling



$$\boxed{H_{\mathrm{c}} = F_{\mathrm{e}} X \hat{n}} \qquad F_{\mathrm{e}} > 0$$

Intrinsic coupling



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$\hat{n} = 0, 1:$ stochastic fluctuations of charge on the dot

Electromechanical coupling

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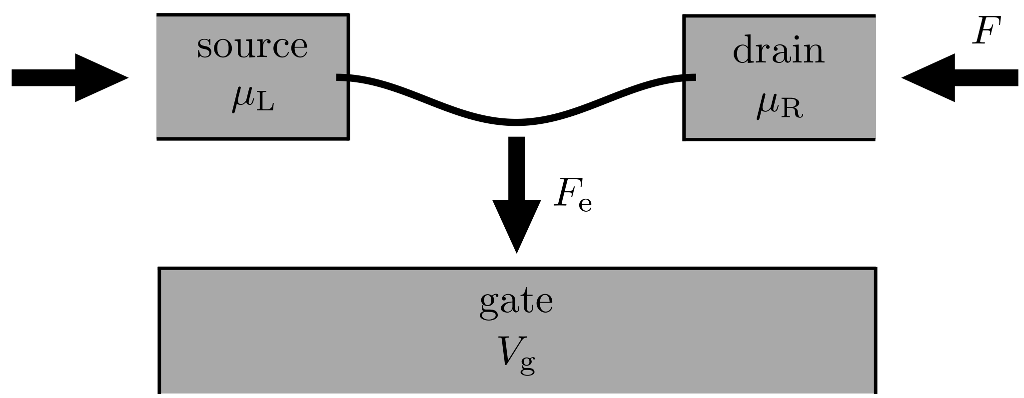

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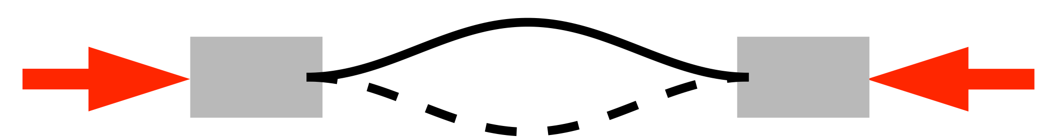

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	capacitive coupling	intrinsic coupling
molecular quantum dot	‣ more easily realized experimentally ‣ more pronounced effect on Coulomb blockade [GW *et al.*, arXiv:1010.0800]	
metallic quantum dot		‣ consistent w/ symmetry of pristine Euler instability ‣ more pronounced effect on Euler [GW *et al.*, Phys. Rev. B '10]

Electromechanical coupling

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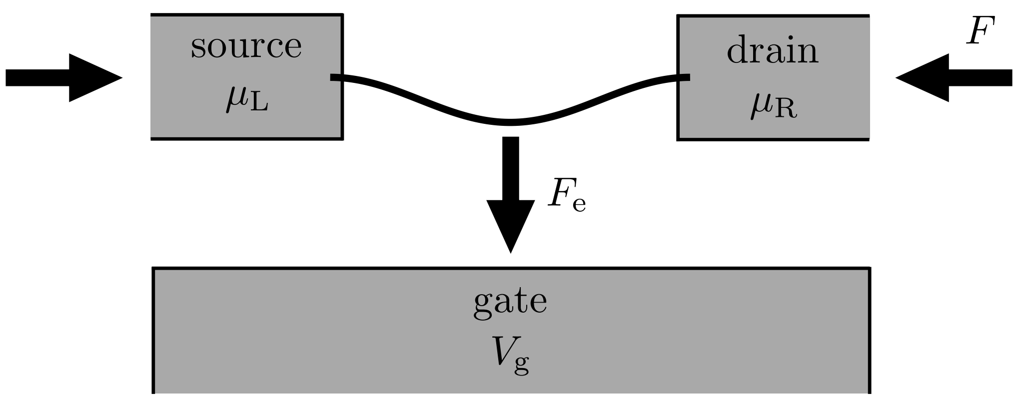

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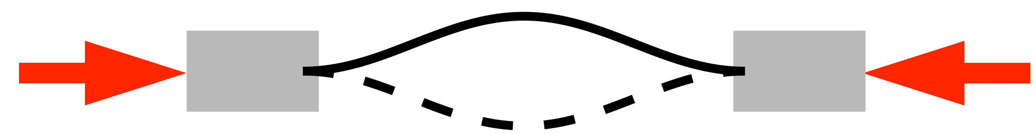
Intrinsic coupling



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- near instability, resonator much slower than electrons $(|\omega| \ll \Gamma)$

  ➡ asymptotically **exact** solution

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Non-equilibrium Born-Oppenheimer approximation:

(similar to Blanter *et al.*, PRL '04 & Mozyrsky *et al.*, PRB '06)

- to leading order: current-induced conservative force acting on vibrational mode

$$\boxed{F_{\text{c-i}}(X) = -(F_{\text{e}} + gX)\langle\hat{n}\rangle_X}$$

$$H_{\text{c}} = \left(F_{\text{e}}X + \frac{g}{2}X^2\right)\hat{n}$$

average occupation of the dot for fixed X

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- next-to-leading order: fluctuations of current-induced force & corresponding dissipation

➡ leads to **Langevin dynamics**

$$\boxed{m\ddot{X} + \frac{\eta(X)}{m}\dot{X} = F_{\text{eff}}(X) + \delta F_{\text{c-i}}(X,t)}$$

$$F_{\text{eff}}(X) = -\partial_X H_{\text{vib}} + F_{\text{c-i}}(X)$$

$$\langle \delta F_{\text{c-i}}(X,t)\delta F_{\text{c-i}}(X,t')\rangle = D(X)\delta(t-t')$$

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$$\boxed{m\ddot{X} + \frac{\eta(X)}{m}\dot{X} = F_{\text{eff}}(X) + \delta F_{\text{c-i}}(X,t)}$$

$$F_{\text{eff}}(X) = -\partial_X H_{\text{vib}} + F_{\text{c-i}}(X)$$

$$\langle \delta F_{\text{c-i}}(X,t) \delta F_{\text{c-i}}(X,t') \rangle = D(X)\delta(t-t')$$

➡ **Fokker-Planck description**

Fokker-Planck description

$$H_{\mathrm{vib}} = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2 + \frac{\alpha}{4}X^4 \qquad H_{\mathrm{c}} = h(X)\hat{n} \qquad h(X) = F_{\mathrm{e}}X + \frac{g}{2}X^2$$

Boltzmann equation:

$$\mathcal{H}_n = H_{\mathrm{vib}} + h(X)n$$

classical vibrations $(\hbar|\omega| \ll k_{\mathrm{B}}T)$

sequential tunneling $(\hbar\Gamma \ll k_{\mathrm{B}}T)$

$$\partial_t \mathcal{P}_n(X,P,t) = \{\mathcal{H}_n, \mathcal{P}_n\} - (-1)^n \Gamma_{01}(X)\mathcal{P}_0(X,P,t) + (-1)^n \Gamma_{10}(X)\mathcal{P}_1(X,P,t)$$

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adiabatic transport $(|\omega| \ll \Gamma) \rightarrow \delta\mathcal{P} \ll \mathcal{P}$ small!

$$\mathcal{P}_0 = \frac{\Gamma_{10}}{\Gamma}\mathcal{P} - \delta\mathcal{P} \qquad \mathcal{P} = \mathcal{P}_0 + \mathcal{P}_1$$

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$$\boxed{\partial_t \mathcal{P} = -\frac{P}{m}\partial_X \mathcal{P} - F_{\text{eff}}(X)\partial_P \mathcal{P} + \frac{\eta(X) + \eta_{\text{e}}}{m}\partial_P(P\mathcal{P}) + \left(\frac{D(X)}{2} + \eta_{\text{e}}k_{\text{B}}T\right)\partial_P^2\mathcal{P}}$$

