Diffusions conditioned on occupation measures

Florian Angeletti

NITheP
National Institute for Theoretical Physics

Work in collaboration with Hugo Touchette

15 December 2015

Out-of-equilibrium systems

How to describe out-of-equilibrium systems?

Out-of-equilibrium systems

How to describe out-of-equilibrium systems?

Idea

- Start with an equilibrium system
- Study fluctuations of this system far away from equilibrium

Out-of-equilibrium systems

How to describe out-of-equilibrium systems?

Idea

- Start with an equilibrium system
- Study fluctuations of this system far away from equilibrium

Application

- Start simple
- Markov process
- Diffusion process

Diffusion process

- X_T diffusion process

SDE

$$dX_t = F(X_t)dt + \sigma dW_t$$

Master equation:

$$\partial_t p(x,t) = L^\dagger p(x,t)$$

Generator :

$$L = F \cdot \nabla + \frac{1}{2}\nabla \cdot D\nabla$$

- Stationary state
- Fluctuation around stationary state

Fluctuations far away from equilibrium?

Occupation observable

- Set S
  - $\mathrm{S} = [a, b]$
  - $\mathrm{S} = [a, \infty]$
  - $\mathrm{S} = \{a\}$?
- Occupation rate

$$R_T = \frac{1}{T} \int_0^T \mathbb{1}_S(X_t)\, dt$$

- What happens during a rare fluctuation of $R(t)$?

Occupation observable

- Set S
  - $S = [a, b]$
  - $S = [a, \infty]$
  - $S = \{a\}$?
- Occupation rate

$$R_T = \frac{1}{T}\int_0^T \mathbb{1}_S(X_t)\,dt$$

- What happens during a rare fluctuation of $R(t)$?

Fluctuations far away from equilibrium

- Large deviation function?
- Conditioning?

Occupation observable

- Set S
  - $S = [a, b]$
  - $S = [a, \infty]$
  - $S = \{a\}$?
- Occupation rate

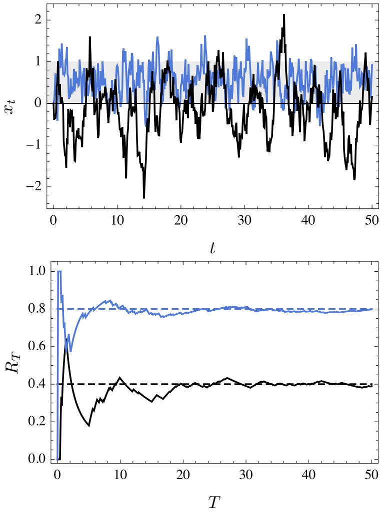
$$R_T = \frac{1}{T} \int_0^T \mathbb{1}_S(X_t)\, dt$$

- What happens during a rare fluctuation of $R(t)$?

Fluctuations far away from equilibrium

- Large deviation function?
- Conditioning?

$S = [0; +\infty]$: softer version of brownian bridge?



x_t
2
1
0
−1
−2
0
10
20
30
40
50
t
R_T
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50
T

Large deviation principle

- R additive observable
- Exponentially decreasing probability

$$P(R_T = r) = e^{-TI(r)+o(T)}$$

- $I(r)$ decay rate: rate function
- Concentration point r_0: $I(r_0) = 0$

Cramer theorem

Scaled cumulant generating function

$$\lambda(k) = \frac{1}{T} \ln \mathbb{E}\left[e^{kTR(X_T)}\right]$$

- Rate function:

$$I(r) = \inf_k \{rk - \lambda(k)\}$$

- Tilted operator:

$$\mathcal{L}_k = L + k\mathbb{1}_S$$

- $\lambda(k)$ maximal eigenvalue of $\mathcal{L}_k$

Conditioned process

$X_t | R_T = r$

- R_T: Non-local observable
- Non homogeneous

Conditioned process

$X_t | R_T = r$

- R_T: Non-local observable
- Non homogeneous

- Strong constraint
- Microcanonical process

Canonical process

- Canonical process C_t
- "generator": $L = \mathcal{L}_k = L + k\mathbb{1}_S$, i.e.

