Statistical forces and stabilization out-of-equilibrium

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10 April 2019

in honor of François Dunlop

Where do more interesting dynamical systems come from?

Some physics motivating some mathematical studies.

Forces around equilibrium are entropic:

The mere power of large numbers

“Strife is not for the component substances, for these component substances of all organism, as air, water, and earth, are abundant;
neither is the strife for energy as such, for this occurs in abundance, as the heat content of matter of our environment;
but strife is for the *free energy* available
for the performance of work.” (Boltzmann, 1886)

Reason: time-reversal invariance
cf detailed balance

$$\exp S(Y)\ k(Y,Y') = \exp S(Y')\ k(Y',Y)$$

where S(Y) = entropy of condition Y and k(Y,Y’) are transition rates.

Ad 1: Convergence to equilibrium determined by GRADIENT FLOW

Steepest descent in free energy landscape…

Static fluctuations in equilibrium:

Connects with work and forces via the miraculous relation,

Force on X is

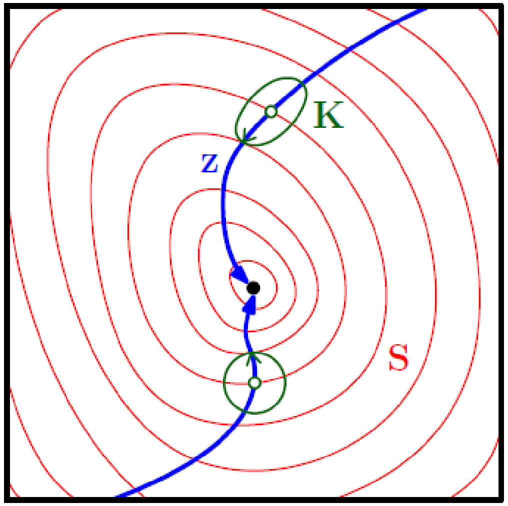
$$-\int \mathrm{d}\eta \, \frac{1}{Z(X)} e^{-\beta H(\eta,X)} \, \nabla_X H(\eta, X) = -\nabla_X \mathcal{F}(X)$$

for free energy acting *truly* as

thermodynamic potential,

$$\mathcal{F}(X) = -k_B T \log Z(X)$$

$$\dot{z} = K(z)\, S'(z) = D j_z,\ K = D\, X\, D^\dagger,\quad X \geq 0$$



- state z: position x, density ρ, etc.
- entropy S
- kinetics K symmetric positive

$$\dot{S}(z) = S'(z) \cdot \dot{z} = S'(z) \cdot K(z)\, S'(z) \geq 0$$

Examples:

$\dot{x} = -\chi(x) V'(x)$	$\dot{\rho}(x) = -\nabla \cdot [-\rho(x)\chi(\rho, x)\nabla V(x) - \chi(\rho, x)\nabla \rho(x)]$
$S = -V$ $K = \chi$	$S(\rho) = -\int(\rho \log(\rho) + \rho V)\mathrm{d}x$ $K(\rho, x) = -\nabla \cdot \rho(x)\chi(\rho, x)\nabla$

Kraaij, Lazarescu, CM and Peletier, Deriving GENERIC from a generalized fluctuation symmetry. Journal of Statistical Physics **170**, 492-508 (2018).

Statistical force

Probe (x) coupled to nonequilibrium medium through energy U(x,η)

Systematic force:

$$f(x) = -\int \rho_x(\mathrm{d}\eta)\, \nabla_x U(x,\eta) = -\langle \nabla_x U(x,\eta) \rangle^x$$

Equilibrium :

$$f_{\mathrm{eq}}(x) = -\nabla_x \mathcal{F}(x)$$

Free energy

The questions

Q1

- What is (involved in) the vector potential?
- What determines the direction of the induced current?

Q2

- Can nonequilibria make fixed points (more) stable?
- Can nonequilibria stabilize patterns/phases?

Q3

- What are the friction/noise relations? How to modify the Einstein (second fluctuation-dissipation) relation?