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$$F_{\text{c-i}}(X) = -(\partial_X h)\langle\hat{n}\rangle_X \qquad D(X) = \frac{2\,(\partial_X h)^2\,\langle\hat{n}\rangle_X(1-\langle\hat{n}\rangle_X)}{\Gamma}$$

η_{e} : accounts for finite Q of resonator

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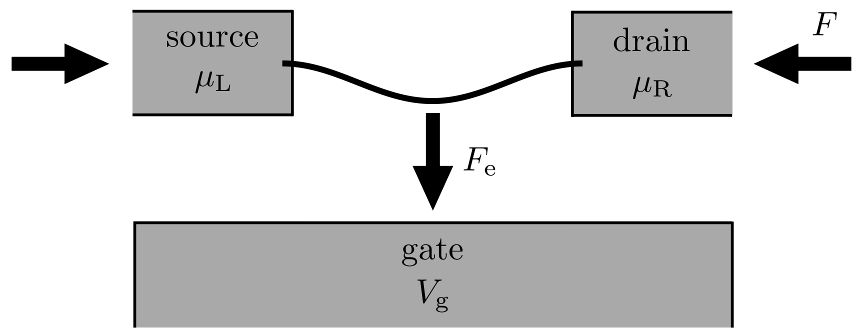
Transport characteristics

$$I = \iint \mathrm{d}X\mathrm{d}P\,\mathcal{P}_{\rm st}(X,P)\mathcal{I}(X)$$

Mechanical properties

$$F_{\rm eff}(X) = 0, \quad \frac{\mathrm{d}F_{\rm eff}}{\mathrm{d}X} < 0$$

Classical current blockade

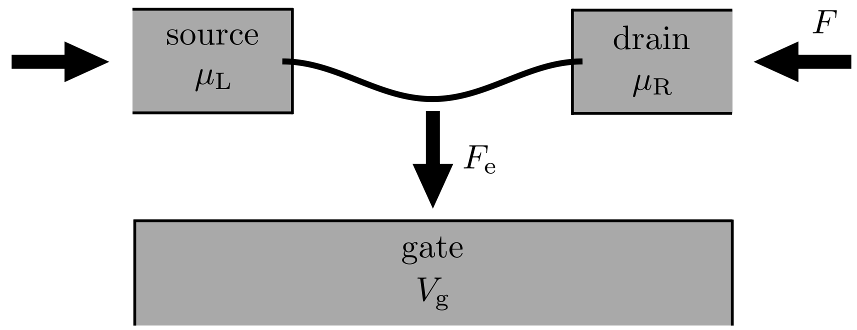


$$\boxed{H_c = F_e X \hat{n}}$$

effective gate voltage:

$$V_g(X) = V_g - F_e X$$

Classical current blockade



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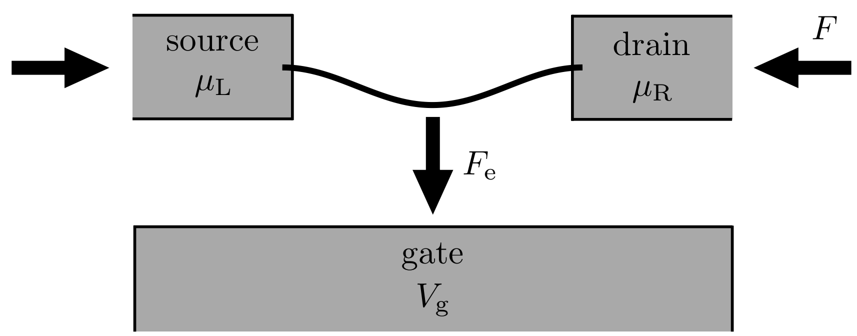
addition of a single electron, $\Delta n = 1$:

- displacement $\Delta X = F_e / m\omega^2$
- effective shift of gate voltage $\Delta V_g = F_e^2 / m\omega^2$

Classical current blockade



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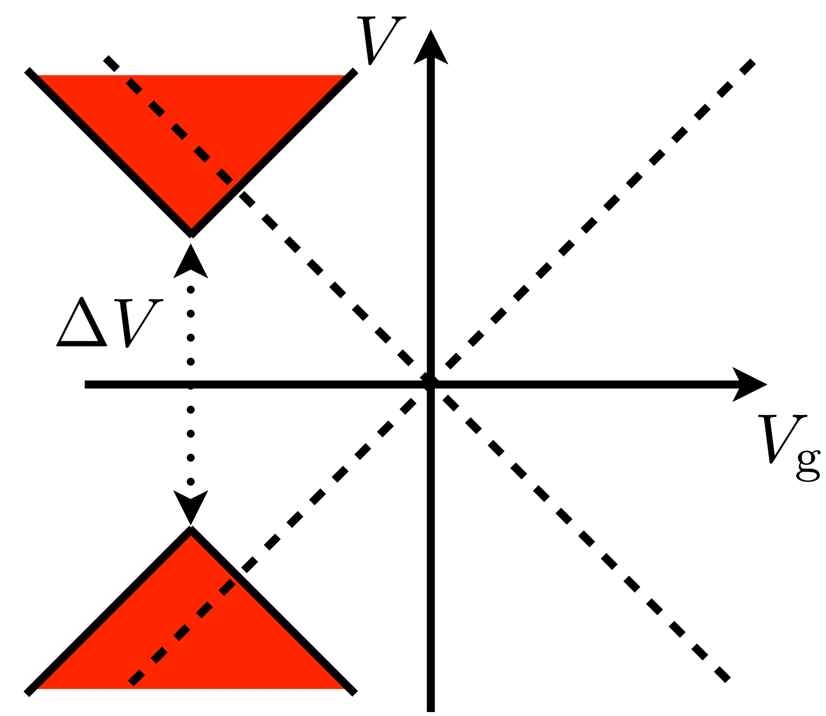
- current blockade for $V < \Delta V$

$$\Delta V(F=0) = F_e^2 / m\omega^2 \sim 3 - 5\ \mu\text{eV}$$

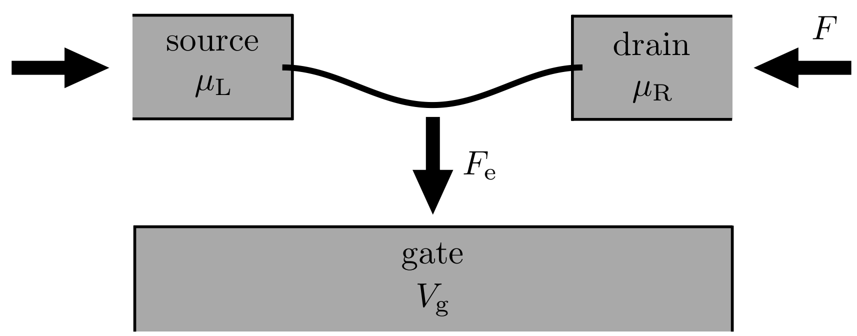


classical current blockade

[Pistolesi, Labarthe, PRB '07]

quantum analog:
Franck-Condon blockade
[Koch, von Oppen, PRL '05]
[Leturcq *et al.*, Nature Phys. '09]

