Scattering theory of current-induced forces

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Overview

Current-induced forces in mesoscopic systems:

- In molecule/dot with slow mechanical modes: Conduction electrons exert current-induced forces on slow modes
- All forces can be expressed in terms of scattering matrix
- Applications: Limit cycle motion, quantum motor, destabilization of vibrations…

*Bode, Kusminskiy, Egger & von Oppen, PRL **107**, 036804 (2011)*

*& Beilstein J Nanotech. **3**, 144 (2012)*

Current induced forces

- Molecule or quantum dot with finite number (M) of relevant electronic states
- Contacted by source and drain electrodes (normal metals)
  - Chemical potential imbalance → bias voltage → nonequilibrium current flows through dot
- Dot hosts N slow ‚mechanical' modes
  - Influence of current flow on dynamics of these modes? Current-induced forces?
  - Separation of time scales: Nonequilibrium Born Oppenheimer (NEBO) approximation

Some examples

- Transport through single hydrogen molecule
  - Slow variables describe center-of-mass motion and rigid rotation of molecule
- Spintronics: spin torques
  - Slow variable: magnetization vector of grain
- Current-induced domain wall motion in ferromagnetic wires
  - Slow variable: center position and angular variable characterizing domain wall center
- Cooling and amplification of mechanical motion in NEMS by backaction forces

Langevin dynamics

Current flow through a mesoscopic system (‚dot‘) with N slow ‚mechanical‘ modes $X_\nu \rightarrow$ current-induced forces on those modes

Langevin equations contain them on rhs:

$$M_\nu \ddot{X}_\nu + \frac{\partial U}{\partial X_\nu} = F_\nu - \sum_{\nu'} \gamma_{\nu\nu'} \dot{X}_{\nu'} + \xi_\nu$$

General form of these forces? Properties? Theoretical concepts?

Current-induced forces

- Mean (average) force $F_\nu(X_t)$
  - Nonconservative away from thermal equilibrium
  - Can do mechanical work in cyclic processes: molecular motor
- Velocity-dependent force, with matrix $\gamma_{\nu\nu'}(X_t)$
  - Symmetric part: dissipation matrix (damping). Negative eigenvalues (‚negative damping') possible out of equilibrium → mechanical instabilities, nonlinear effects
  - Antisymmetric part: Pseudo-magnetic Lorentz force due to Berry phase
- Noisy Gaussian random force $\xi_\nu(X_t)$

General model

- Dot Hamiltonian (including the coupling to slow modes): $$H_{dot} = \sum_{mm'} d_m^+ \left(H_0 + \sum_\nu \Lambda_\nu X_\nu \right)_{mm'} d_{m'}$$
  - M x M matrix Λ_ν: coupling of X_ν to electrons
  - H_0 describes electronic structure of dot
- Leads : $N_0 = N_{left} + N_{right}$ channels
  - Scattering state with complex amplitudes $c_n^{in,out}(t)$

$$\Psi(x<0, r_\perp, t) = \sum_{n=1}^{N_0} \left(c_n^{in} e^{ik_n x} + c_n^{out} e^{-ik_n x} \right) \Phi_{\perp,n}(r_\perp)$$

…captures essential physics of all examples…

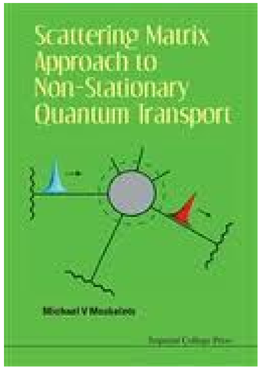
Scattering matrix

- Incoming amplitudes fixed by Fermi functions

$$\left|c_n^{in}(\varepsilon)\right|^2 = f_{a=left/right}(\varepsilon)$$

- Outgoing amplitudes depend on scattering processes within dot
  - Time dependence of mechanical modes → unitary S matrix is also time-dependent
  - Taking into account causality:

$$c^{out}(t) = \int_{-\infty}^{t} dt'\, S(t,t')\, c^{in}(t')$$



NEBO approximation

- Force operator: $\hat{F}_\nu = -\sum_{mm'} d_m^+ [\Lambda_\nu]_{mm'} d_{m'}$
- X slow on electronic time scales: NEBO
  - for given trajectory X_t , average over the fast electronic motion: $\hat{F}_\nu \to tr\left[i\Lambda_\nu G^<(t,t)\right] + \xi_\nu(t)$

$$G^<_{mm'}(t,t') = i\left\langle d^+_{m'}(t') d_m(t)\right\rangle$$

  - Time average replaced by ensemble average (ergodicity assumption)
- Needed: Lesser Green´s function (GF) of dot

Scattering matrix from GF

$$S = 1 - 2\pi i W G^R W^+$$

- Retarded GF: $G^R_{mm'}(t,t') = -i\Theta(t-t')\left\langle \left[d_m(t), d^+_{m'}(t') \right]_+ \right\rangle$
- Tunnel amplitudes connecting dot and leads are collected in $N_0 \times M$ matrix *W*
- Langreth rules connect retarded and lesser GF →

S matrix theory of current-induced forces

Bode, Kusminskiy, Egger & von Oppen, PRL 2011

- very flexible & intuitive approach, often used in mesoscopic physics and quantum transport theory
- Direct calculation of electric current (backaction!) also possible through S matrix