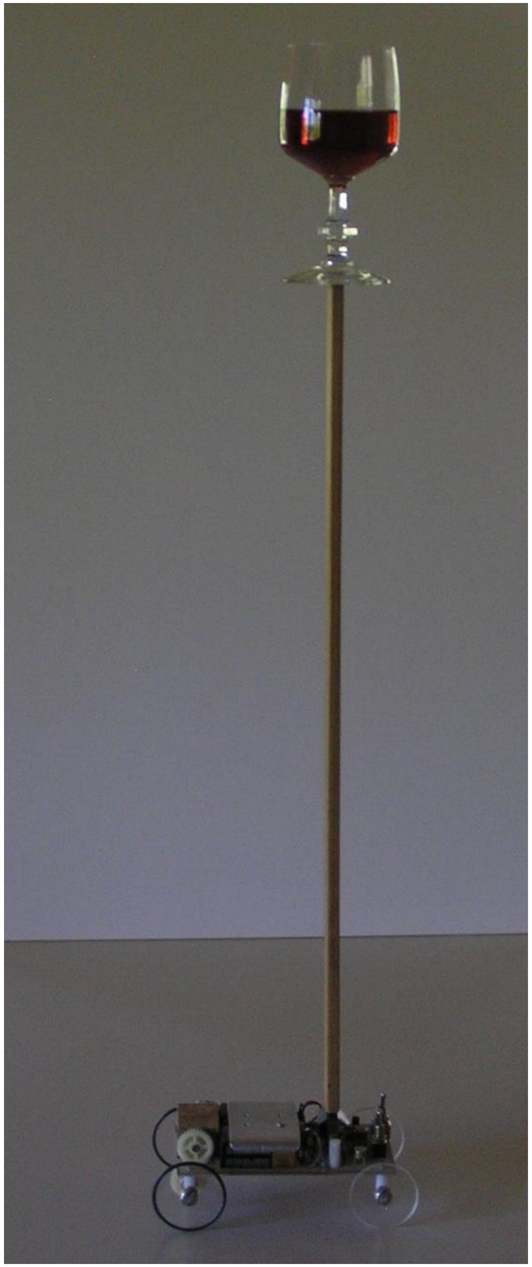
Statistical forces out-of-equilibrium

- Christian Maes and Karel Netočný, Nonequilibrium corrections to gradient flow. arXiv:1904.00379v1 .
- Thibaut Demaerel, Christian Maes and Karel Netočný, Stabilization in the Eye of a Cyclone. Annales Henri Poincaré **19**, 2673 (2018).
- Christian Maes and Karel Netočný, Non-reactive forces and pattern formation induced by a nonequilibrium medium. arxiv:1711.05168 .
- Christian Maes and Thimothée Thiery, The induced motion of a probe coupled to a bath with random resettings. J. Phys. A: Math. Theor. **50**, 415001 (2017) .
- Urna Basu, Pierre de Buyl, Christian Maes and Karel Netočný, Driving-induced stability with long-range effects. EPL **115**, 30007 (2016).
- Urna Basu, Christian Maes and Karel Netočný, Statistical forces from close-to-equilibrium media. New Journal of Physics **17**, 115006 (2015).

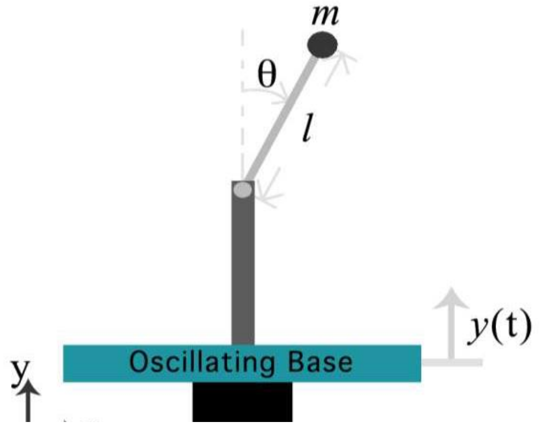
Stabilizing the metastable or even the unstable…

Standard examples:

-Via feedback, dynamical control



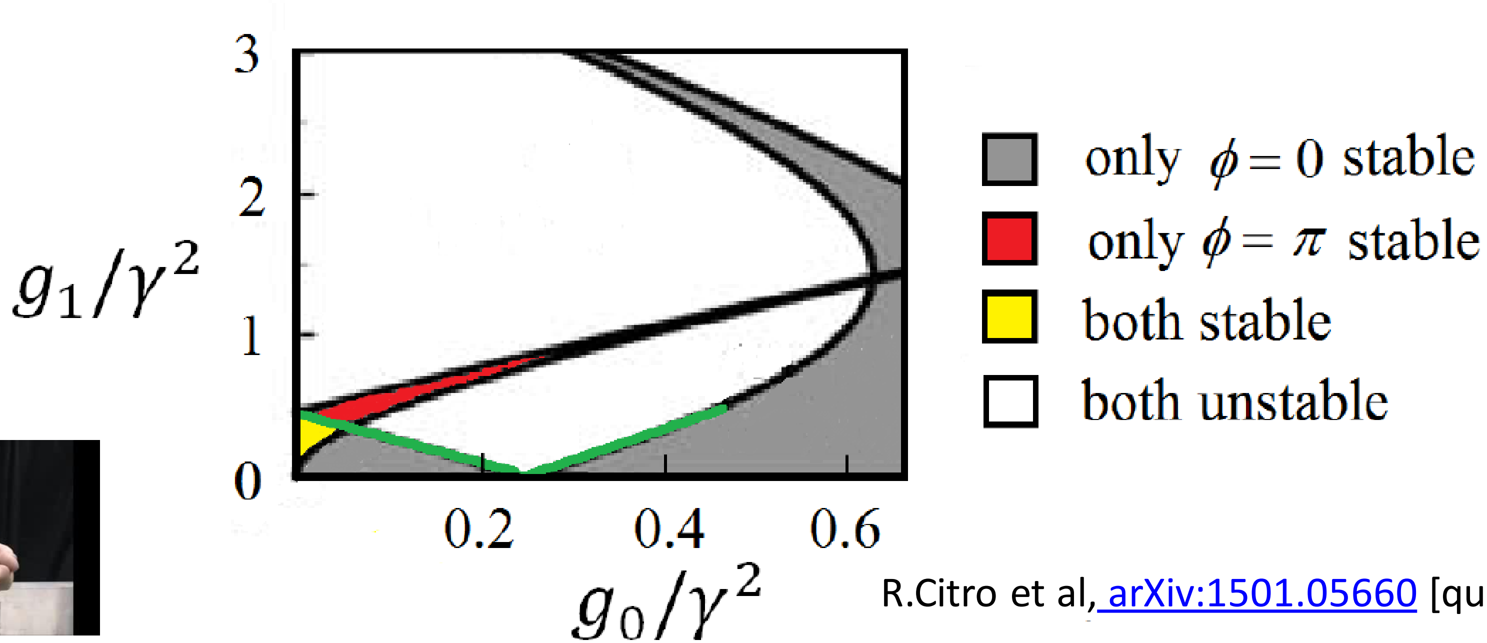
Stabilizing the metastable or even the unstable…

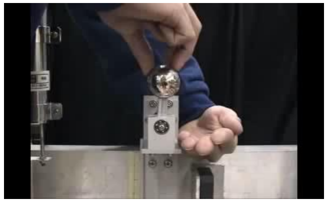


Much less trivial:

Stephenson-Kapitza (inverted) pendulum

$$H(t) = \frac{1}{2}p^2 - g(t)\cos(\phi), \quad \text{with} \quad g(t) = g_0 + g_1 \cos(\gamma t)$$





