NONEQUILIBRIUM RESPONSE -III

RECAP

- General response formula in Nonequilibrium from dynamical ensembles
- Decomposition according to time-reversal symmetry
- Consistent with Kubo and Green-Kubo around equilibrium
- Examples: Jump processes
- Random walk and boundary/bulk driven SEP

DIFFUSION PROCESSES

- Single particle/ many particles diffusing in potential
- Time evolution governed by Langevin equation: overdamped/ underdamped
- Response to external force
- General formalism remains same
- How to compute the path probability? Action?

OVERDAMPED DIFFUSION

- Single particle in a thermal bath of temperature T
- Nonconservative force field : out of equilibrium
- Overdamped regime $$\dot{x} = \mu[f(x) + \varepsilon h_s \nabla V(x)] + \sqrt{2\mu T}\,\eta_t$$

Nonconservative force (d>1)

Perturbation

- Discretise the trajectory to write the probability

$$\omega = \{x_s; 0 \leq s \leq t\} := \{x_{i\Delta t}\}_{i=0}^{N}$$ With $t = N\Delta t$

- Path-weight $P(\omega) = \lim_{N\to\infty} \prod_{i=0}^{N} P_{\Delta t}(x_i | x_{i-1})$ (Markov)

- Discretize Langevin equation:

$$\Delta x = \mu F(x)\Delta t + \sqrt{2D\Delta t}\ \xi$$

Where

$F(x) = f(x) + \varepsilon h_t \nabla V(x)$

$$D = \mu T$$

- Gaussian variable ξ from $N(0,1)$: $P(\xi) \propto \exp[-\xi^2/2]$

$$P_{\Delta t}(\Delta x_i) \propto \exp\left[-\frac{\Delta t}{4D}\left(\frac{\Delta x_i}{\Delta t} - \mu F(x_i)\right)^2\right]$$

- Multiply and $\Delta t \to 0$

$$P(\omega) \propto \exp\left[-\frac{1}{4D}\int_0^t ds\ \left(\dot{x}_s - \mu F(x_s)\right)^2\right]$$

Trajectory weight for an overdamped particle moving under force F(x)

- Reference process: pure diffusion

$$P_0(\omega) \propto \exp\left[-\frac{1}{4D} \int_0^t ds\ \dot{x}_s^2 \right]$$

- Action from the ratio

$F(x) = f(x) + \varepsilon h_t \nabla V(x)$

$$A_\varepsilon(\omega) = -\log \frac{P(\omega)}{P_0(\omega)} = -\frac{\beta}{2} \int_0^t dx_s\ F(x_s) + \frac{\beta\mu}{4} \int_0^t ds\ F(x_s)^2$$

- Response : excess wrt ε (around $\varepsilon = 0$)

Stochastic integrals

$$\boxed{A_0'(\omega) = -\frac{\beta}{2} \int_0^t dx_s\ h_s \nabla V(x_s) + \frac{\beta\mu}{2} \int_0^t ds\ h_s\ f(x_s) \nabla V(x_s)}$$

- Identify entropy and frenesy
- Time-reversal: protocol h_s also to be reversed $\theta h_s = h_{t-s}$

$$A_0'(\omega) = -\frac{\beta}{2}\int_0^t dx_s\ h_s \nabla V(x_s) + \frac{\beta\mu}{2}\int_0^t ds\ h_s\ f(x_s)\nabla V(x_s)$$

Not well defined symmetry

Symmetric

- Recast in terms of Stratonovich integral

Calculate explicitly

$$\int_0^t dx_s\ h_s \nabla V(x_s) = \int_0^t dx_s \circ h_s \nabla V(x_s) - D\int_0^t ds\ h_s \nabla^2 V(x_s)$$

Anti-symmetric

Symmetric

- Excess entropy

$$S_0' = \beta \int_0^t dx_s \circ h_s \nabla V(x_s)$$

$$= \beta \left[V(x_t) h_t - V(x_0) h_0 - \int_0^t ds \; \dot{h}_s V(x_s) \right]$$

Work done by the perturbing force along the trajectory

Same as Kubo

- Excess frenesy

$$D_0' = \frac{\beta}{2} \int_0^t ds \; h_s \; [D \nabla^2 V(x_s) + \mu f(x_s) \nabla V(x_s)]$$

- Depends on diffusion constant and μ: medium dependent

- Equilibrium response can be obtained by just knowing the perturbation protocol
- In nonequilibrium medium property enters through frenesy
- Same perturbation in different medium results in different response

ACTIVE RUN-AND-TUMBLE PARTICLE (RTP)

- Overdamped particle with an internal `orientation' $\sigma = \pm 1$

- Flips with rate α

$$\dot{x} = v_0 \sigma_t + \sqrt{2T}\, \eta_t + \varepsilon \quad \text{and } \sigma \overset{\alpha}{\leftrightarrow} -\sigma$$