Adiabatic expansion of S matrix

- Wigner transform: $S_{full}(\varepsilon,t)=\int d\tau\ e^{i\varepsilon\tau}S(t+\tau/2,t-\tau/2)$
- NEBO expansion (in $\dot{X}$): $S_{full}=S+A+\cdots$
  - Lowest order: frozen (strictly adiabatic) S matrix

$$S(\varepsilon;X_t)=1-2\pi iW\left(\varepsilon-H_0-\sum_\nu \Lambda_\nu X_\nu+i\pi W^+W\right)^{-1}W^+$$

  - Leading correction: A matrix *Moskalets & Büttiker, PRB 2004*

$$A(\varepsilon,t)=\sum_\nu A_\nu(\varepsilon;X_t)\dot{X}_\nu$$

$$A_\nu=\pi W\left(\frac{\partial G^R}{\partial\varepsilon}\Lambda_\nu G^R-G^R\Lambda_\nu\frac{\partial G^R}{\partial\varepsilon}\right)W^+$$

For M=1 : A=0

Mean current-induced force

- Average force follows from frozen S matrix

$$F_\nu(X_t) = \sum_a \int \frac{d\varepsilon}{2\pi i} \; f_a \; Tr\left(P_a S^+ \frac{\partial S}{\partial X_\nu} \right)$$

  - P_a = projection operator to left/right lead
  - Tr = trace over lead channel space
- Conservative only in thermal equilibrium (no applied bias), otherwise nonconservative force
- Cyclic process: work can be done $\sum_\nu \oint F_\nu dX_\nu \neq 0$
  - Adiabatic quantum motor

Bustos-Marun, Refael & von Oppen, PRL 2013

  - „waterwheel" or „electron wind" force

Todorov, Dundas & McEniry, PRB 2010

Random Langevin force

- Random force $\xi_\nu(t)$ in Langevin equation obeys Gaussian statistics
- NEBO: Force correlations are local in time

$$\left\langle \xi_\nu(t)\xi_{\nu'}(t')\right\rangle_{Langevin} = D_{\nu\nu'}(X_t)\,\delta(t-t')$$

  - Symmetric fluctuation matrix

$$D_{\nu\nu'} = \sum_{aa'}\int \frac{d\varepsilon}{2\pi}\; f_a(1-f_{a'})\,Tr\left(P_a\left(S^{+}\frac{\partial S}{\partial X_\nu}\right)^{+}P_{a'}\,S^{+}\frac{\partial S}{\partial X_{\nu'}}\right)_{sym}$$

  - D is always positive definite & determined by frozen S matrix alone

Velocity dependent forces

- Velocity dependent forces also involve the A matrix
- Scattering matrix form of (symmetric) damping matrix:

$$\gamma_{\nu\nu'}^{sym} = \sum_a \int \frac{d\varepsilon}{4\pi} \left(-\frac{df_a}{d\varepsilon} \right) Tr \left(P_a \frac{\partial S^+}{\partial X_\nu} \frac{\partial S}{\partial X_{\nu'}} \right)_{sym}$$

$$+ \sum_a \int \frac{d\varepsilon}{2\pi i} f_a \; Tr \left(P_a \left[\frac{\partial A_{\nu'}^+}{\partial X_\nu} S - S^+ \frac{\partial A_{\nu'}}{\partial X_\nu} \right] \right)_{sym}$$

  - Second term is pure nonequilibrium contribution
  - In equilibrium connected to noise correlator through fluctuation-dissipation relation $D = 2kT\gamma^{sym}$

Fluctuations must always accompany damping!

Negative damping?

- In thermal equilibrium (no applied voltage): D>0 implies positivity of damping matrix
- Negative eigenvalues of damping matrix are possible out of equilibrium (second term!)
  - Electrons pump energy into collective modes: „phonon emission“
  - nonlinear phenomena & ‚run away‘ instabilities

Lü, Brandbyge & Hedegard, Nano Lett. 2010, PRL 2011

  - Limit cycles possible near X configurations with zero damping eigenvalue *Bode et al., PRL 2011*

Non-dissipative velocity-dependent force

- Antisymmetric part of γ matrix
  → „Lorentz"-like force

$$F_\nu^{Lorentz} = -\sum_{\nu'} \gamma_{\nu\nu'}^{anti} \dot{X}_{\nu'}$$

$$\gamma_{\nu\nu'}^{anti} = \sum_a \int \frac{d\varepsilon}{2\pi i} f_a \, Tr\left(P_a \left[\frac{\partial A_{\nu'}^{+}}{\partial X_\nu} S - S^{+} \frac{\partial A_{\nu'}}{\partial X_\nu} \right] \right)_{antisym}$$

