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…

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 $X_v \rightarrow$ current-induced forces on those modes

Langevin equations contain them on rhs:

$$M_v \ddot{X}_v + \frac{\partial U}{\partial X_v} = F_v - \sum_{v'} \gamma_{vv'} \dot{X}_{v'} + \xi_v$$

General form of these forces? Properties? Theoretical concepts?
Current-induced forces

- Mean (average) force $F_v(X_t)$
  - Nonconservative away from thermal equilibrium
  - Can do mechanical work in cyclic processes: molecular motor

- Velocity-dependent force, with matrix $\gamma_{vv'}(X_t)$
  - Symmetric part: dissipation matrix (damping). Negative eigenvalues ('negative damping') possible out of equilibrium $\rightarrow$ mechanical instabilities, nonlinear effects
  - Antisymmetric part: Pseudo-magnetic Lorentz force due to Berry phase

- Noisy Gaussian random force $\xi_v(X_t)$
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 \( \Lambda_{\nu} \): coupling of \( X_{\nu} \) 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
  \[ |c_n^{in}(\epsilon)|^2 = f_{a=left/right}(\epsilon) \]

- 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:
  \[ \hat{F}_v = -\sum_{mm'} d_m'^+ \Lambda_{\nu}^{mm'} d_{m'} \]

- \( X \) slow on electronic time scales: NEBO
  - for given trajectory \( X_t \), average over the fast electronic motion:
    \[ \hat{F}_v \rightarrow tr[i\Lambda_{\nu} G^<(t,t)] + \xi_{\nu}(t) \]
    \[ G^<(t,t') = i\langle d_m'^+(t')d_m(t) \rangle \]
  - 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:**
  \[ G^R_{mm'}(t, t') = -i\Theta(t - t')\langle [d_m(t), d_{m'}^+(t')]_+ \rangle \]

- 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
    \[
    S(\varepsilon; X_t) = 1 - 2\pi i W (\varepsilon - H_0 - \sum_v \Lambda_v \dot{X}_v + i \pi W^+ W)^{-1} W^+
    \]
- Leading correction: A matrix
  \[
  A(\varepsilon, t) = \sum_v A_v(\varepsilon; X_t) \dot{X}_v
  \]
  \[
  A_v = \pi W \left( \frac{\partial G^R}{\partial \varepsilon} \Lambda_v G^R - G^R \Lambda_v \frac{\partial G^R}{\partial \varepsilon} \right) W^+
  \]
  For \( M=1 \) : \( A=0 \)
Mean current-induced force

- Average force follows from frozen S matrix

\[ F_v(X_t) = \sum_a \int \frac{d\epsilon}{2\pi i} f_a \ Tr \left( P_a S^+ \frac{\partial S}{\partial X_v} \right) \]

- \( P_a \) = 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
  \[ \sum_v \oint F_v dX_v \neq 0 \]
  - 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 $\xi_v(t)$ in Langevin equation obeys **Gaussian statistics**
- NEBO: Force correlations are **local in time**
  $$\langle \xi_v(t)\xi_{v'}(t') \rangle_{\text{Langevin}} = D_{vv'}(X_t) \delta(t-t')$$
- Symmetric fluctuation matrix
  $$D_{vv'} = \sum_{aa'} \int \frac{d\xi}{2\pi} f_a (1 - f_{a'}) \text{Tr} \left( P_a \left( S^+ \frac{\partial S}{\partial X_v} \right)^+ P_{a'} S^+ \frac{\partial S}{\partial X_{v'}} \right)_{\text{sym}}$$
- 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:

\[
\gamma_{vv'}^{\text{sym}} = \sum_a \int \frac{d\varepsilon}{4\pi} \left( -\frac{df_a}{d\varepsilon} \right) \text{Tr} \left( \frac{\partial S^+}{\partial X_v} \frac{\partial S}{\partial X_{v'}} \right)_{\text{sym}} \\
+ \sum_a \int \frac{d\varepsilon}{2\pi i} f_a \text{Tr} \left( P_a \left[ \frac{\partial A^+_{v'}}{\partial X_v} S - S^+ \frac{\partial A_{v'}}{\partial X_v} \right] \right)_{\text{sym}}
\]