Perturbation

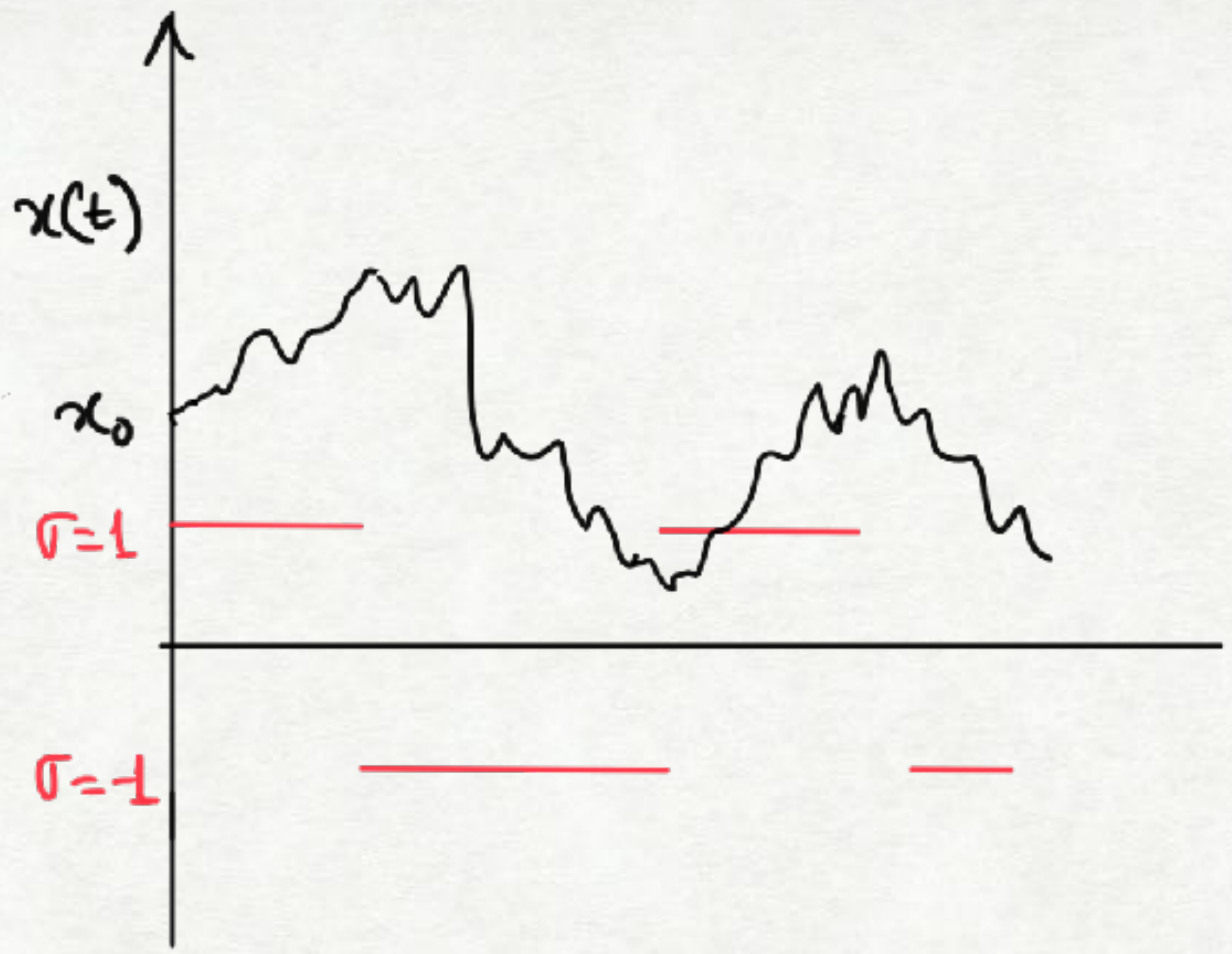
- Two sources of stochasticity: σ and η

- White noise $\langle \eta_t \rangle = 0, \ \ \langle \eta_t \eta_{t'} \rangle = \delta(t - t')$

- Dichotomous noise (memory) $\langle \sigma_t \rangle = 0, \ \ \langle \sigma_t \sigma_{t'} \rangle = \exp[-2\alpha \,|\, t - t' \,|\,]$: coloured

- Position: non-Markov evolution

TRAJECTORY



- Trajectory $\omega = \{x_s, \sigma_s; 0 \leq s \leq t\}$
- Joint $x - \sigma$ process is Markov
- σ evolution independent of position
- Weight $P(\omega) = P(\{x_s\} \mid \{\sigma_s\}) P(\{\sigma_s\})$
- σ trajectory: 2 state jump process –> $\{(\sigma_0, t_0), (\sigma_1, t_1), \ldots (\sigma_n, t_n)\}$
- $P(\{\sigma_s\}) \propto \rho(\sigma_0)\, e^{-\alpha \sum t_i} \alpha^n$

With $\rho(\sigma_0) = \dfrac{1}{2}$

P denotes probability generically, not the specific function

- Position trajectory weight- piecewise:

$$P(\{x_s\} \mid \{\sigma_s\}) = \prod_{i=0}^{n} P(\{x_s; 0 \le s \le t_i\} \mid \sigma_i)$$