Classical current blockade



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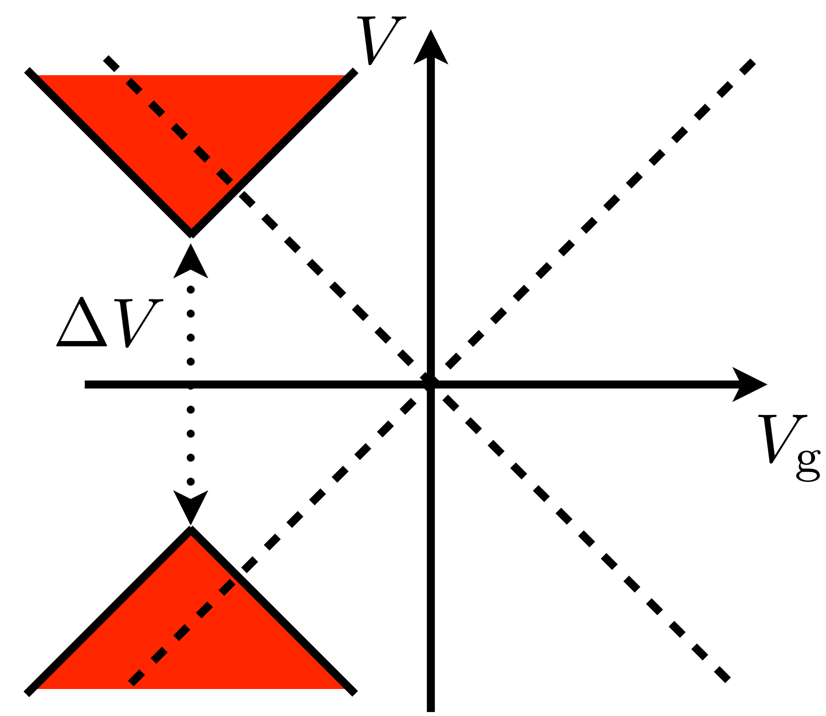
$$\Delta V(F = 0) = F_e^2 / m\omega^2 \sim 3 - 5\ \mu\text{eV}$$

$$\boxed{\Delta V(F \to F_c) = F_e^2 / m\omega^2 \to \infty}$$

diverges at the Euler instability!



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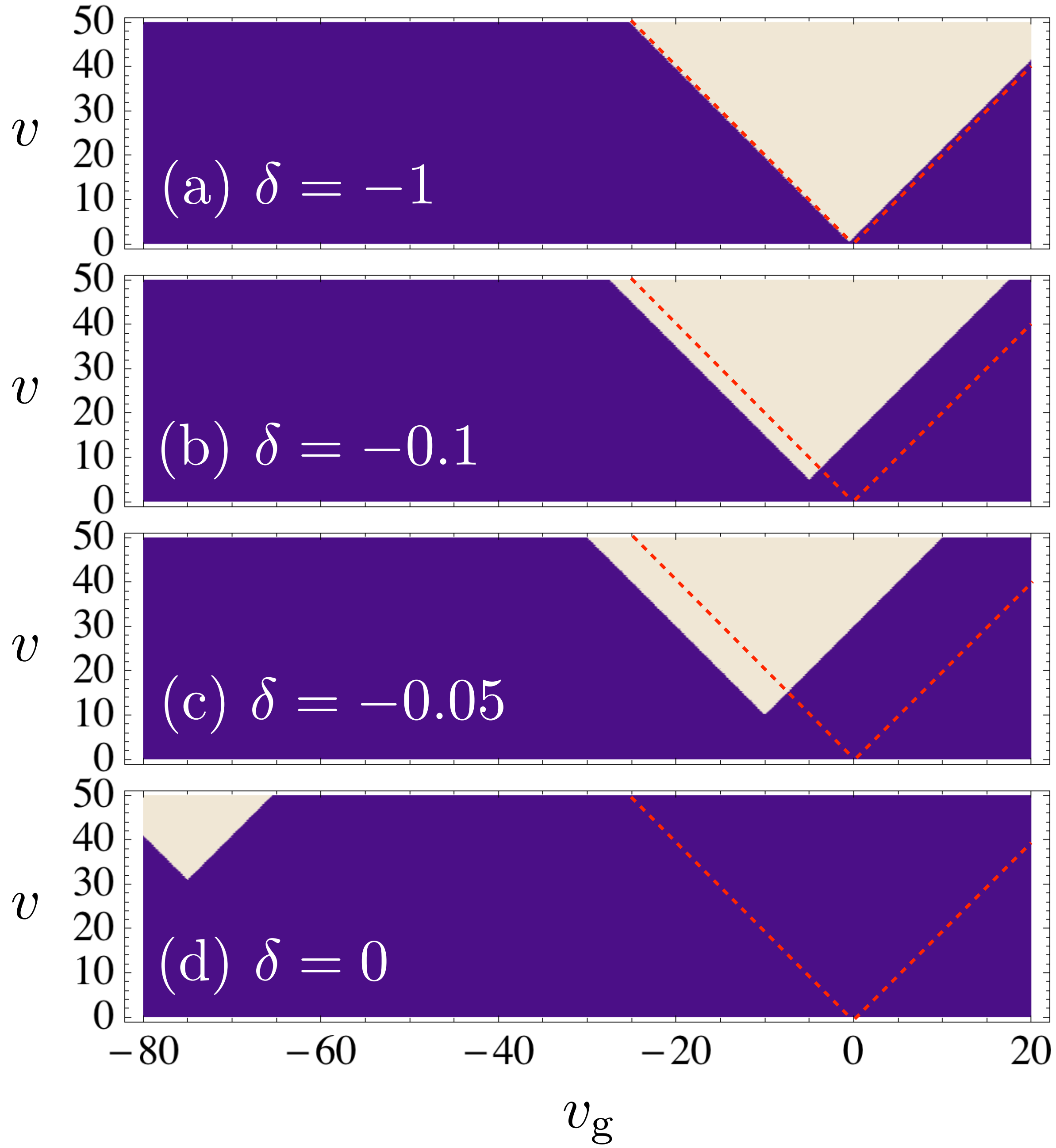
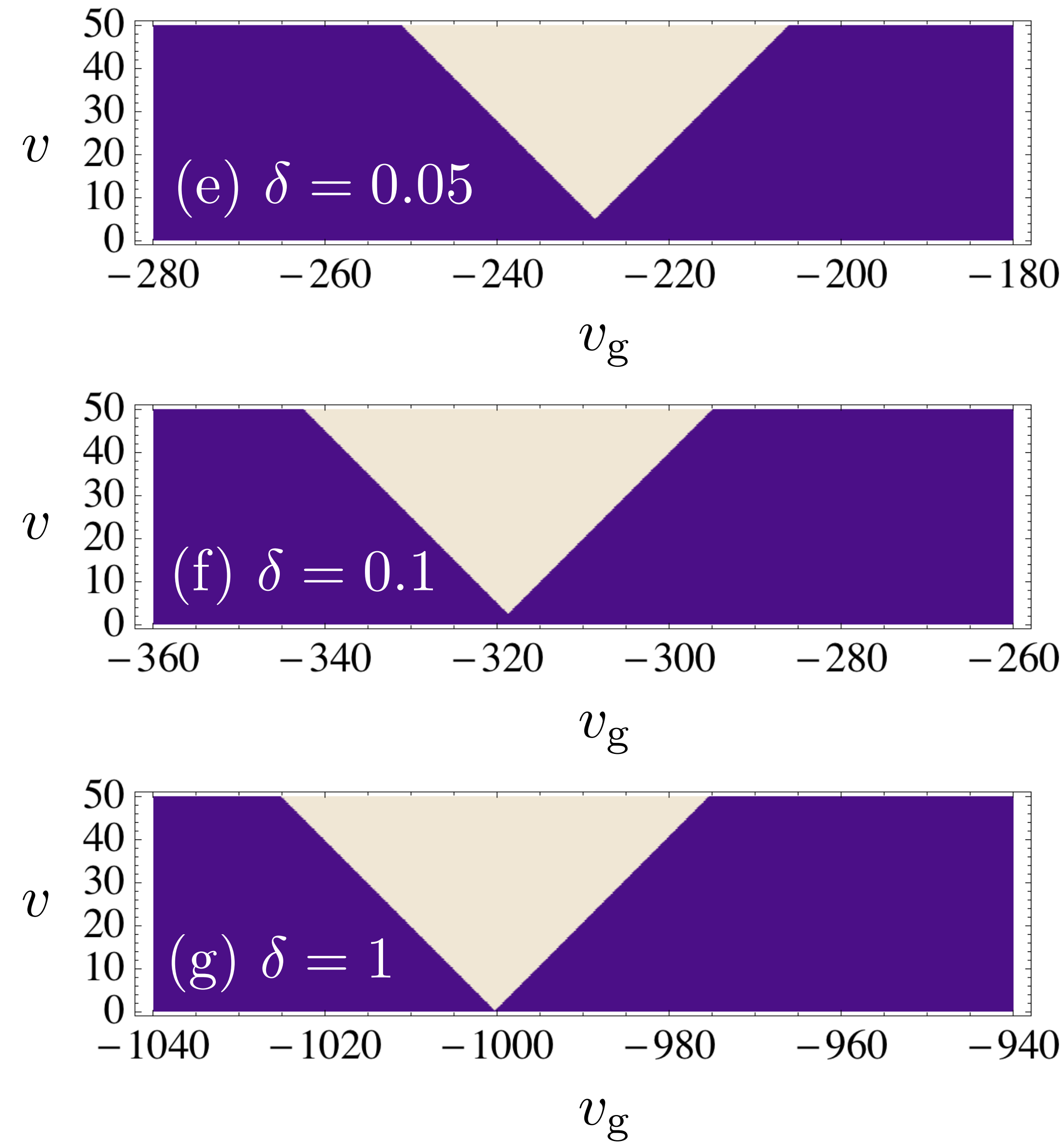
Enhanced current blockade