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

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 $\gamma$ matrix
  $\rightarrow$ "Lorentz"-like force

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

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

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

Lü, Brandbyge & Hedegard, Nano Lett. 2010
„Toy model“ applications

- 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 $\tilde{\varepsilon}(X) = \varepsilon_0 + \lambda X$
- $\gamma$ scalar: pseudo-Lorentz force absent
- $M=1 \rightarrow A=0 \rightarrow$ "nonequilibrium" contribution to $\gamma$ is zero $\rightarrow$ 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 $N=M=1$

$\bar{U}(x)\quad eV_{\text{bias}} = 0$
$\quad eV_{\text{bias}} = 0.4$
$\quad eV_{\text{bias}} = 0.8$

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

(energy unit set by polaron energy)
Two almost degenerate electronic levels
Occupation difference couples to single vibration mode X with strength $\lambda$
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:

\[
A = \lambda X \frac{\Gamma t}{\Delta^2} \begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix}
\]
Effective potential: \( M=2, \, N=1 \)

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

\[ \omega_{osc} = 0.01, \, t = \Gamma = 0.1, \]
\[ \varepsilon_0 = 0.2, \, T = 0 \]

Again: multistability, tunable by bias voltage
Damping constant: $M=2$, $N=1$

Negative damping now possible out of equilibrium (A finite for $M=2$)
Conditions for negative damping?

- Both dot levels $\tilde{\varepsilon}_\pm(X) = \varepsilon_0 \pm \lambda X$ should be inside 'bias window'
- otherwise effectively $M=1 \rightarrow A=0 \rightarrow \gamma > 0$
- Level alignments at $\pm eV/2 \rightarrow$ up to four peaks in $\gamma(X)$
- For $X>0$: 'downhill' transport
  - energy transfer to vibration mode: amplitude growth, negative damping
  - $\lambda X \approx t$ for resonant transfer: negative damping peak

$eV_{\text{gate}} = \varepsilon_0$

(a) $x > 0$

(b) $x < 0$
**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 \( X_1 \)
    \[ \varepsilon_0 \rightarrow \tilde{\varepsilon}(X_1) = \varepsilon_0 + \lambda_1 X_1 \]
  - Stretch mode \( X_2 \) (or rigid rotation)
    \[ t \rightarrow \tilde{t}(X_2) = t + \lambda_2 X_2 \]
S matrix for $M=N=2$

- Closed results in wide band limit
  - Frozen S matrix
    \[
    S(\varepsilon, X_{1,2}) = 1 - \frac{2i}{\Delta} \left( \begin{array}{cc}
    \left( \varepsilon - \bar{\varepsilon} + i\Gamma_R \right)\Gamma_L & \tilde{t}\sqrt{\Gamma_L\Gamma_R} \\
    \tilde{t}\sqrt{\Gamma_L\Gamma_R} & \left( \varepsilon - \bar{\varepsilon} + i\Gamma_L \right)\Gamma_R
    \end{array} \right)
    \]
    \[
    \Delta = \left( \varepsilon - \bar{\varepsilon} + i\Gamma_L \right)\left( \varepsilon - \bar{\varepsilon} + i\Gamma_R \right) - \tilde{t}^2
    \]
  - A matrix
    \[
    A = i\lambda_2 \dot{X}_2 \left( \frac{\Gamma_R - \Gamma_L}{\Delta^2} \sqrt{\Gamma_R\Gamma_L} \right) \begin{pmatrix}
    0 & 1 \\
    -1 & 0
    \end{pmatrix}
    \]

- 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 is nonzero:
Nonconservative force for all X configurations

\[
\frac{(\nabla \times F)_1}{(M\omega_0^2)} = \Gamma = \Gamma_{RL,osc}
\]

\[
\omega_{osc} = 0.014 \\
\Gamma_L = 1.8, \quad \Gamma_R = 0.2 \\
t = 0.9, \quad \varepsilon_0 = 0 \\
\lambda_1 = 1.5\lambda_2 \\
eV_{bias} = 10
\]
Damping eigenvalue

- One eigenvalue of $\gamma$ 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

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...