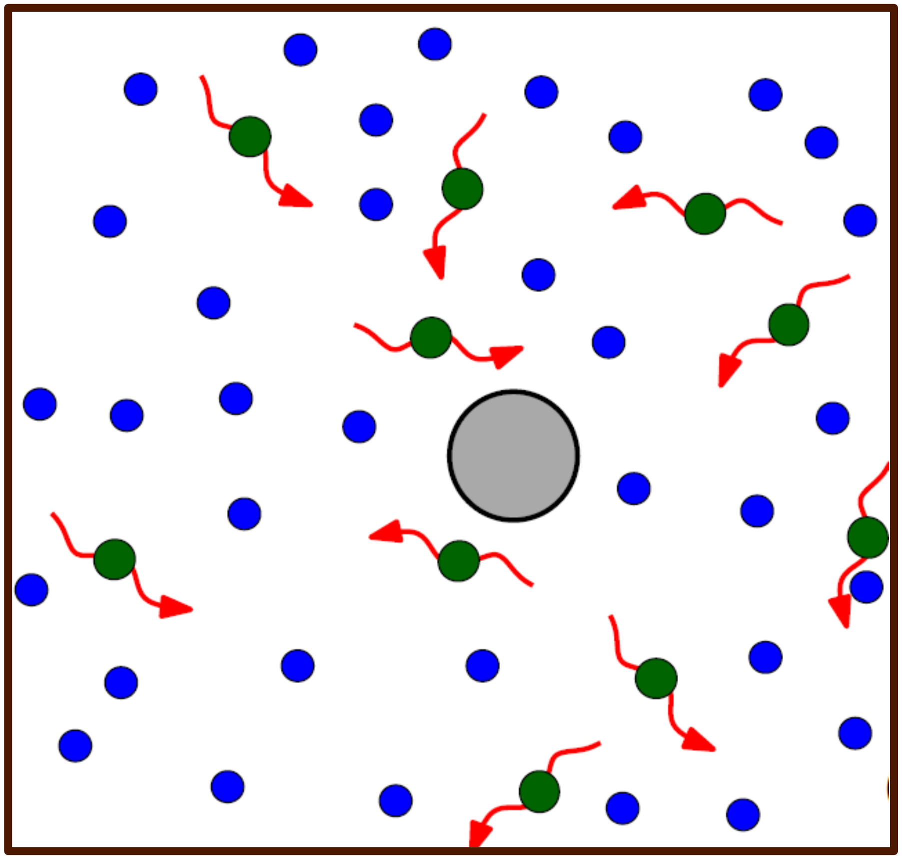
R.Citro et al, arXiv:1501.05660 [quant-ph]