below instability



above instability

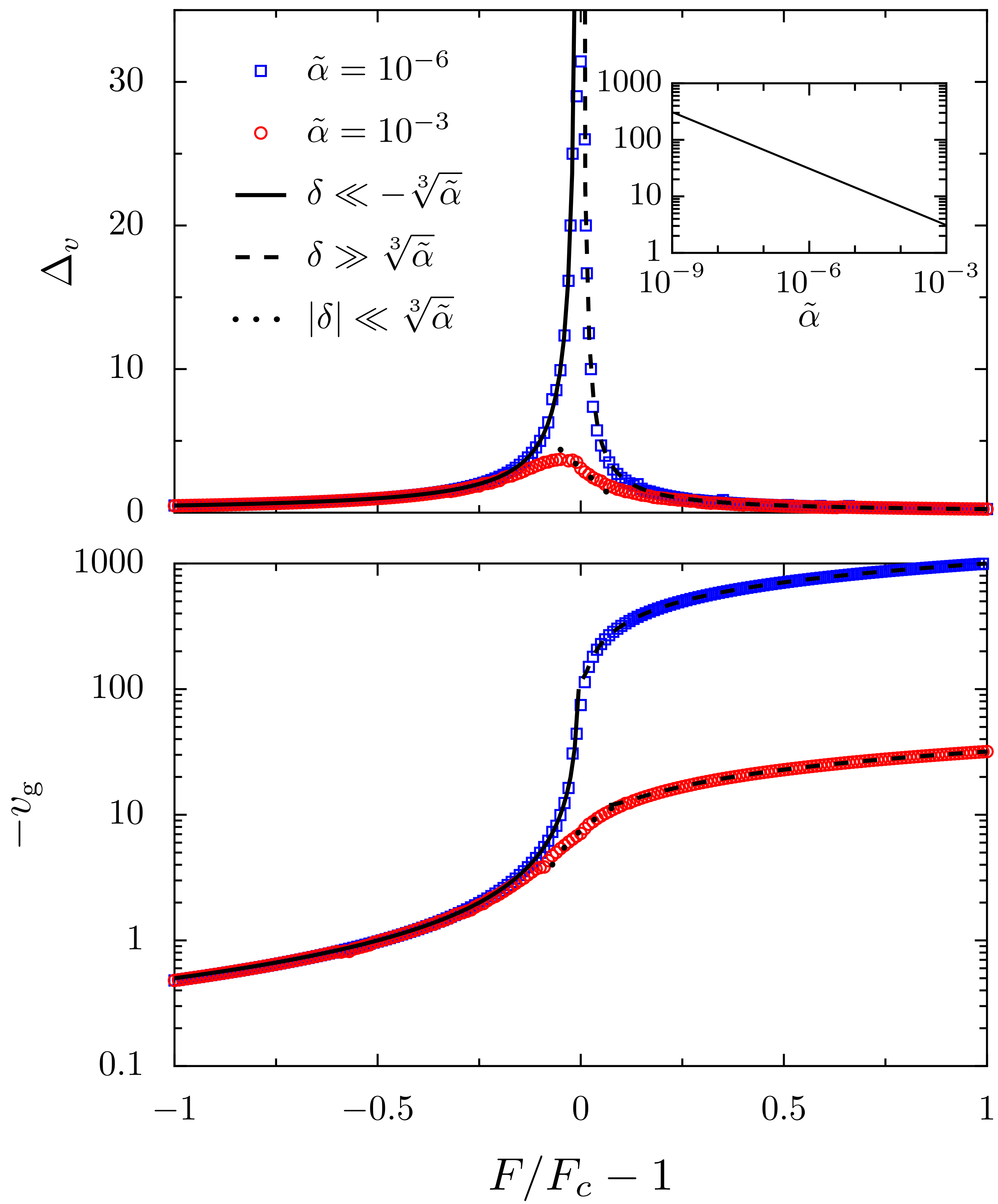


$\delta = F/F_c - 1$

mean-field results

energy unit:
$F_{\mathrm{e}}^2/m\omega_0^2 \sim \mu\mathrm{eV}$

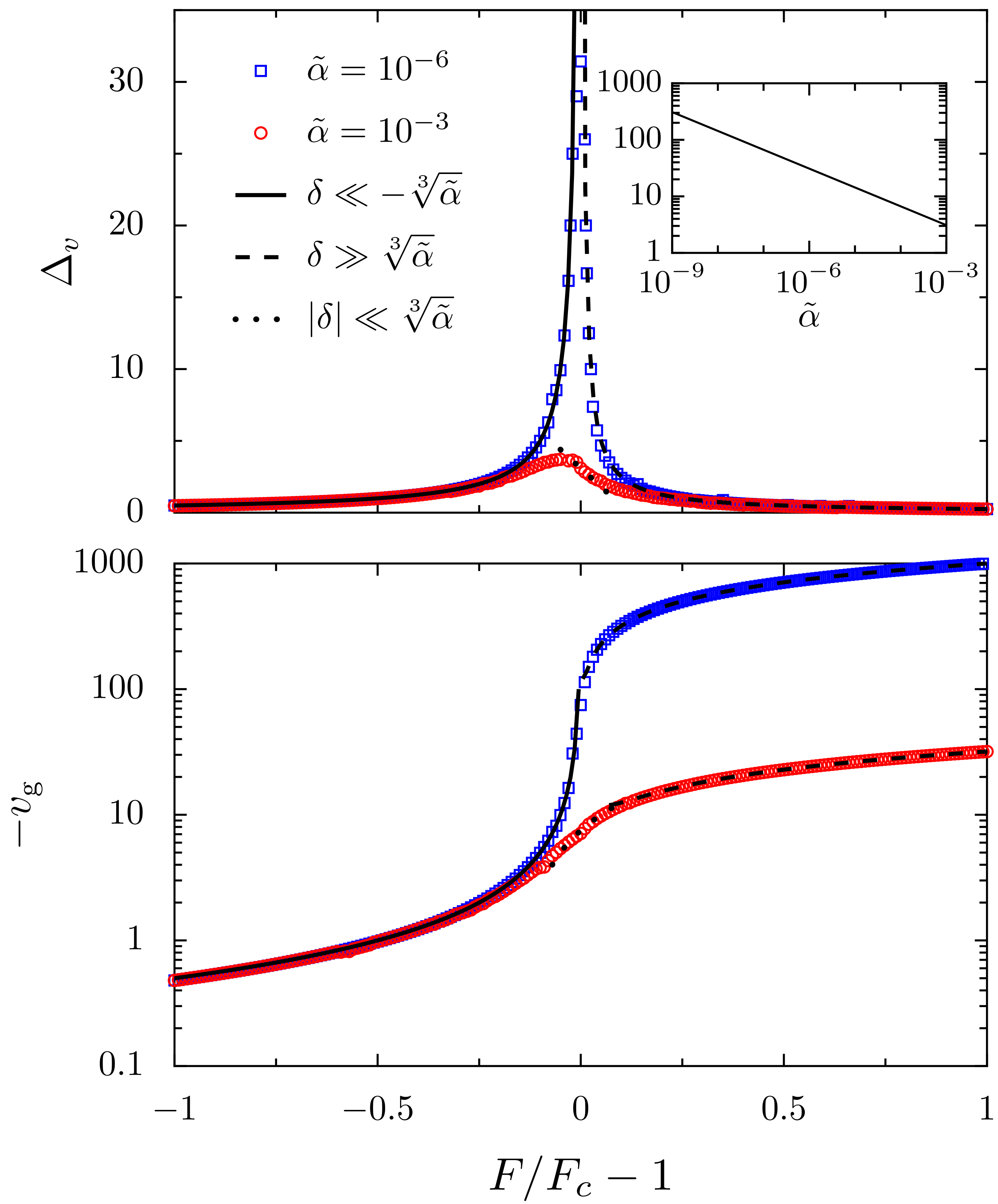
Enhanced current blockade



- gap increases sharply near F_c
- increase limited by anharmonic term
- relative increase stronger for weaker electromechanical coupling