$$\mathbb{E}\left[f_1(C_{t_1})\dots C_{t_n}\right] = \frac{1}{Z(t_n)}\int p_0(x_0)e^{t_1 L}f(x_1)\dots e^{(t_n-t_{n-1})L}f(x_n)dx_0\dots dx_n$$

- Non-homogeneous
- $k = I(r)$: same average as the conditioned process

Driven process Y_T

- Generalized Doubbs transform of C_t:

$$L_k = r_k^{-1}\mathcal{L}_k r_k - r_k^{-1}(\mathcal{L}_k r_k)$$

- r_k maximal eigenvalue of $\mathcal{L}_k$
- homogeneous

Driven process

- Y_t diffusion process with effective force:

$$dY_t = F_k(Y_t)dt + \sigma dW_t$$

- Effective force:

$$F_k(x) = F(x) + D\nabla \ln r_k(x)$$

Process equivalence

$$X_T \asymp C_T \asymp Y_T$$

$$X \asymp y \iff \lim_T \frac{1}{T} \ln \frac{P_X}{P_Y} = 0$$

Spectral problem

How to find $\lambda(k)$ and $r(k)$

$$L_k r_k = \lambda_k r_k$$

Case 1 L_k self-adjoint:

- reversible process with respect to Lebesgue measure
- Quantum mechanics results

Spectral problem

How to find $\lambda(k)$ and $r(k)$

$$L_k r_k = \lambda_k r_k$$

Case 1 L_k self-adjoint:

- reversible process with respect to Lebesgue measure
- Quantum mechanics results

Case 2 L_k is not self-adjoint, real eigenvalues

- if $F = \nabla U$
- reversible with respect to the stationary measure $p = e^{-U}$
- symmetrisation: quantum eigenvalue problems $H\Psi = \lambda\Psi$

Spectral problem

How to find $\lambda(k)$ and $r(k)$

$$L_k r_k = \lambda_k r_k$$

Case 1 L_k self-adjoint:

- reversible process with respect to Lebesgue measure
- Quantum mechanics results

Case 2 L_k is not self-adjoint, real eigenvalues

- if $F = \nabla U$
- reversible with respect to the stationary measure $p = e^{-U}$
- symmetrisation: quantum eigenvalue problems $H\Psi = \lambda\Psi$

Case 3 True out-of-equilibrium system

Ornstein-Uhlenbeck process

$$dX_t = -\gamma X_t dt + \sigma dW_t,$$

- Case 2:

$$U(x) = \frac{\alpha x^2}{2}$$

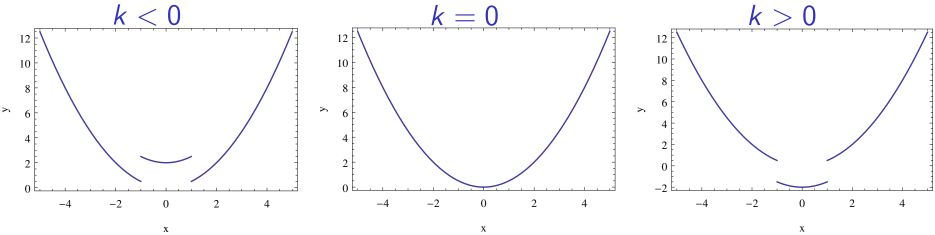
with $\alpha = 2\gamma/D$ and $D = \sigma^2$.

Quantum problem

$$\Psi''(x) - \left(\frac{x^2}{4} + \nu(x)\right)\Psi(x) = 0$$

- Weber equation with piecewise constants
- where
$$\nu(x) = \frac{2}{\alpha D}\left(\lambda - \frac{\alpha D}{4} - k\mathbb{1}_{\sqrt{\alpha}S}(x)\right)$$

Perturbed potential



- $S = [-1, 1]$

Exact solutions

- Solution space spanned by:

$$s_1(\nu,x) = e^{-\frac{x^2}{4}}\,{}_1F_1\left(\frac{\nu}{2}+\frac{1}{4};\frac{1}{2};\frac{x^2}{2}\right)$$

$$s_2(\nu,x) = xe^{-\frac{x^2}{4}}\,{}_1F_1\left(\frac{\nu}{2}+\frac{3}{4};\frac{3}{2};\frac{x^2}{2}\right),$$

where ${}_1F_1\left(a;b;x\right)$ is the confluent hypergeometric function of the first kind.