  - vanishes in thermal equilibrium
  - can be traced to Berry phase effects

Lü, Brandbyge & Hedegard, Nano Lett. 2010

„Toy model" applications

Bode, Kusminskiy, Egger & von Oppen,
Beilstein J. Nanotechn. 2012

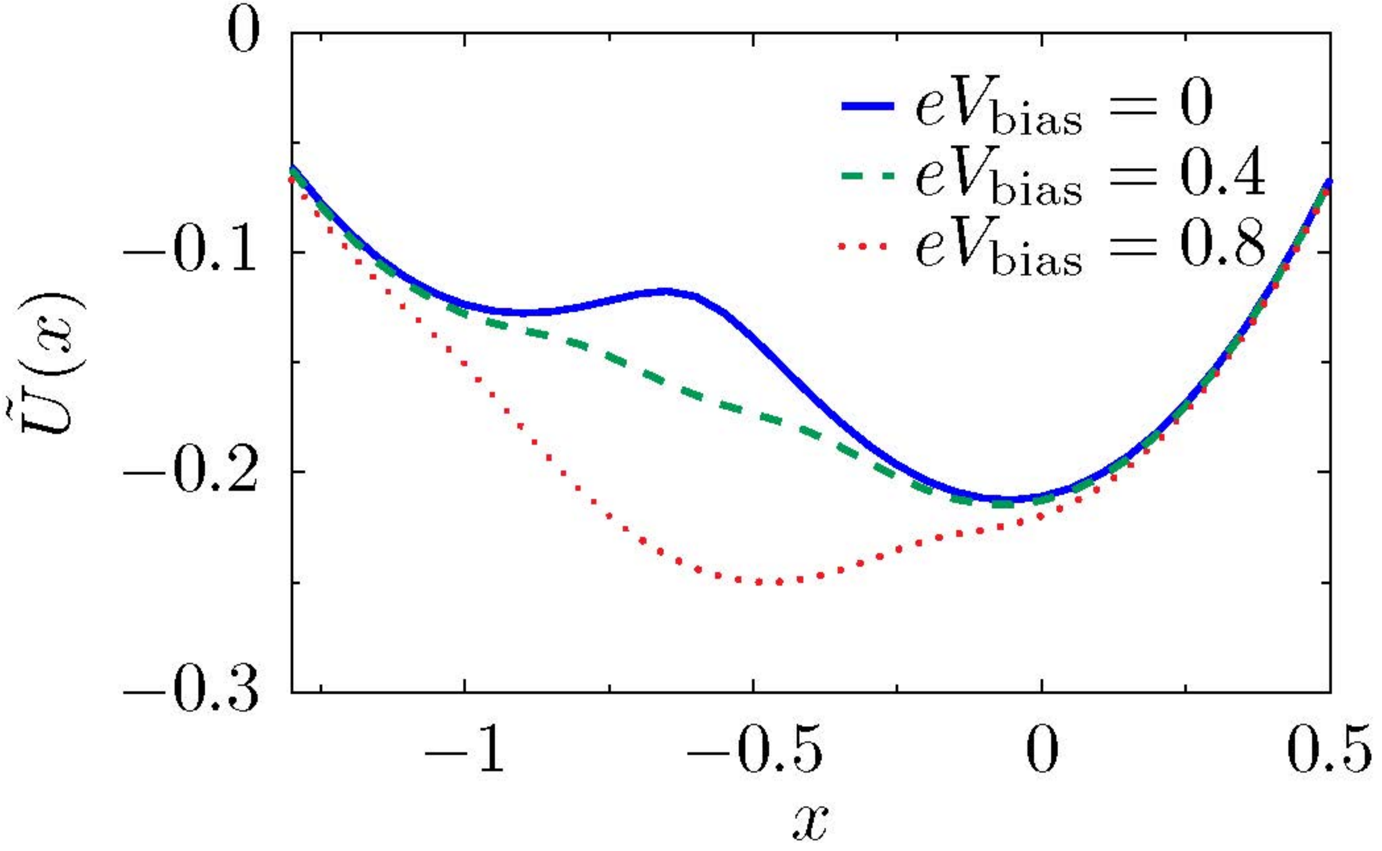
- Resonant level with single vibration mode: M=1, N=1
- Two electronic levels, single vibration mode: M=2, N=1
- Two levels, two modes: M=N=2
  - Limit cycle dynamics
  - Nonlinear frequency locking for transport through hydrogen molecule with N=2 vibrational modes

Resonant level M=N=1

- Analytically solvable: local level $\tilde{\varepsilon}(X) = \varepsilon_0 + \lambda X$
- γ scalar: pseudo-Lorentz force absent
- M=1 → A=0 → „nonequilibrium“ contribution to γ is zero → negative damping impossible
- Mean force always conservative for N=1
  - derivative of effective potential U(X)
  - U(X) multi-stable: qualitative effect of bias voltage
- Results for force and backaction current in agreement with previous work

Pistolesi, Blanter & Martin, PRB 2008

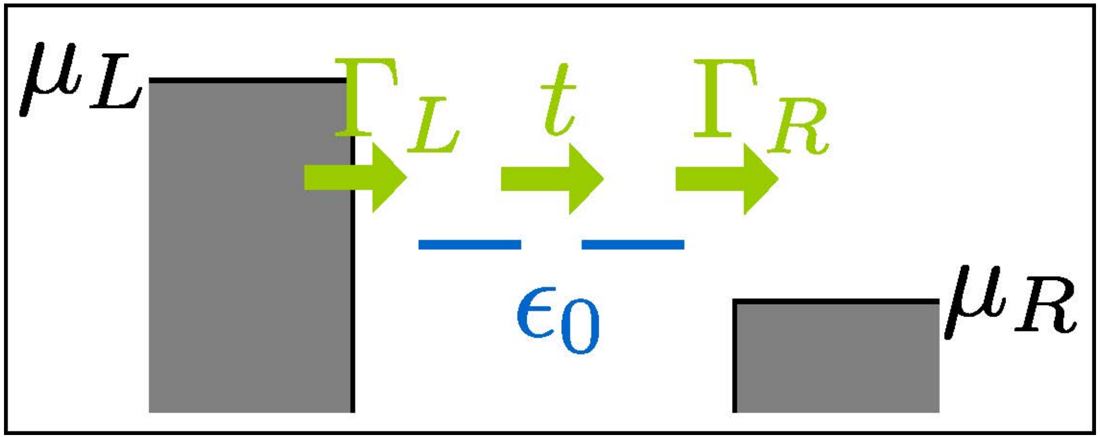
Effective potential for N=M=1



$\omega_{osc} = 0.01,\ \Gamma = 0.1,\ \varepsilon_0 = 0,\ T = 0$

(energy unit set by polaron energy)