- Coulomb diamond shifts in gate voltage
- small shift below instability
- orders of magnitude larger shift on buckled side

Enhanced current blockade



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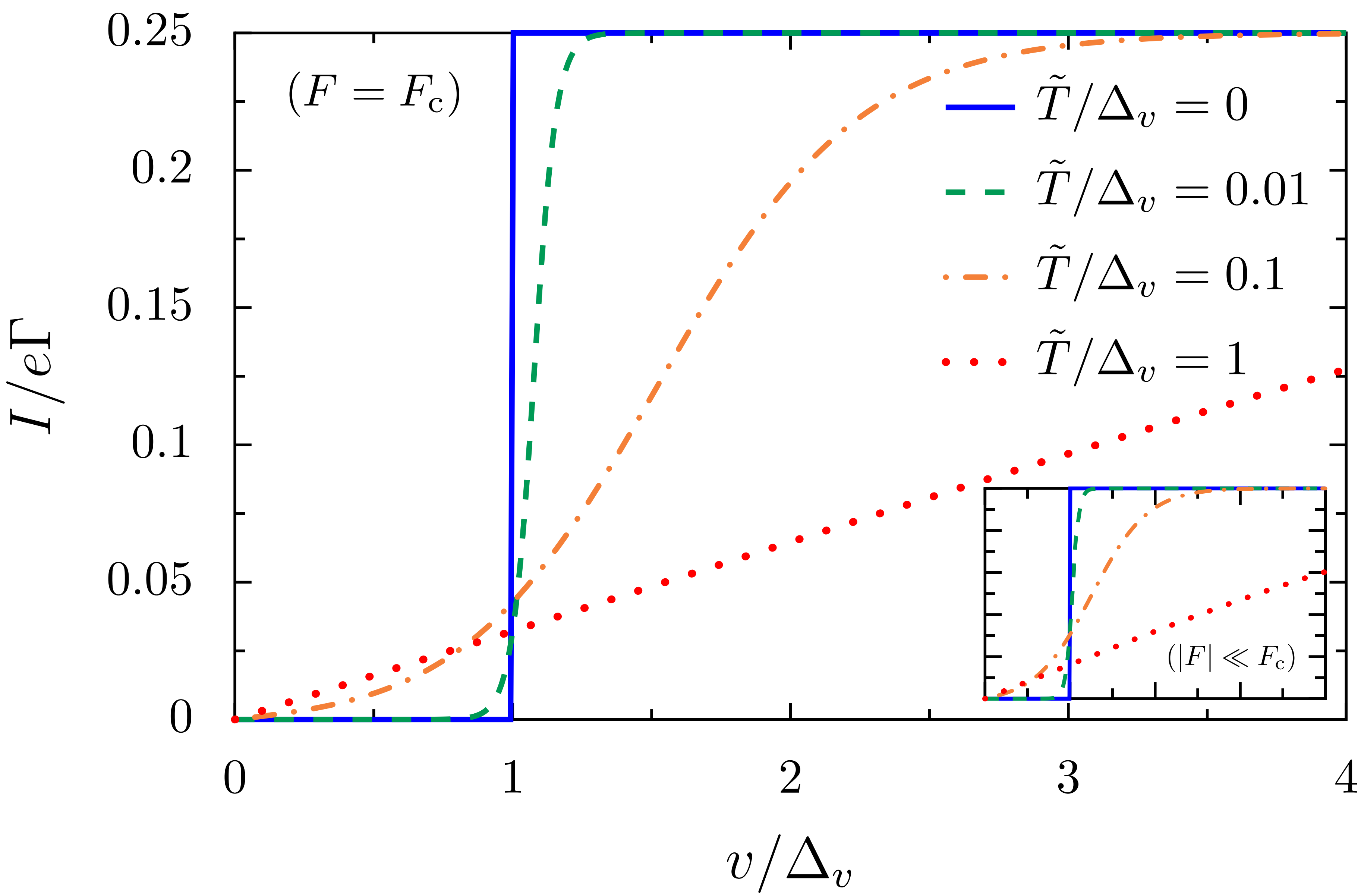
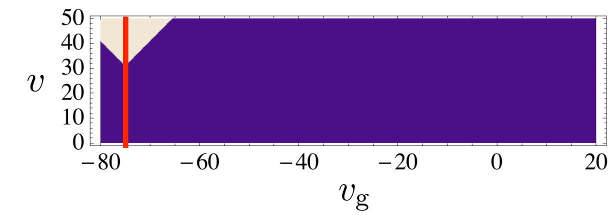
experiments on CNT:
$\Delta V \simeq 5\,\mathrm{meV}$