- Exact solution vanishing at $+\infty$:

$$W(\nu,x) = \frac{1}{2^{\frac{\nu}{2}+\frac{1}{4}}\sqrt{\pi}}\left[\cos\left(\tfrac{\nu}{2}\pi+\tfrac{\pi}{4}\right)\Gamma\left(\tfrac{1}{4}-\tfrac{\nu}{2}\right)s_1(\nu,x)\right.$$
$$\left.-\sqrt{2}\sin\left(\tfrac{\nu}{2}\pi+\tfrac{\pi}{4}\right)\Gamma\left(\tfrac{3}{4}-\tfrac{\nu}{2}\right)s_2(\nu,x)\right].$$

Piecewise solution on interval

$S = [a, b]$

$$\Psi(x) = \begin{cases} K_1 W(\nu', -x) & x < a \\ K_2 s_1(\nu, x) + K_3 s_2(\nu, x) & a < x < b \\ K_4 W(\nu', x) & b < x, \end{cases}$$

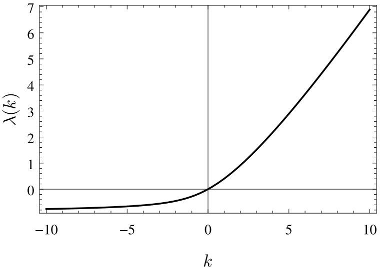
with $\nu' = \nu(S^c)$ and $\nu = \nu(S)$

Continuity condition

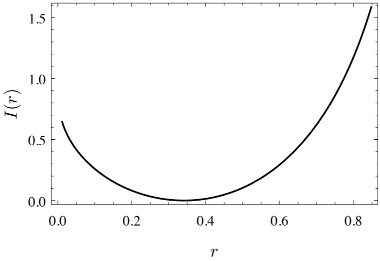
$$\det \begin{pmatrix} -W(\nu', -a) & s_1(\nu, a) & s_2(\nu, a) & 0 \\ \partial_x W(\nu', -a) & \partial_x s_1(\nu, a) & \partial_x s_2(\nu, a) & 0 \\ 0 & s_1(\nu, b) & s_2(\nu, b) & -W(\nu', b) \\ 0 & \partial_x s_1(\nu, b) & \partial_x s_2(\nu, b) & -\partial_x W(\nu', b) \end{pmatrix} = 0$$

Rate functions

$\lambda(k)$



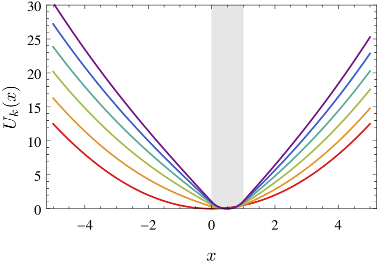
Rate function $I(k)$



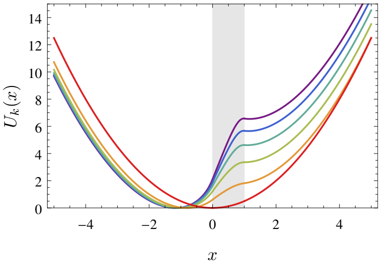
- $S = [0, 1]$
- Parameters: $\alpha = \sigma = 1$

Effective potential

Effective potential $U_k(x)$ for $S = [0, 1]$

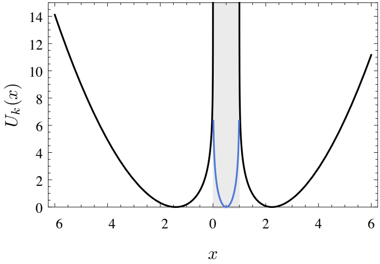


- $k = \{0; 2; 4; ..; 10\}$



- $k = \{0; -2; -4; ..; -10\}$

Asymptotic effective potential



Black: Effective potential $U_{-\infty}(x)$ preventing any occupation in $S = [0, 1]$