Two electronic levels: M=2, N=1



$$H_0 = \begin{pmatrix} \varepsilon_0 & t \\ t & \varepsilon_0 \end{pmatrix}$$

$$\Lambda = \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}$$

- Two almost degenerate electronic levels
- Occupation difference couples to single vibration mode X with strength λ
- Hybridization parameters $\Gamma_a = \pi W^+ P_a W$
- inspired by double dot on suspended CNT

Scattering matrix: M=2, N=1

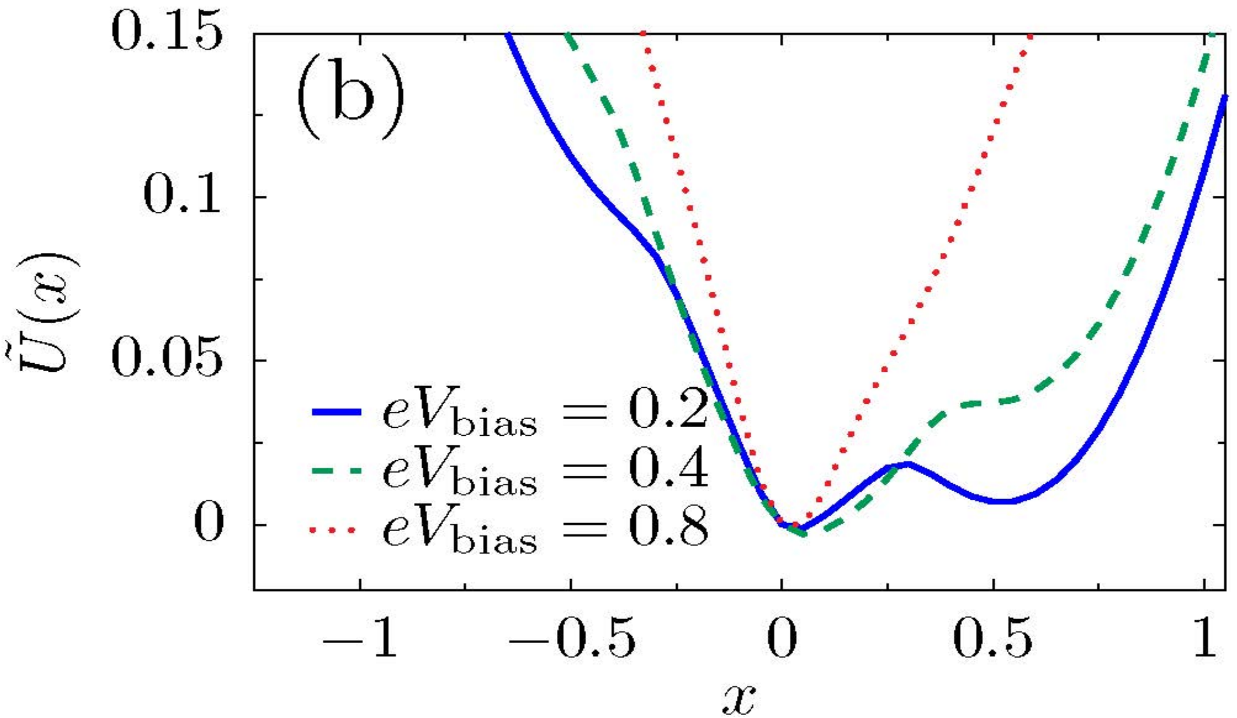
- Analytical results for S in wide-band limit
  - Assume symmetric contacts $\Gamma_L = \Gamma_R = \Gamma / 2$
  - Each lead couples to single dot state (in good basis): S is 2 x 2 matrix
- Frozen S matrix

$$S(\varepsilon, X) = 1 - i\frac{\Gamma}{\Delta}\begin{pmatrix} \varepsilon - \tilde{\varepsilon}_+ + i\Gamma/2 & t \\ t & \varepsilon - \tilde{\varepsilon}_- + i\Gamma/2 \end{pmatrix}$$

$$\tilde{\varepsilon}_\pm = \varepsilon_0 \pm \lambda X, \quad \Delta = (\varepsilon - \tilde{\varepsilon}_+ + i\Gamma/2)(\varepsilon - \tilde{\varepsilon}_- + i\Gamma/2) - t^2$$

- A matrix now finite: $A = \lambda \dot{X}\frac{\Gamma t}{\Delta^2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Effective potential: M=2, N=1