Set-up

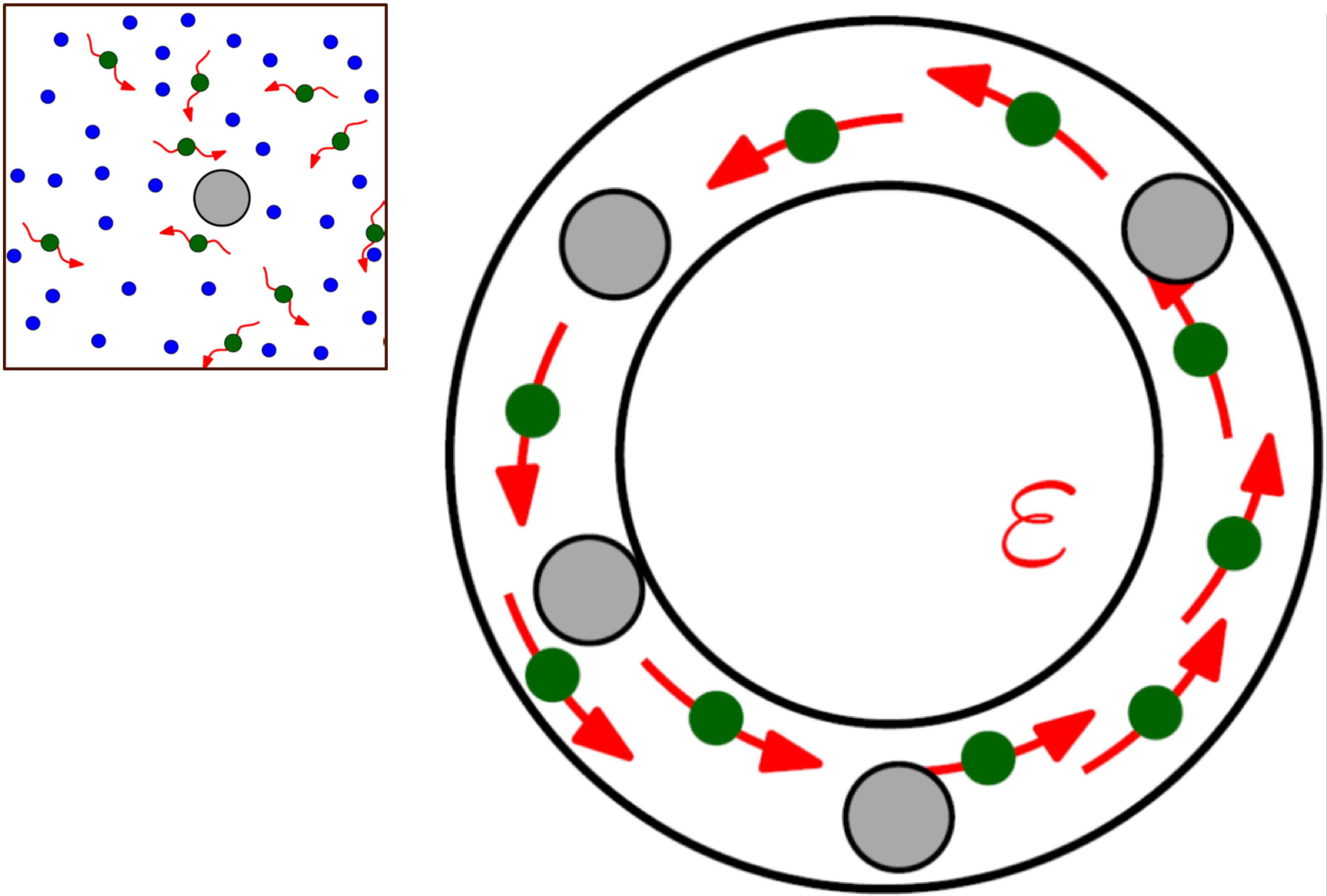
Probe interacting with

nonequilibrium medium

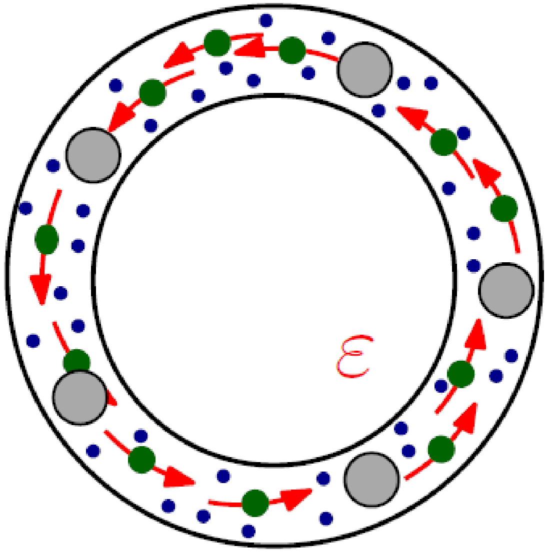
connected to equilibrium reservoir(s)



Time-scale separation: probe is slow, medium relaxes fast to stationary state


ε

PARTICLE SYSTEM on circle S^1.
blue = viscous heat bath at some temperature T.
green = many colloidal particles driven by emf of strenth ε.
grey = some slow undriven particles in short range interaction with colloids.



LENGTH SCALES:
L = circle, with L/N equidistance between grey particles
$(\beta\,\epsilon)^{-1}$ = dissipation length
δ = short range of interaction.

That is

Overdamped stationary diffusion in non-conservative force field: for $x \in S^1$, $Y = (Y_\alpha)_1^n \in S^1$,

$$0 = \partial_x \left(\left[\varepsilon + \sum_\alpha u'(x - Y_\alpha) \right] \rho(x, Y) \right) + T\, \partial^2_{xx} \rho(x, Y)$$

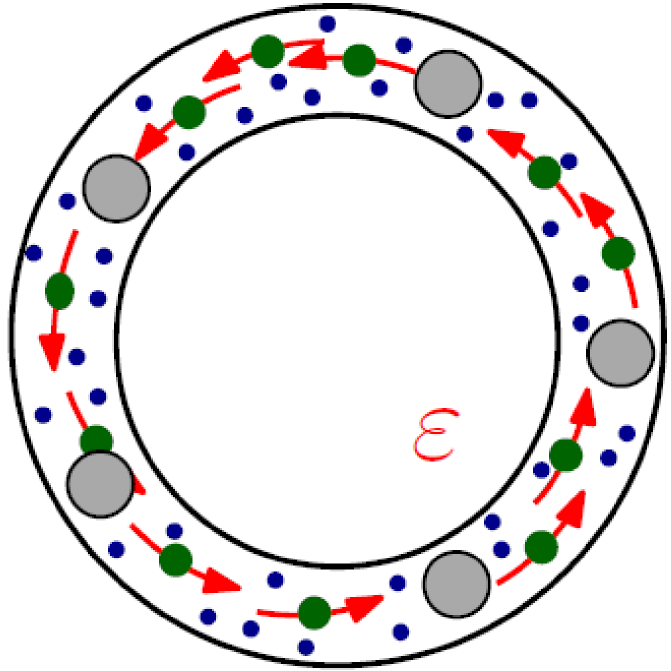
for prob density $\rho(x, Y)$ wrt dx on S^1 for fixed Y.

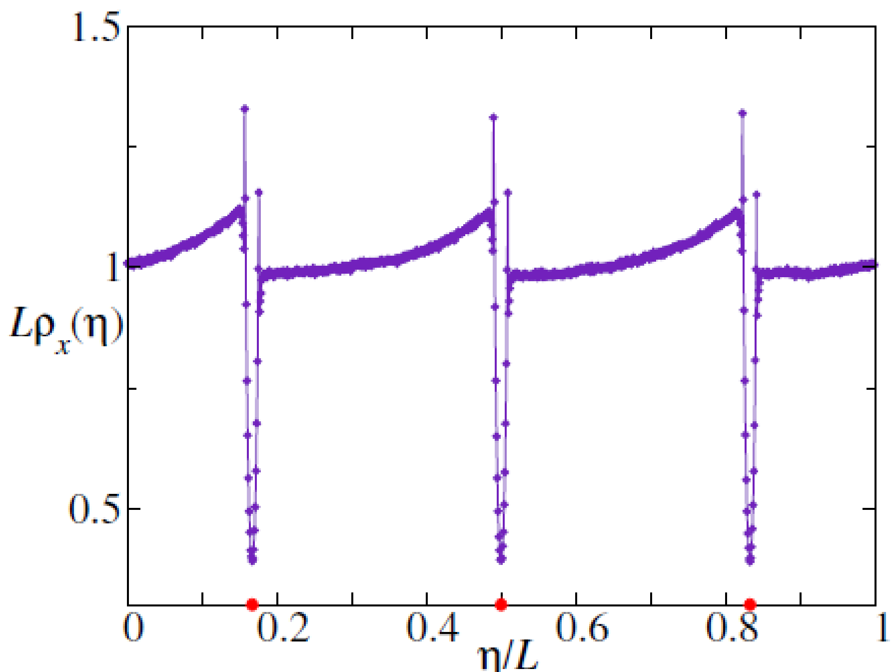
Potential $u(z)$ is even and short-ranged.

Imagine all is "well" (which is easy enough): unique smooth solution.