Blue: Effective potential $U_{\infty}(x)$ forcing a total occupation in $S = [0, 1]$

arameters: $\alpha = \sigma = 1$

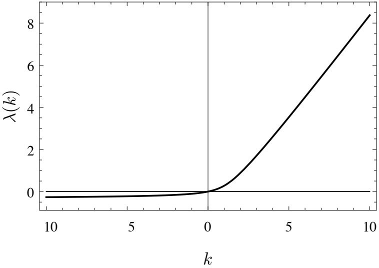
Half-line

$$S = [a, +\infty)$$

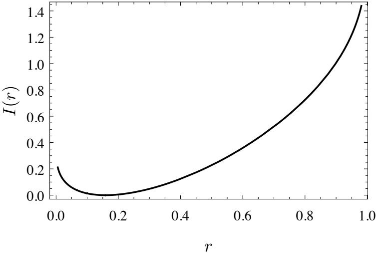
$$\Psi(x) = \begin{cases} K_1 W(\nu', -x) & x < a \\ K_2 W(\nu, x) & x > a \end{cases}$$

Rate function

$\lambda(k)$

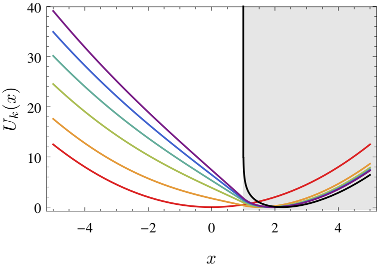


Rate function $I(k)$

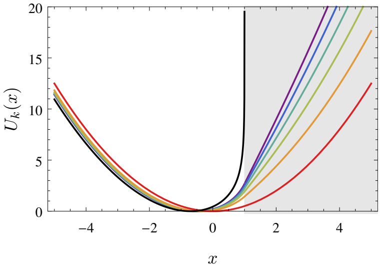


- $S = [1, \infty)$
- $\alpha = \sigma = 1.$

Effective potential



- $k = 0 : 2 : 10$



- $k = 0 : 2 : 10$

Black : asymptotic effective potential $U_{\pm\infty}(x)$

- $S = [1, \infty)$
- $\alpha = \sigma = 1.$

Punctual occupation

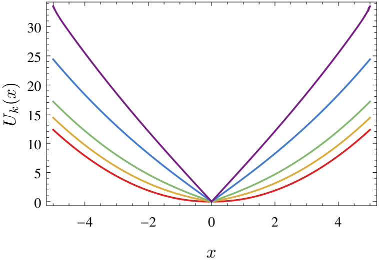
$$S = \{a\} = \lim_{\epsilon \to 0} \{a + \epsilon, a - \epsilon\}$$

$$\Psi(x) = \begin{cases} K_1 W(\nu', -x) & x < a \\ K_2 W(\nu', x) & x > a \end{cases}$$

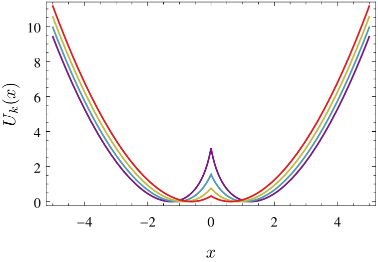
Continuity conditions

$$K_1 W(\nu, -a) - K_2 W(\nu, a) = 0$$
$$K_1 \partial_x W(\nu, -a) + K_2 \partial_x W(\nu, a) = k\Psi(a).$$