$\omega_{osc} = 0.01,\ t = \Gamma = 0.1,$

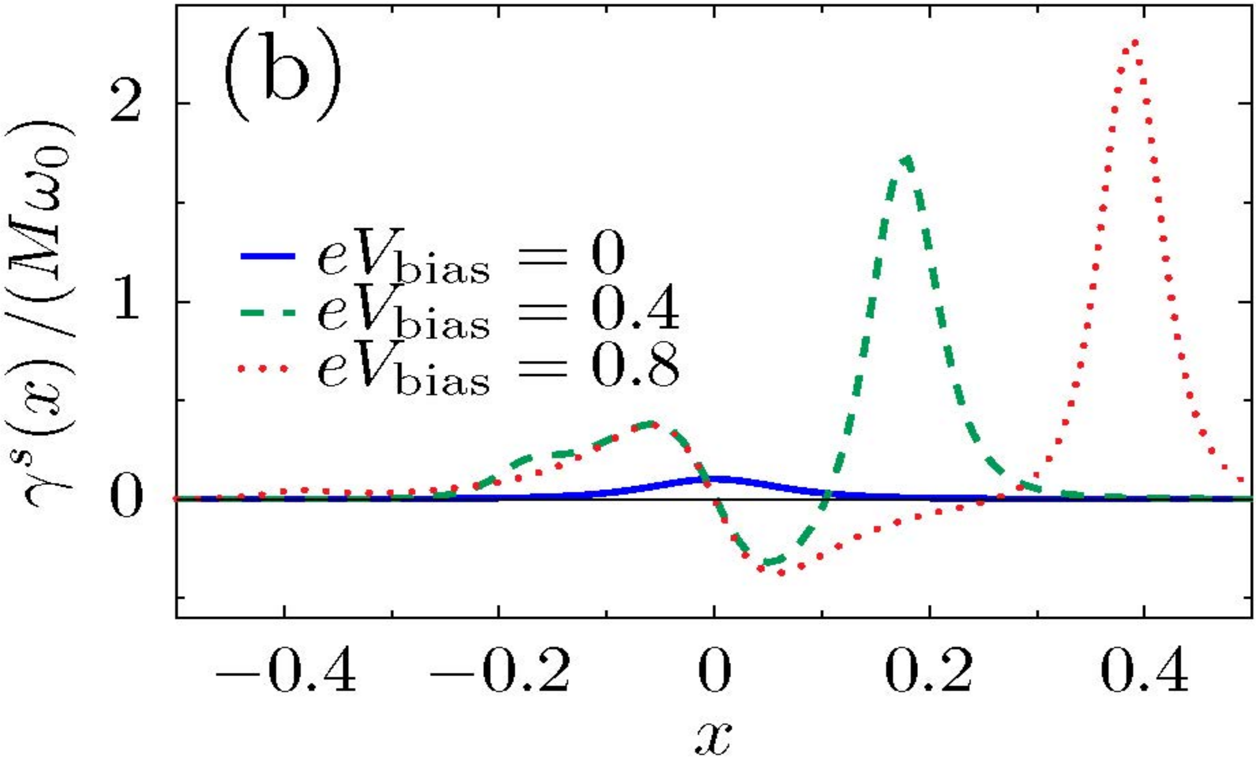
$\varepsilon_0 = 0.2,\ T = 0$

Current-induced mean force follows from this effective potential (single X variable!)

Again: multistability, tunable by bias voltage

Damping constant: M=2, N=1

Negative damping now possible out of equilibrium (A finite for M=2)



$\omega_{osc} = 0.01$

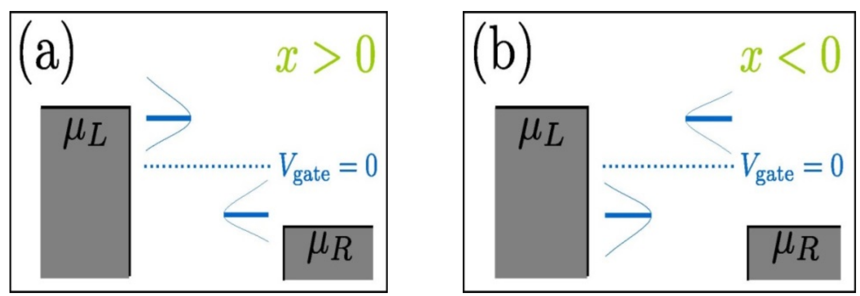
$t = \Gamma = 0.1$

$\varepsilon_0 = T = 0$

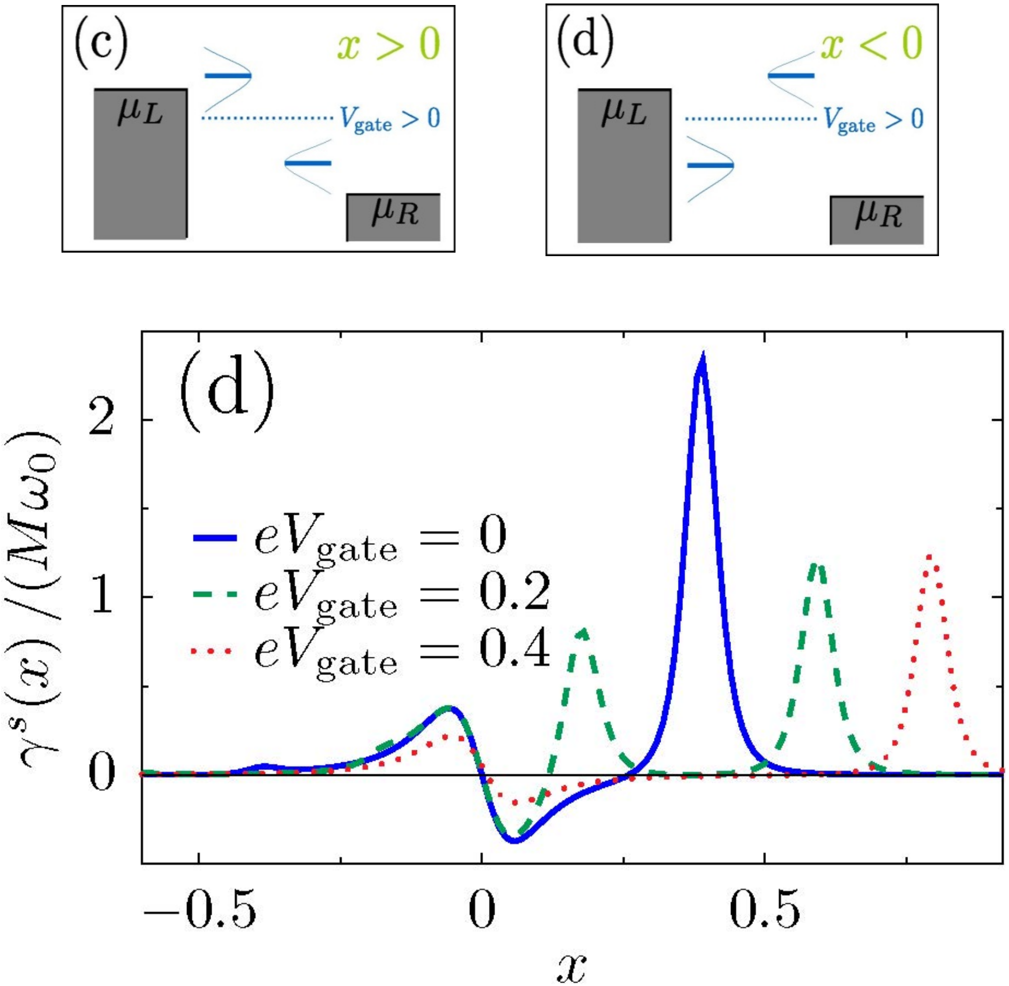
Conditions for negative damping?