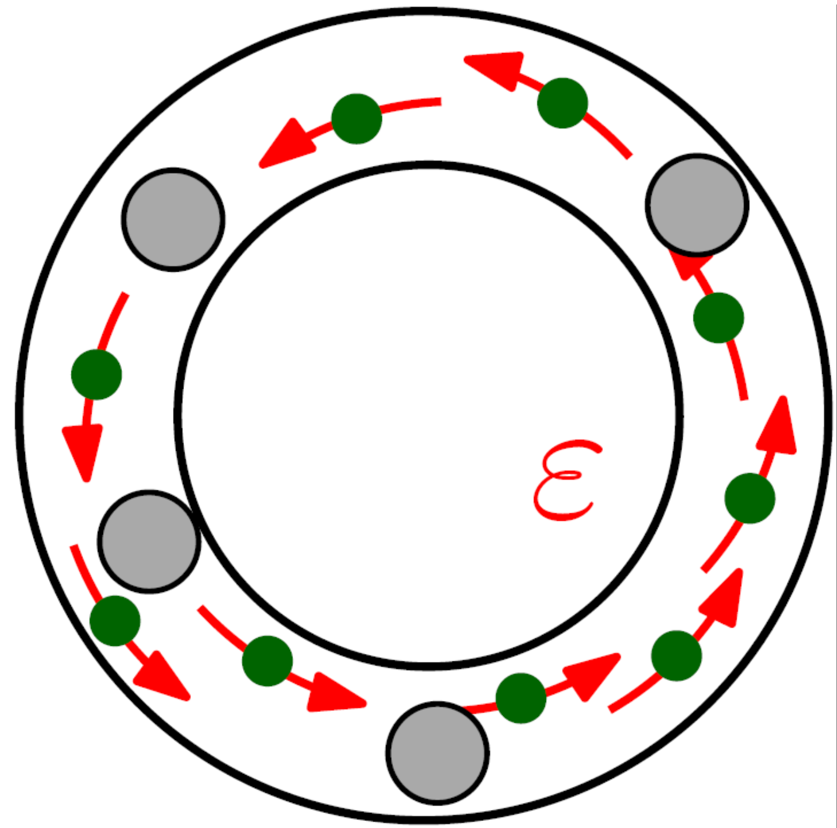
Study statistical force on αth probe,

$$f_\alpha(Y) = \oint dx\, \rho(x, Y)\, u'(x - Y_\alpha)$$


ε


1.5
1
0.5
$L\rho_x(\eta)$
0
0.2
0.4
0.6
0.8
1
η/L

Multiple probes in short-range interaction with driven medium



medium

$$\gamma \frac{d\eta_t}{dt} = \varepsilon - \frac{\partial U(x,\eta)}{\partial \eta} + \left(\frac{2\gamma}{\beta}\right)^{1/2} \xi_t$$

coupling

$$u(z) = \begin{cases} u_0 \left[1 - \left(\frac{z}{\delta}\right)^2\right]^2 & \text{for } |z| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$

Statistical force on αth-probe

$$f_\alpha(x) = -\oint \frac{\partial U(x,\eta)}{\partial x_\alpha} \rho_x(\eta)\, d\eta = -\oint u'(x_\alpha - \eta)\, \rho_x(\eta)\, d\eta$$

1.

$x \in S^1$, $Y = (Y_\alpha)_1^N \in S^1$:

$$0 = \partial_x \left(\left[\varepsilon + \sum_\alpha u'(x - Y_\alpha) \right] \rho(x, Y) \right) + T\, \partial^2_{xx} \rho(x, Y)$$

$$f_\alpha(Y) = \oint dx\, \rho(x, Y)\, u'(x - Y_\alpha)$$

Result: equidistant probe configuration is "fixed point" and "stable" whenever $\varepsilon \neq 0$.

fixed point: $Y_\alpha = v^* t + L\, \frac{\alpha}{N}$

stable: linear stability + Lyapunov property

Stability of equidistant "crystal" configuration

$$x^*_\alpha(t) = v^* t + \frac{L}{N}\,\alpha \quad (\alpha \bmod N)$$

$$\Gamma \dot{y}_\alpha = \sum_\gamma M_{\alpha\gamma} y_\gamma\,, \qquad M_{\alpha\gamma} = \frac{\partial f_\alpha(x^*)}{\partial x_\gamma}$$

$$x_\alpha = x^*_\alpha + y_\alpha$$

$$M_{\alpha\alpha} = -\sum\nolimits_{\gamma\neq\alpha} M_{\alpha\gamma} \qquad M_{\alpha\gamma} = m_{\gamma-\alpha}$$

$$m_\alpha = \frac{\zeta j^* B}{\ell_d^2\,(1 - e^{-L/\ell_d})}\, e^{-\frac{L}{N\ell_d}\alpha}\,, \quad \alpha = 1, \ldots, N-1$$