Thermal fluctuations



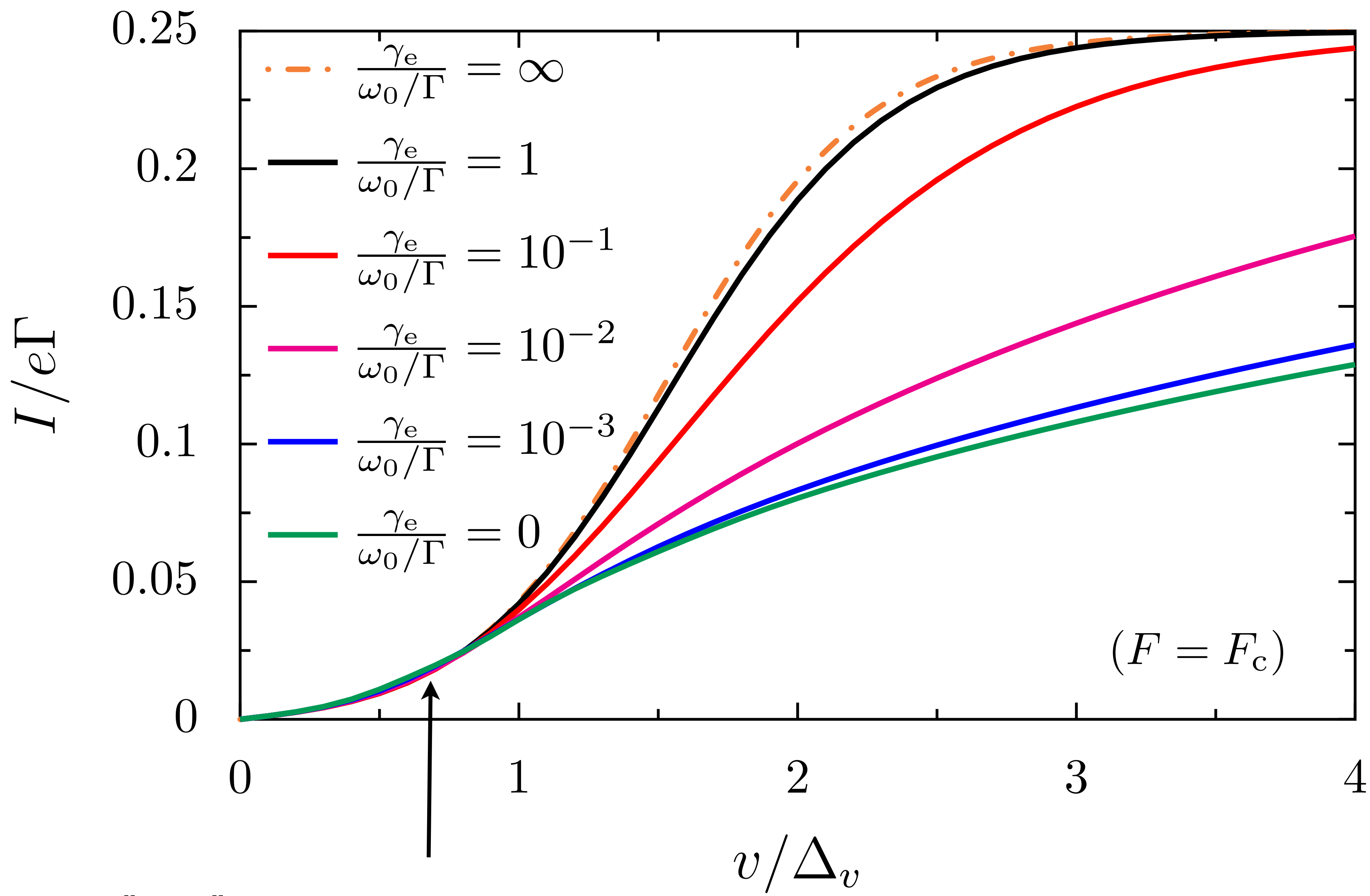


$$\mathcal{P}_{st}(X, P) \sim \exp\left(-\frac{P^2/2m + V_{eff}(X)}{k_B T}\right)$$

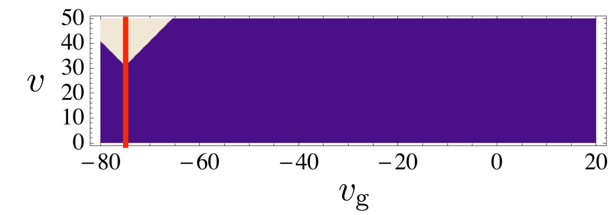
$$V_{eff}(X) = -\int^X dX\, F_{eff}(X)$$

- gap observable as long as $T \ll$ gap
- scaling law
- tuning system near instability enlarges temperature region

Full Langevin dynamics



"local" fluctuation-dissipation theorem



$\tilde{T}/\Delta_v = 0.1$

$\tilde{\alpha} = 10^{-6}$

current blockade more pronouced for:

- low Q
- slow oscillator

Conclusion

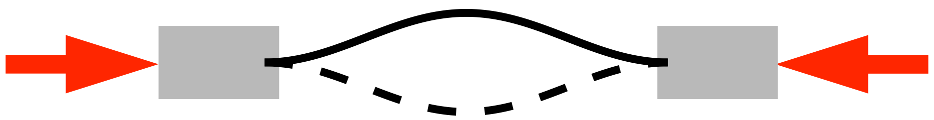
Nanoelectromechanical systems near mechanical instabilities:

- Euler instability as paradigm of mechanical instability
- "critical slowing down" makes problem inherently classical, and allows for asymptotically exact solution
- capacitive coupling (molecular quantum dot):
  strong enhancement of current blockade

  [GW, F. von Oppen, F. Pistolesi, submitted to Phys. Rev. B (arXiv:1010.0800)]
- intrinsic coupling (metallic quantum dot):
  discontinuous Euler instability

  [GW, F. Pistolesi, E. Mariani, F. von Oppen, Phys. Rev. B **81**, 121409(R) (2010)]