- Both dot levels $\tilde{\varepsilon}_{\pm}(X) = \varepsilon_0 \pm \lambda X$ should be inside ‚bias window‘
  - otherwise effectively M=1 → A=0 → γ>0
  - Level alignments at ±eV/2 → up to four peaks in γ(X)
- For X>0: ‚downhill‘ transport
  - energy transfer to vibration mode: amplitude growth, negative damping
  - $\lambda X \approx t$ for resonant transfer: negative damping peak

$eV_{gate} = \varepsilon_0$



Effect of finite gate voltage



Finite gate voltage:

Asymmetry → four peaks visible

Negative damping again possible…

$$\omega_{osc} = 0.01$$
$$t = \Gamma = 0.1$$
$$eV_{bias} = 0.8$$

Two vibrational modes: N=2

- „Lorentz“ force exists only for N>1
- Current-induced mean force can be nonconservative only for N>1
- Minimal case: N=2, with M=2 electronic levels
- Toy model for H_2 molecule between left/right lead: two near-degenerate vibrational modes
  - Center-of-mass vibration mode X_1

$$\varepsilon_0 \to \tilde{\varepsilon}(X_1) = \varepsilon_0 + \lambda_1 X_1$$

  - Stretch mode X_2 (or rigid rotation)

$$t \to \tilde{t}(X_2) = t + \lambda_2 X_2$$

S matrix for M=N=2

- Closed results in wide band limit
  - Frozen S matrix

$$S(\varepsilon, X_{1,2}) = 1 - \frac{2i}{\Delta} \begin{pmatrix} (\varepsilon - \tilde{\varepsilon} + i\Gamma_R)\Gamma_L & \tilde{t}\sqrt{\Gamma_L \Gamma_R} \\ \tilde{t}\sqrt{\Gamma_L \Gamma_R} & (\varepsilon - \tilde{\varepsilon} + i\Gamma_L)\Gamma_R \end{pmatrix}$$

$$\Delta = (\varepsilon - \tilde{\varepsilon} + i\Gamma_L)(\varepsilon - \tilde{\varepsilon} + i\Gamma_R) - \tilde{t}^2$$

  - A matrix

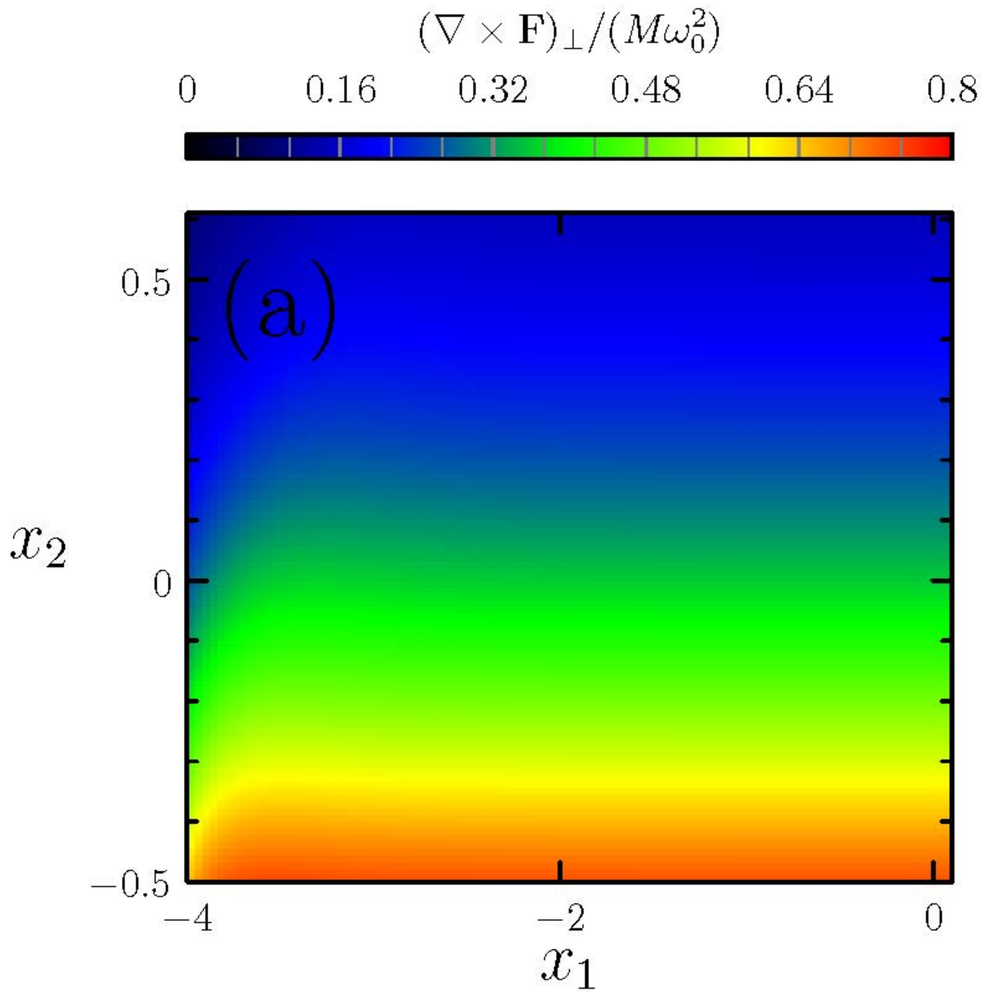
$$A = i\lambda_2 \dot{X}_2 \frac{(\Gamma_R - \Gamma_L)\sqrt{\Gamma_R \Gamma_L}}{\Delta^2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