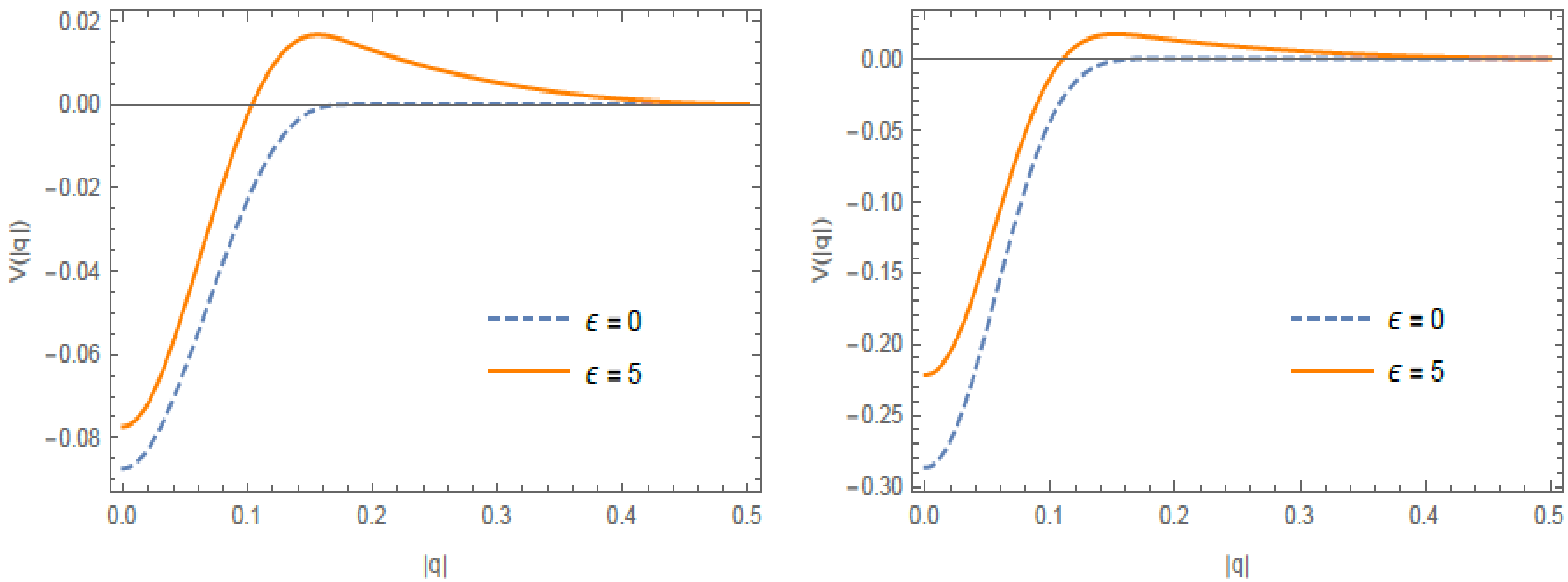


FIG. 1: Induced probe–probe interaction potential for (a) repulsive ($u_0 = 1$) and (b) attractive ($u_0 = -1$) probe–medium coupling. The other parameters are $\varepsilon = 5$, $\delta = 0.1$, $\beta = 1$, $\gamma = 1$, $\rho^o = 1$, and $L = 1$.

NEW ATTRACTOR: stable EQUIDISTANT CONFIGURATION OF PROBES

FLOW TOWARDS *CRYSTAL* FORMATION

Asymmetric springs
(via overdamped Langevin equation for real $y_\alpha, \alpha = 1, \ldots, N$)

$$\Gamma \dot{y}_\alpha = \sum_\gamma M_{\alpha\gamma} y_\gamma + \sqrt{2\Gamma}\, \xi_\alpha$$

with $M_{\alpha\gamma} = m_{\gamma-\alpha}$ effective "spring constants" though not symmetric $m_\gamma \neq m_{-\gamma}$, due to the non-reactivity of the forces.

Stationary distribution is still

$$\nu(y) = \frac{1}{\mathcal{Z}}\, e^{-V(y)}$$

for the effective potential

$$V(y) = \frac{1}{2} \sum_{\alpha,\gamma} y_\alpha M_{\alpha\gamma} y_\gamma = \frac{1}{4} \sum_{\gamma>0} m_\gamma \sum_\alpha (y_{\alpha+\gamma} - y_\alpha)^2$$

despite the absence of detailed balance

Dynamical system

$$\Gamma \dot{y}_\alpha = \sum_\gamma M_{\alpha\gamma} y_\gamma = \sum_{\gamma=1}^{N-1} m_\gamma (y_{\alpha+\gamma} - y_\alpha)$$

conserves the zero mode $Y = \sum_\alpha y_\alpha$. On the invariant hypersurface $\sum_\alpha y_\alpha = 0$ the configuration $y_\alpha \equiv 0$ is stable:
check the Lyapunov property of the function

$$\Lambda(y) = \frac{1}{2\Gamma} \sum_\alpha y_\alpha^2$$

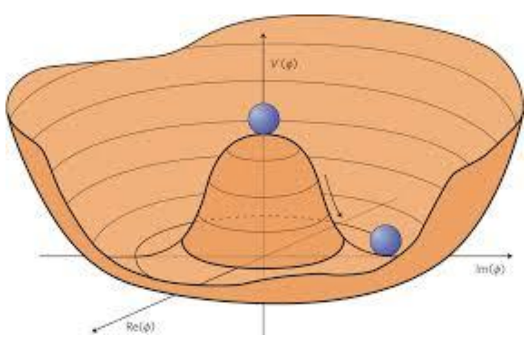
Indeed, $\dot{\Lambda}(y) = -\frac{1}{2} \sum_{\gamma=1}^{N-1} m_\gamma \sum_{\alpha=0}^{N-1} (y_{\alpha+\gamma} - y_\alpha)^2$

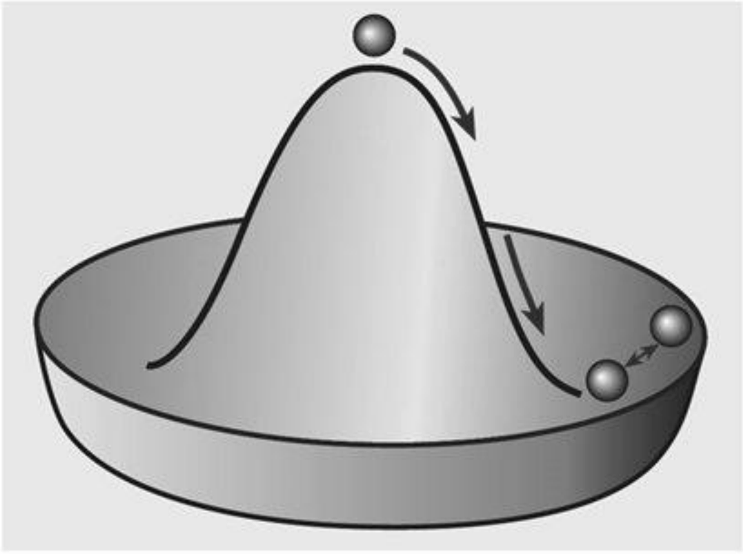
Stabilizing the metastable or even the unstable…

Consider many particles undergoing a Mexican-shape self-potential (2 dim).