Discontinuous Euler instability



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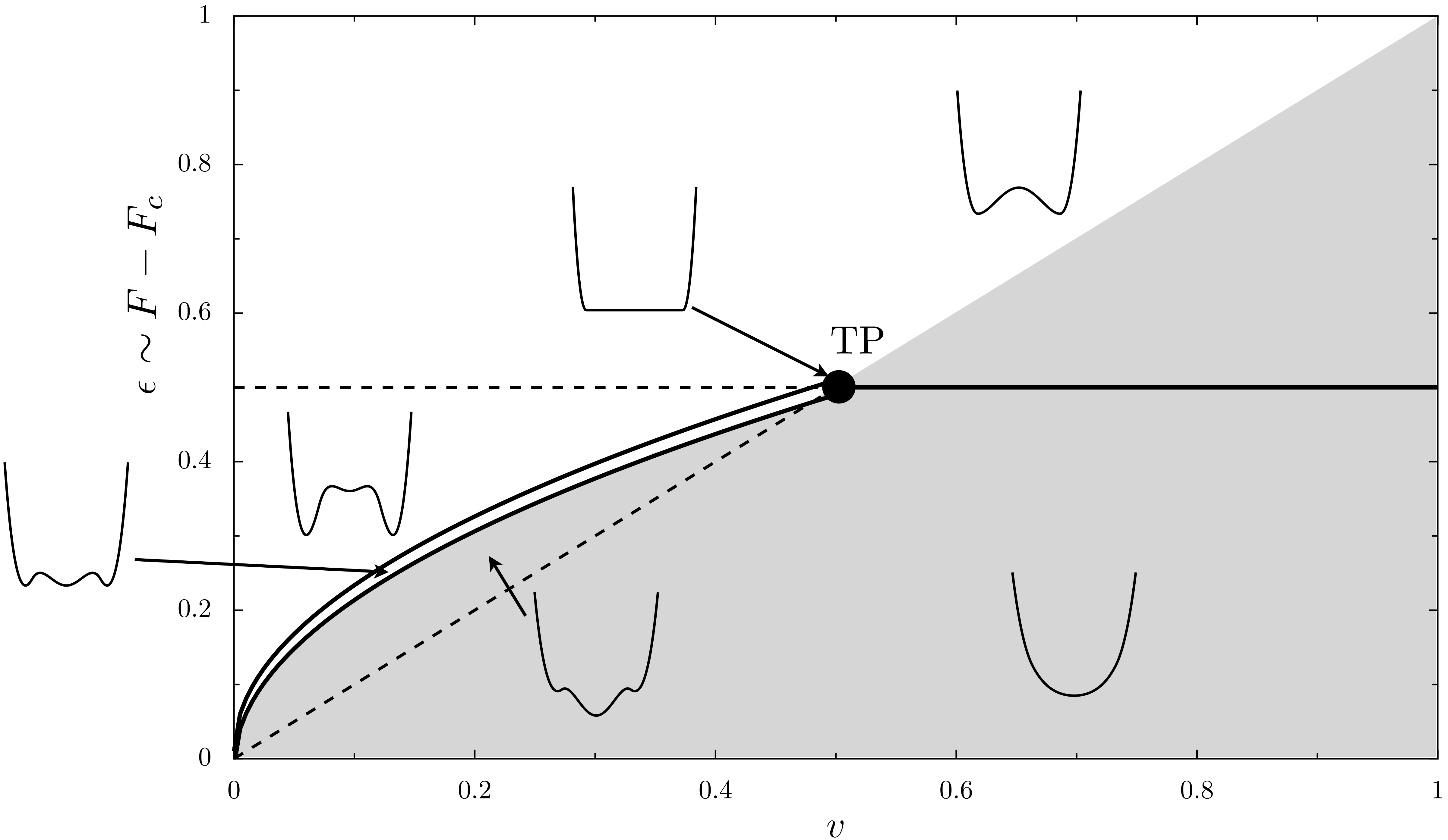
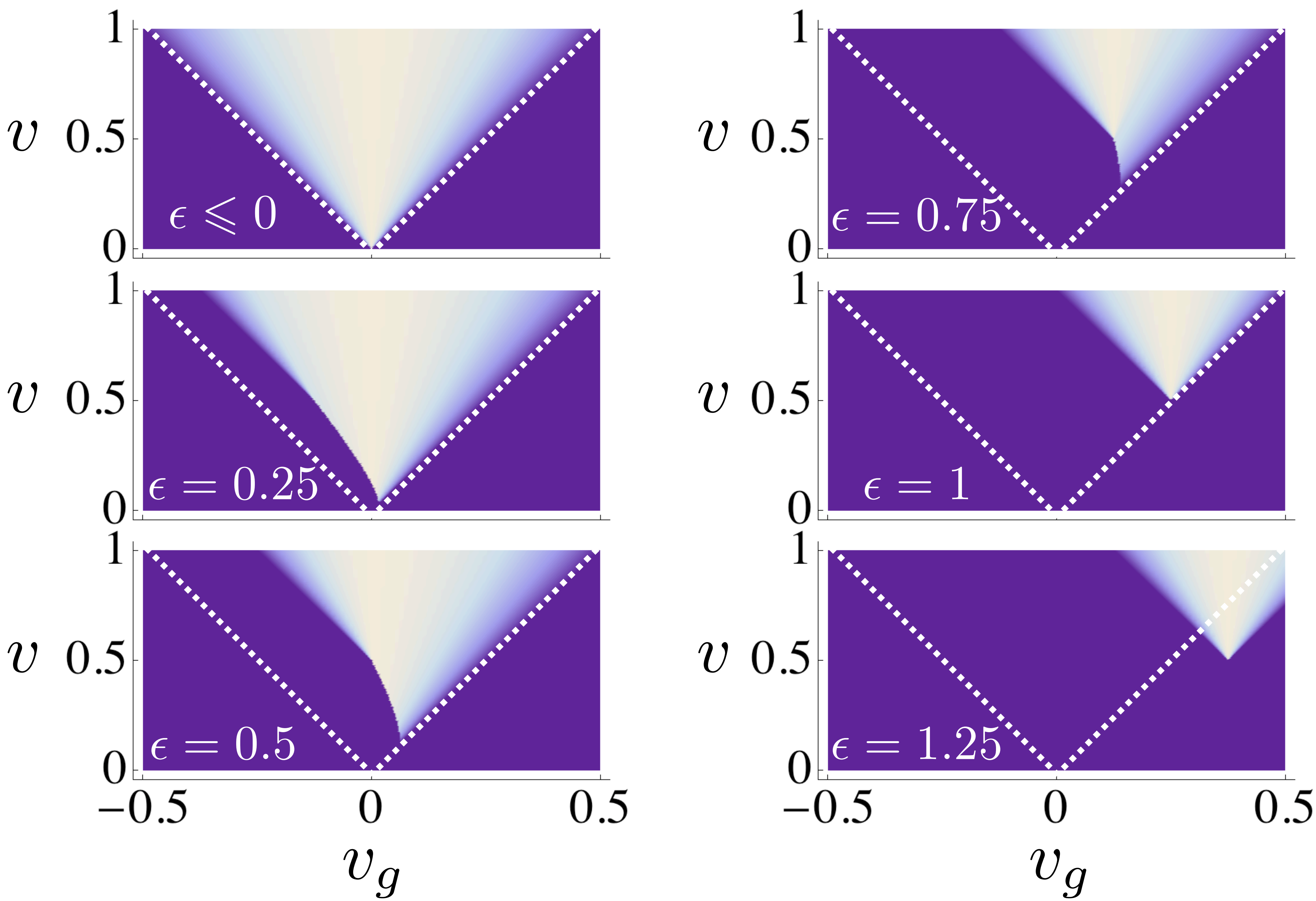
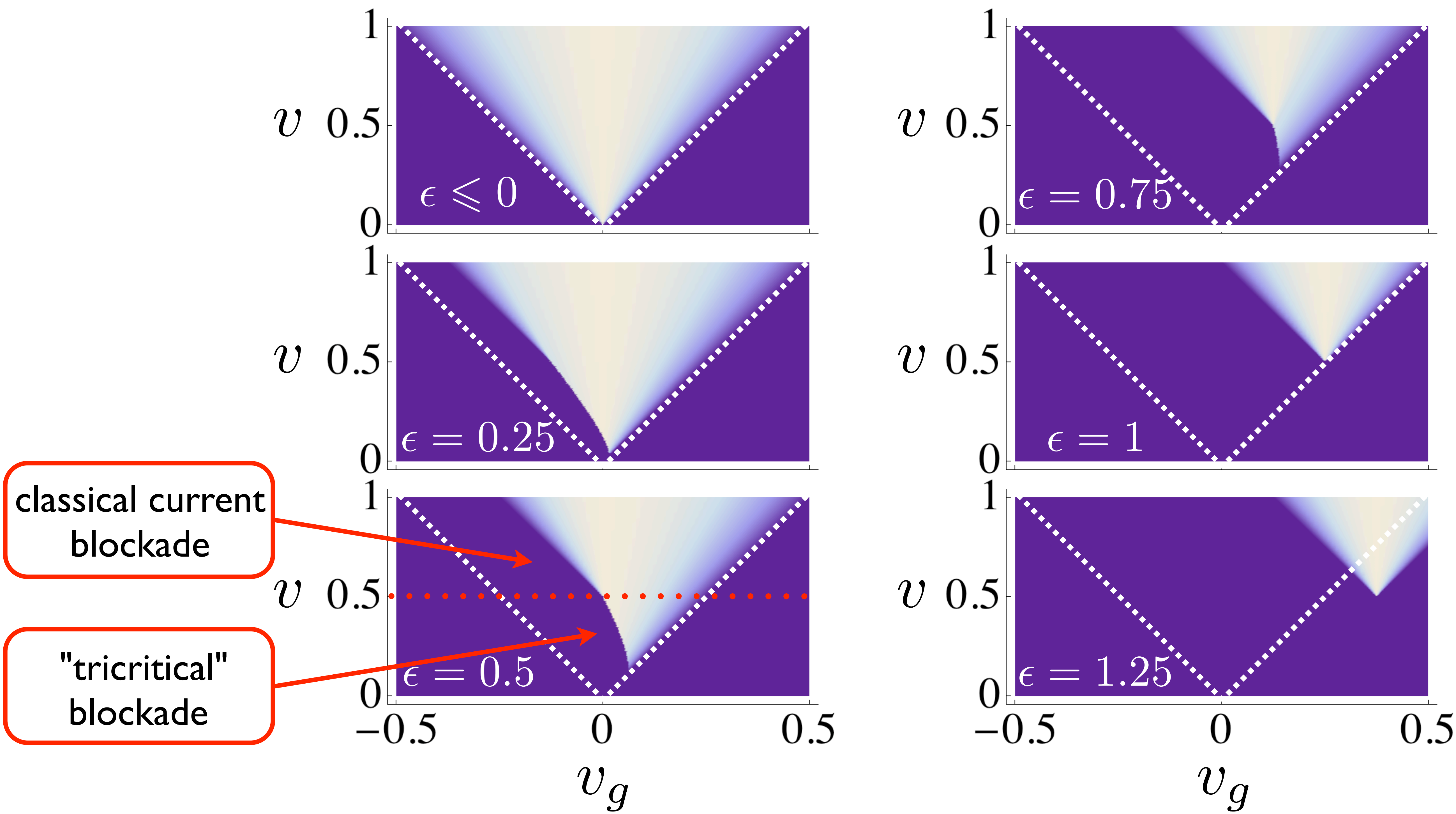