    - Needs asymmetry in contacts, only due to stretch mode!
- all current induced forces at T=0 follow in analytical (but lengthy) form…

Mode dynamics for M=N=2

- Numerical solution of coupled Langevin equations for $X_1(t)$ and $X_2(t)$, including all current-induced forces and full nonlinearity
- Study interplay of
  - Nonconservative mean force
  - Negative damping causes instabilities of linearized theory: amplitude growth, run-away modes
  - „Lorentz“ force
  - Random force, not linked to damping by FDT

Curl of mean force



Curl of mean force is nonzero: Nonconservative force for all X configurations

$$\omega_{osc} = 0.014$$

$$\Gamma_L = 1.8,\ \Gamma_R = 0.2$$

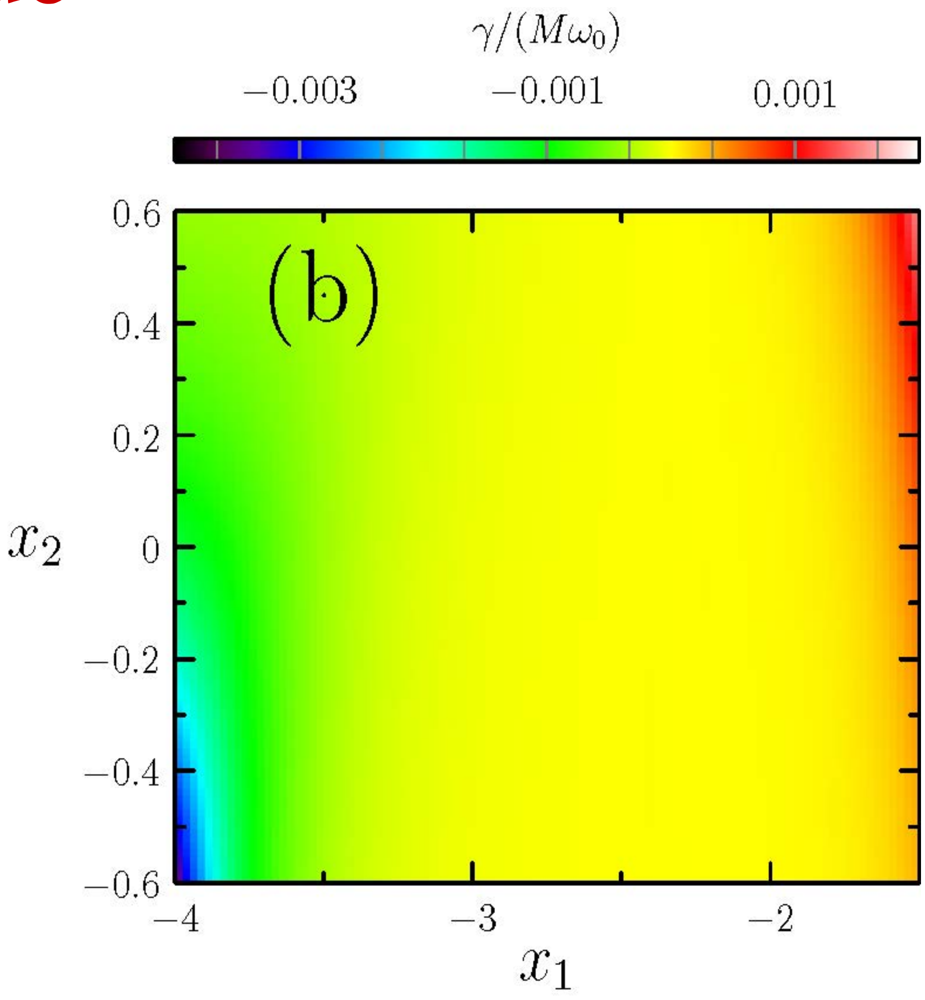
$$t = 0.9,\ \varepsilon_0 = 0$$

$$\lambda_1 = 1.5\lambda_2$$

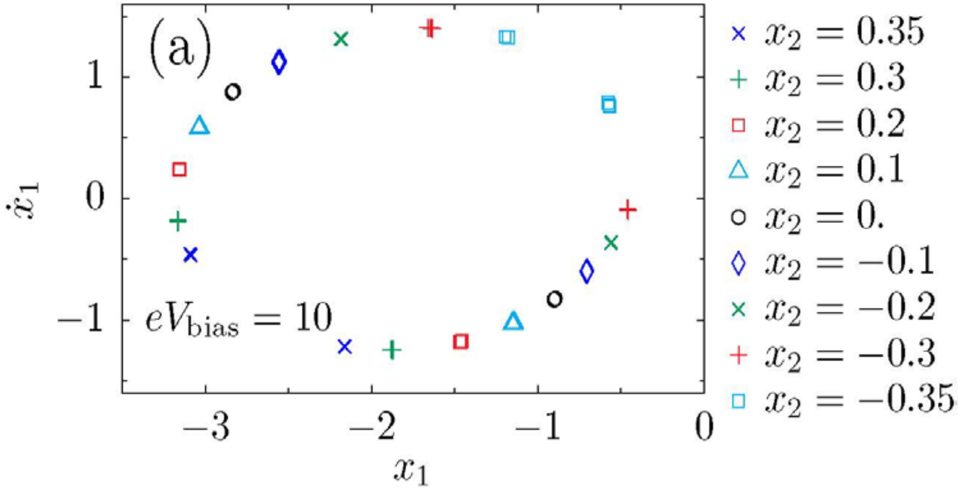
$$eV_{bias} = 10$$

Damping eigenvalue

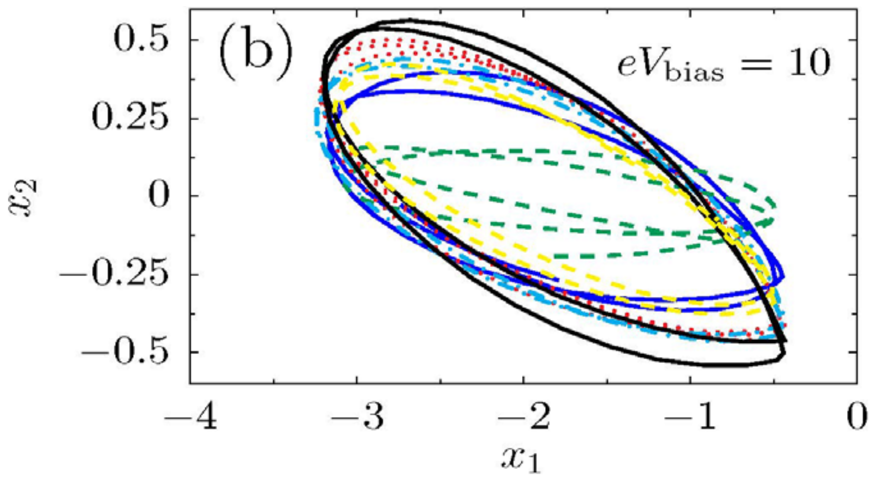
- One eigenvalue of γ matrix is shown