Effective potential



- $k = 0, 1.01, 2.02, 4.04, 6.06$



- $k = -1.01, -2.02, -4.04, -10.1$

- $\alpha = \sigma = 1$

Perturbative methods

- Rewrite the hamiltonian $\mathcal{H}_k$ as a perturbed hamiltonian

$$\mathcal{H}_{k+\Delta k} = \mathcal{H}_k + \Delta k \, \mathbb{1}_S$$

- First order approximation for eigenvalues:

$$\partial_k \lambda_n(k) = \langle \Psi_n(k) | \mathbb{1}_S | \Psi_n(k) \rangle$$

- Eigenvectors:

$$\partial_k \Psi_n(k) = \sum_{m \neq n} \frac{\langle \Psi_m(k) | \mathbb{1}_S | \Psi_n(k) \rangle}{\lambda_m(k) - \lambda_n(k)} \Psi_m(k).$$

Orthogonality matrix

$$N_{i,j}(k) = \langle \Psi_i(k) | \mathbb{1}_S | \Psi_j(k) \rangle$$

$$\partial_k \lambda_n(k) = N_{n,n}$$

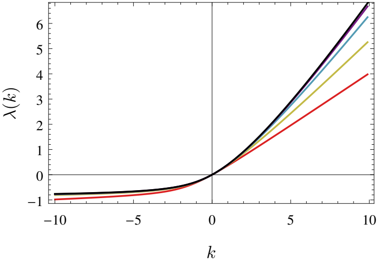
$$\partial_k N_{i,j}(k) = \sum_{m \neq i} \frac{N_{i,m}(k) N_{m,j}(k)}{\lambda_i(k) - \lambda_m(k)} + \sum_{m \neq j} \frac{N_{j,m}(k) N_{m,i}(k)}{\lambda_j(k) - \lambda_m(k)},$$

Methods: Truncate higher eigenvalues terms and use a numerical solvers

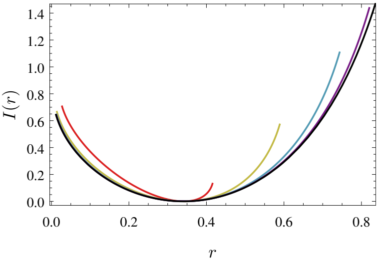
Rate function

- $S = [0, 1]$

$\lambda(k)$



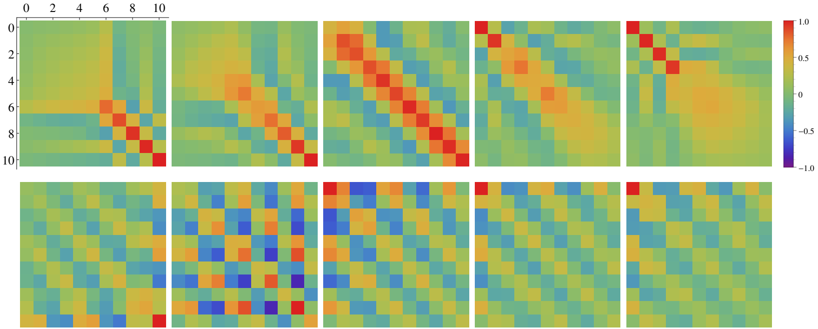
RatefunctionI(k)



Black: exact function

- number of modes $M = 2, 5, 10, 20$
- $\alpha = \sigma = 1$

Orthogonality matrix evolution



- $k = -10, -5, 0, 5, 10$

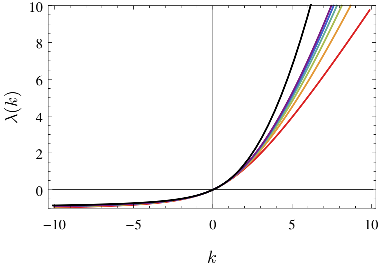
Top: $S = [1, \infty)$

Bottom: $S = [0, 1]$

- $M = 10,\ \alpha = \sigma = 1$

Failures

$\lambda(k)$ for point occupation at $x = 0$



Black: exact $\lambda(k)$

- $M = 20, 40, 60, 80, 100, 120$
- $\alpha = \sigma = 1$

Perspectives

- Beyond dimension 1
- Adaptative numerical method for the spectral problem
- Perturbing out-of-equilibrium well-known statistical physics system

Questions?