Discontinuous Euler instability



$\epsilon \sim F - F_c$

Discontinuous Euler instability



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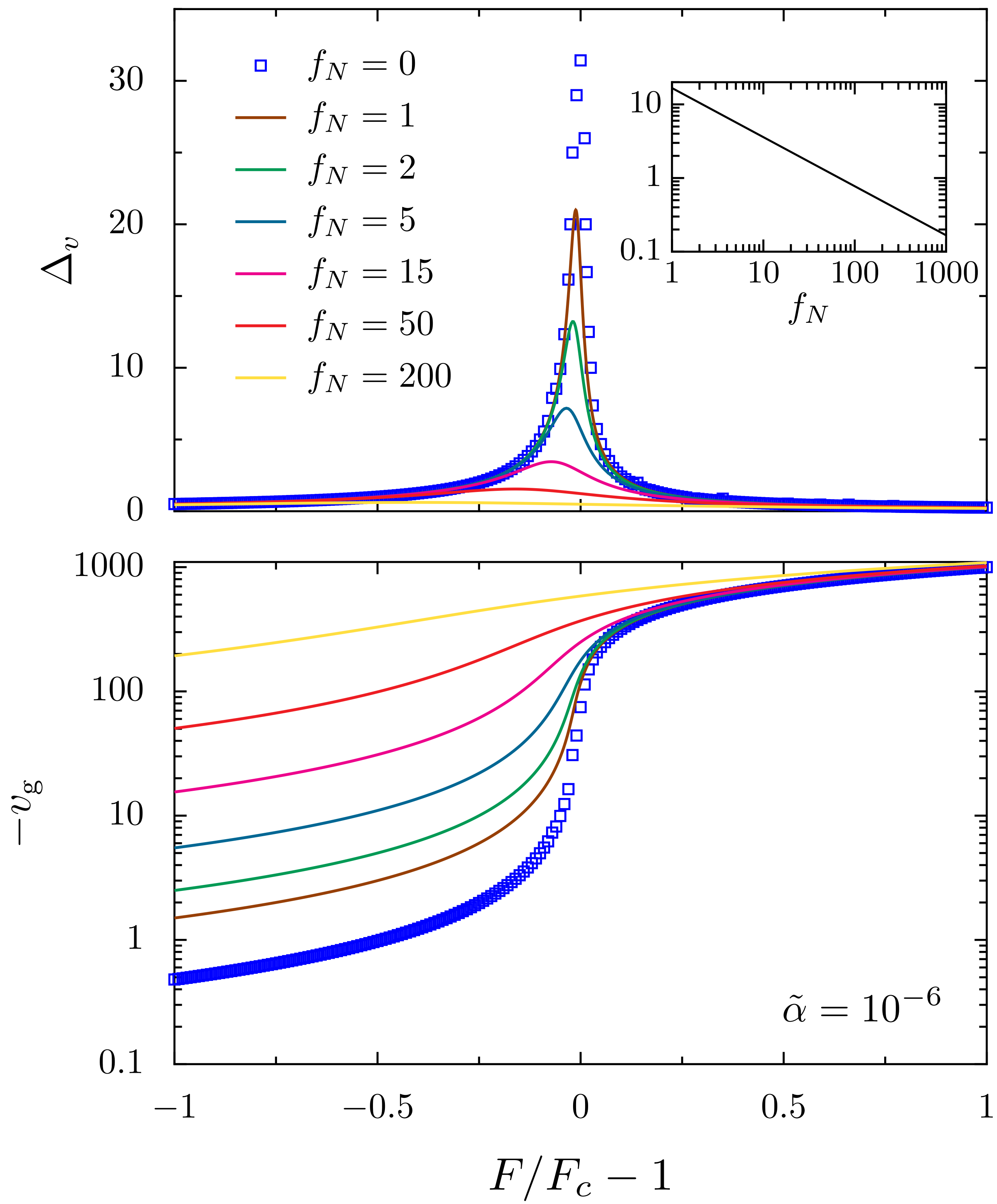
Effect of offset charges



so far: $N = 0$ $\hat{n} = 0, 1$

but gate voltage can be larger than charging energy $\Rightarrow N > 0$

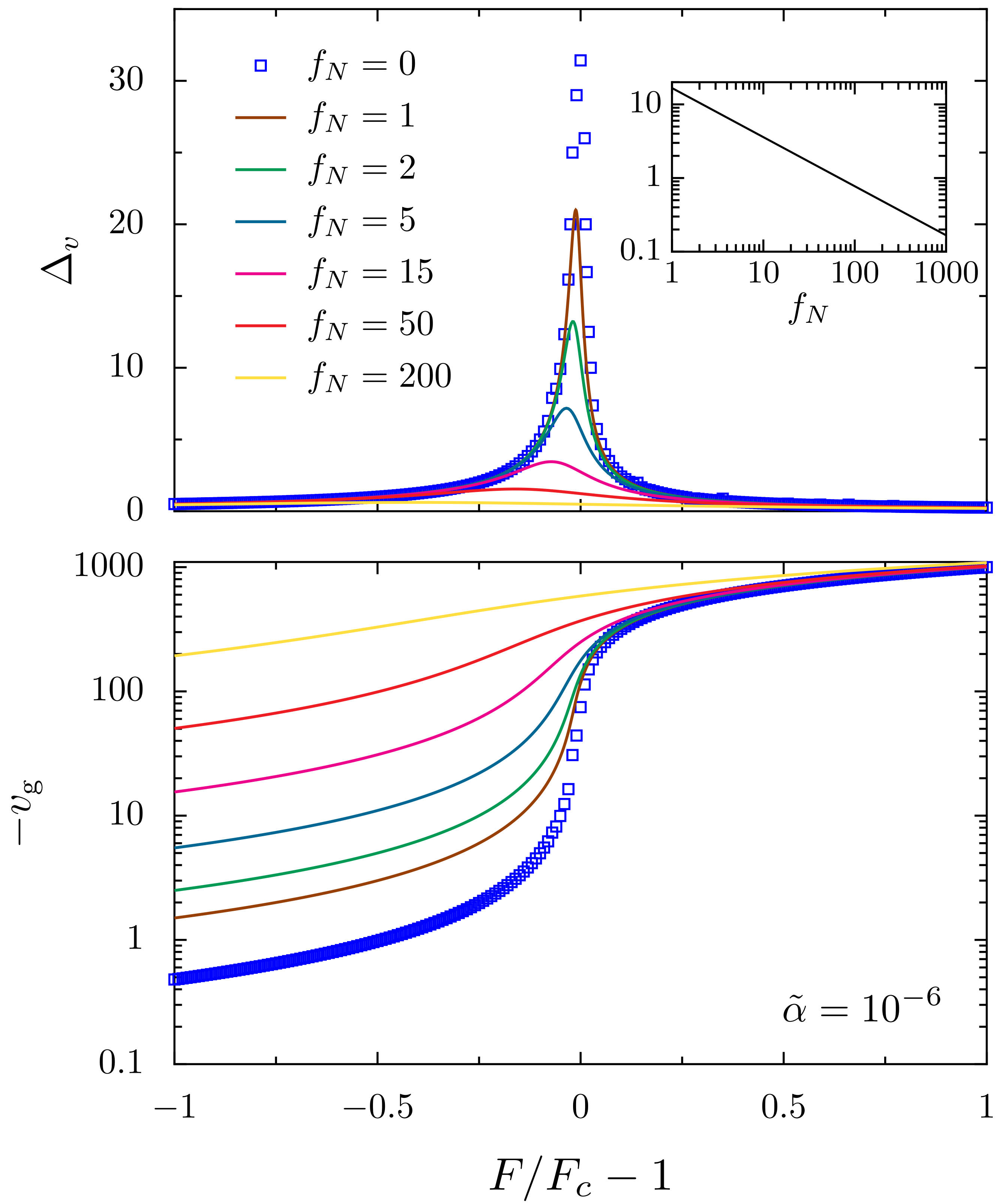
➡ additional force $f_N \sim N$ that bends the tube further

$$V(X) = \frac{m\omega^2}{2}X^2 + \frac{\alpha}{4}X^4 + F_e f_N X$$

cf. symmetry-breaking field in Landau theory

- gap increase suppressed by offset charges

Effect of offset charges



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$N \lesssim 10^3$–10^4