- Sign change with X configuration possible
- Negative damping
- Consequence:
  Limit cycle dynamics
  - Nonlinear oscillations (similar to Van der Pol oscillator)



Limit cycle dynamics



Poincaré sections (without random force) show limit cycle: Periodic solution in parametric (X_1,X_2) space



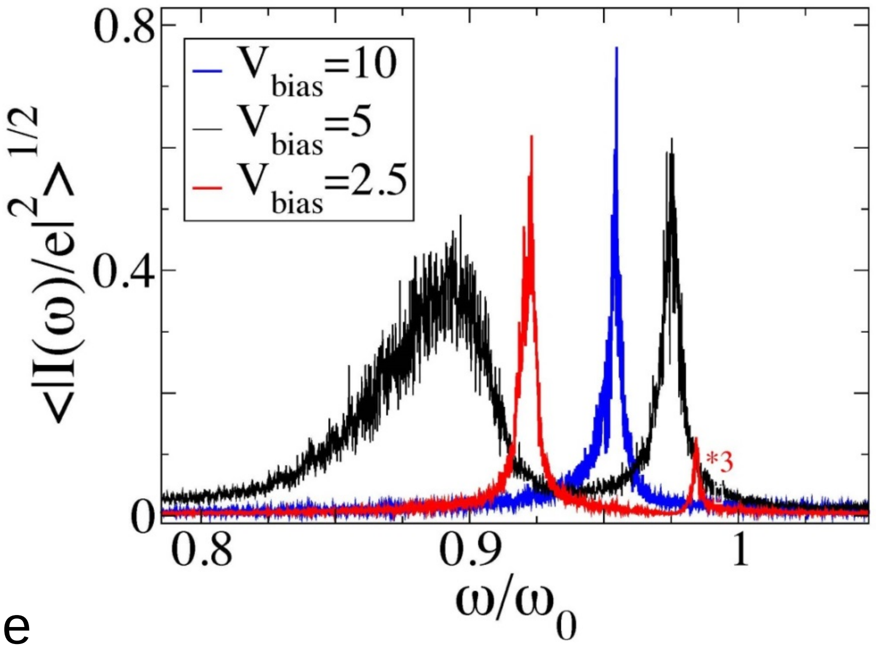
Typical trajectories in (X_1,X_2) space (with different initial conditions): Signatures of limit cycle in presence of random forces

Shot noise frequency locking

Signature of limit cycle in current-current correlations:

Noise peak at limit cycle frequency for large bias voltage: nonlinear frequency locking

For small bias voltage: no limit cycle dynamics → two characteristic frequencies (independent X_1 and X_2 oscillations)



Conclusions

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- Applications: Limit cycle motion, quantum motor, destabilization of vibrations…

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