Short range attraction to probe

Origin is unstable fixed point for probe





$$\dot{y}_t = F(y_t) - \nabla U_x(y_t) + (2T)^{1/2}\xi_t\,, \qquad \nabla \cdot F = 0$$

We take the potential and driving field

$$U_x(y) = V(|y|) + U_I(|y-x|), \qquad F(y) = \varepsilon |y| \omega(|y|)\, \hat{e}_\varphi$$

$$V(r) = \begin{cases} k_0 e^{-\frac{r^2}{2\sigma_0^2}} & \text{for } 0 \le r \le R \\ 0 & \text{for } r > R \end{cases}$$

$$U_I(r) = -\lambda e^{-\frac{r^2}{2\sigma^2}}$$

$$V(r) = k_0 e^{-\frac{r^2}{2\sigma_0^2}} + k_w e^{r-\sigma_w}$$

or

$$U_I(x,y) = -\lambda \left[1 - \frac{(x-y)^2}{\sigma^2}\right]^2$$

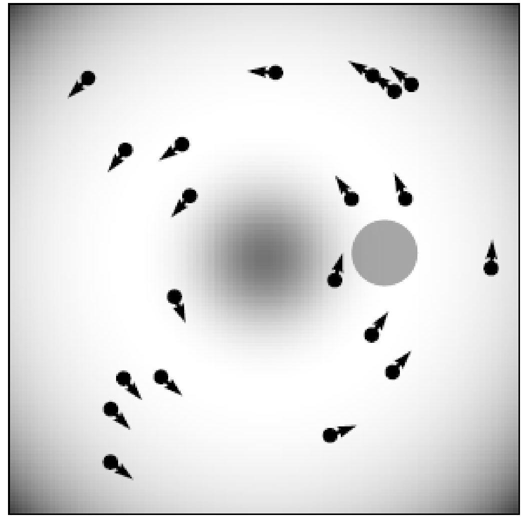
Second result.
$x \in \mathbb{R}^2$, $Y \in \mathbb{R}^2$:

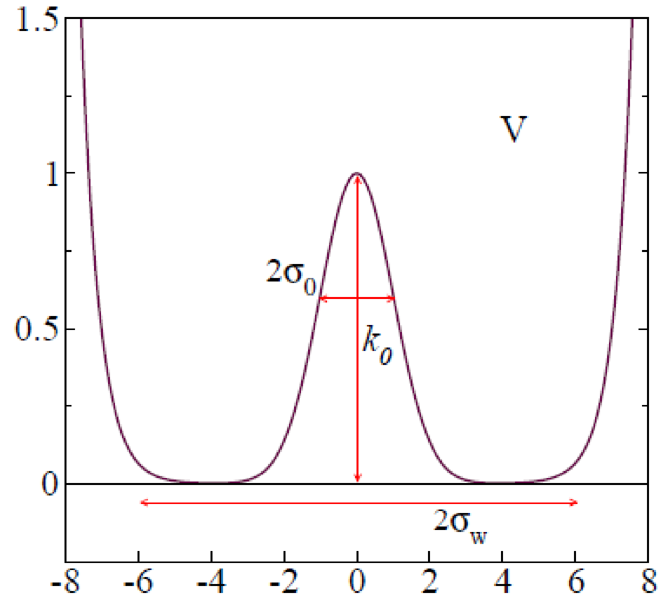
$$0 = \partial_x \left([\varepsilon F(x) + u'(x - Y) + V'(x)] \, \rho(x, Y) \right) + T \, \partial^2_{xx} \rho(x, Y)$$

where F is azimuthal (differenential or rigid rotation), and V is "Mexican."

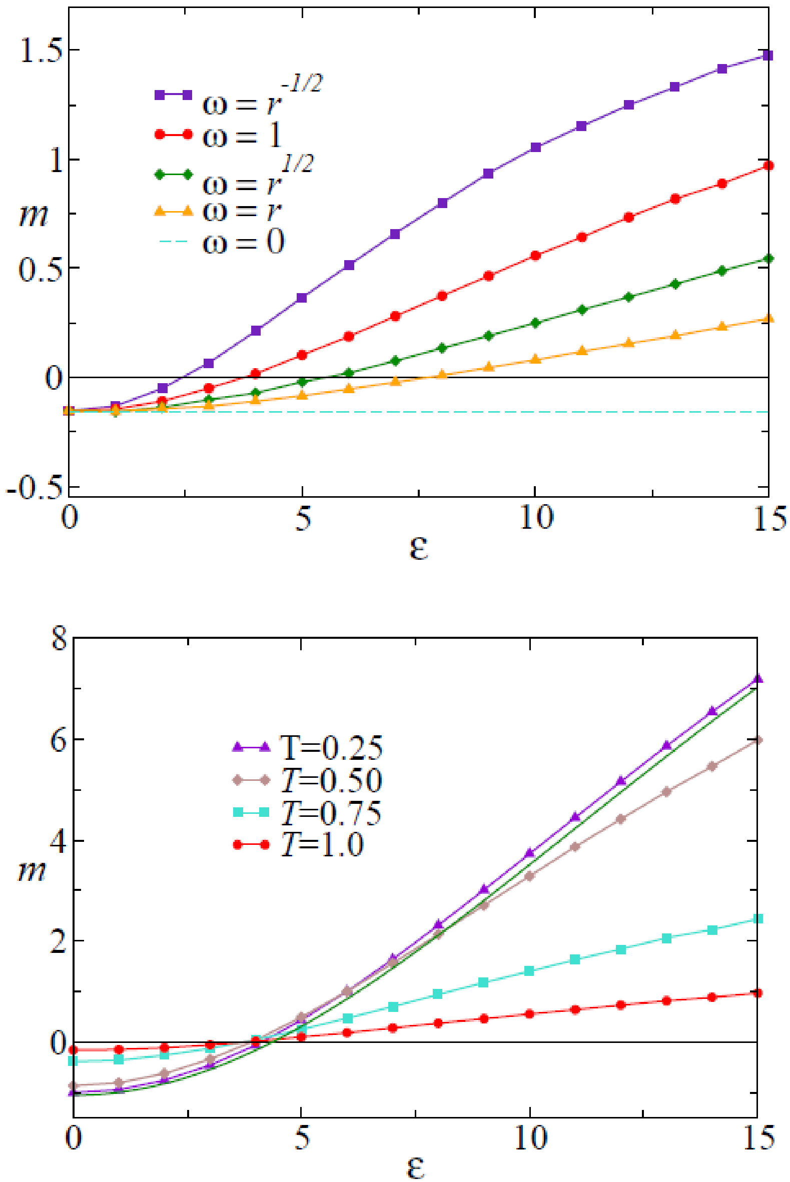
$$f(Y) = \oint dx \, \rho(x, Y) \, u'(x - Y)$$

Result: origin is fixed point and is "linearly stable" whenever $\varepsilon \neq 0$ is large enough.





1.5
1
0.5
0
V
2σ0
k0
2σw
-8
-6
-4
-2
0
2
4
6
8



1.5
1
0.5
0
-0.5
m
$\omega = r^{-1/2}$
$\omega = 1$
$\omega = r^{1/2}$
$\omega = r$
$\omega = 0$
0
5
10
15
ε
8
6
4
2
0
m
T=0.25
T=0.50
T=0.75
T=1.0
0
5
10
15
ε

Shown: stability of origin as fixed point of probe increases with rotation amplitude of medium.

E.g. plot of effective spring constant m, second order effect

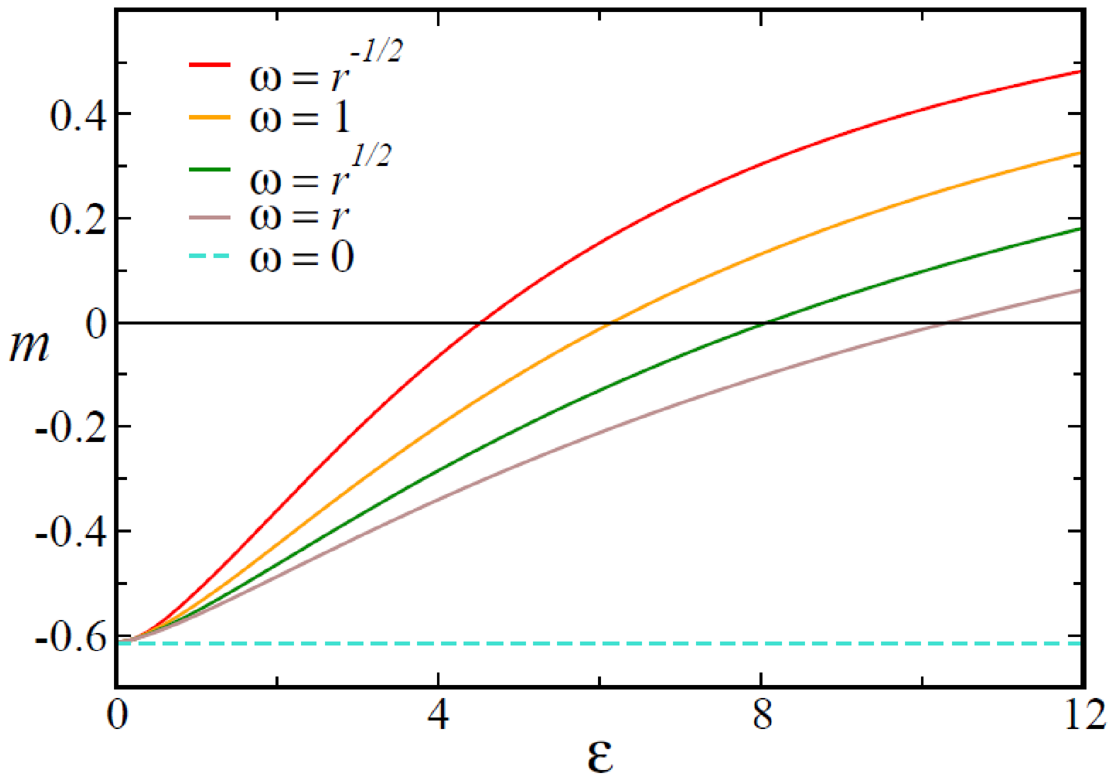


Fig. 1: Stiffness for various rotation profiles as function of the driving ε. Parameters: $T = 1$, $\lambda = 1$, $k_0 = 3/4$, $\sigma = 1/2$, $\sigma_0 = 1$, and $R = 5$.

Q1: Non-Gradient character

Local linear structure: differential stiffness of probe

$$M_{jk}(x) = -\nabla_j f_k(x)$$

Under equilibrium: intrinsic mechanical stiffness diminished by fluctuations in the medium

$$M^{\rm eq}_{jk}(x) = -\beta^{-1}\partial_{jk}\log Z_x = \langle \partial_{jk} U\rangle^x - \beta\,\mathrm{Cov}(\nabla_j U;\nabla_k U)^x$$

With Maxwell symmetries: $M^{\rm eq}_{jk}(x) = M^{\rm eq}_{kj}(x)$

Under contact with nonequilibrium medium: rotational part

$$M^{(a)}_{jk}(x) = \frac{1}{2\beta}\left\langle \nabla_j S\,\nabla_k D - \nabla_k S\,\nabla_j D\right\rangle^x$$

Statistical force: EXPANSION in coupling parameter λ

coupling potential has the form $U_\lambda(x,\eta) = U_0(\eta) + \lambda U_I(x,\eta)$

$$-\nabla_x \Psi_\lambda(x) + f_\lambda^{\mathrm{neq}}(x)$$

with

$$\Psi_\lambda(x) = -\frac{1}{\beta}\log\langle e^{-\beta\lambda U_I}\rangle^0$$

$$f_\lambda^{\mathrm{neq}}(x) = \frac{1}{\beta}\langle (D_\lambda - D_0)\,\nabla_x(S_\lambda - S_0)\rangle^0 + O(\lambda^3)$$

Q3; deriving the Langevin-Smoluchowski dynamics

Force = systematic part + friction + noise

? Systematic force = nature of induced force

? 2nd fluctuation-dissipation theorem in friction/noise relation

? Nature of noise

for a probe in a medium, colloid, Brownian motion,…

$$M'\ddot{Q} + \int_0^{+\infty} \mathrm{d}\tau \, K'_{r'}(\tau)\dot{Q}_{t-\tau} = F_{\mathrm{tot}}(Q_t) + \zeta_t$$

Effective stochastic dynamics

- Christian Maes and Thimothée Thiery, The induced motion of a probe coupled to a bath with random resettings. J. Phys. A: Math. Theor. **50**, 415001 (16pp) (2017) .

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