- Each segment evolves following an overdamped equation

$$P(\{x_s; 0 \le s \le t_i\} \mid \sigma_i) \propto \exp\left[-\frac{1}{4T}\int_0^{t_i} ds\ (\dot{x}_s - v_0\sigma_i + \varepsilon)^2\right]$$

- Full trajectory probability

$$P_\varepsilon(\omega) \propto \alpha^n e^{-\alpha t} \exp\left[-\frac{1}{4T}\int_0^{t} ds\ (\dot{x}_s - v_0\sigma_s + \varepsilon)^2\right]$$

- Reference process: $\varepsilon = 0$
- Weight

$$P_0(\omega) \propto \alpha^n e^{-\alpha t} \exp\left[-\frac{1}{4T}\int_0^t ds\ (\dot{x}_s - v_0\sigma_s)^2\right]$$

- Action

$$A_\varepsilon(\omega) = \frac{1}{4T}\int_0^t ds\ [\varepsilon^2 + \varepsilon(\dot{x} - v_0\sigma_s)]$$

- Excess action (around $\varepsilon = 0$)

$$A_0'(\omega) = \frac{1}{2T}\int_0^t ds\ (\dot{x} - v_0\sigma_s) = \frac{1}{2T}\left[x_t - x_0 - v_0\int_0^t ds\ \sigma_s\right]$$

DECOMPOSITION

- Identify time-symmetric and anti-symmetric components

$$A_0'(\omega) = \frac{1}{2T}\left[x_t - x_0 - v_0 \int_0^t ds\ \sigma_s\right]$$

Anti-symmetric

- Second term: depends on time-reversal behaviour of σ
- Symmetric if $\sigma_{t-s} = \sigma_s$, anti-symmetric if $\sigma_{t-s} = -\sigma_s$ (like velocity)

Generalized reversible

- If $\sigma_{t-s} = \sigma_s$
- Excess entropy $$S'(\omega) = \frac{1}{T}(x_0 - x_t)$$
- Excess freneasy $$D'(\omega) = -\frac{v_0}{2T}\int_0^t ds\ \sigma_s$$
- If $\sigma_{t-s} = -\sigma_s$
- Whole action is anti-symmetric $$S_0'(\omega) = -\frac{1}{T}\left[x_t - x_0 - v_0\int_0^t ds\ \sigma_s\right]$$
- No excess frenesy $D'(\omega) = 0$

- Response of displacement (same irrespective of choice)

$$\langle (x_t - x_0) \rangle_\varepsilon = \varepsilon \Big[\frac{1}{2T} \langle (x_t - x_0)^2 \rangle_0 - \frac{v_0}{2T} \int_0^t \langle \sigma_s (x_t - x_0) \rangle_0 \Big]$$

- Can be verified explicitly
- Equilibrium limit : $v_0 = 0$
- Physical interpretation: response entropic if σ reverses sign under time-reversal
- Also generalised reversible then…

VIOLATION OF EINSTEN-SUTHERLAND RELATION

$$\dot{x} = v_0\sigma_t + \sqrt{2T}\,\eta_t + \varepsilon$$

- Mobility and diffusion are related in equilibrium $\mathscr{D} = \mu T$
- For RTP, mobility $\mu = \lim_{t\to\infty} \frac{1}{\varepsilon t}\langle (x_t - x_0)\rangle_\varepsilon = 1$
- Diffusion $\mathscr{D} = \lim_{t\to\infty} \frac{1}{2t}\langle (x_t - x_0)^2\rangle_0 = T + \frac{v_0^2}{2\alpha} > \mu T$
- Diffusion even when no temperature
- Additive violation of Einstein relation

EFFECTIVE TEMPERATURE

- Enforce Kubo-formula with a modified prefactor
- Example: RTP $\mathscr{D} = \mu T_{eff}$ with $T_{eff} = T + \dfrac{v_0^2}{2\alpha}$
- Strategy: Incorporate the deviation from Kubo-formula via effective temperature
- Does the same temperature work for all observable?

- Recast the Nonequilibrium response formula (around $\varepsilon = 0$):

$$
\begin{aligned}
\frac{1}{\varepsilon}[\langle O(t)\rangle_\varepsilon - \langle O(t)\rangle_0] &= \frac{1}{2}\langle S_0' O(t)\rangle_0 - \langle D_0' O(t)\rangle_0 \\
&= \langle S_0' O(t)\rangle_0 - \left\langle [D_0' + \frac{1}{2} S_0'] O(t) \right\rangle_0 \\
&= \langle S_0' O(t)\rangle_0 \left[1 - \frac{\left\langle [D_0' + \frac{1}{2} S_0'] O(t) \right\rangle_0}{\langle S_0' O(t)\rangle_0}\right] \\
&= \beta \left[1 - \frac{\left\langle [D_0' + \frac{1}{2} S_0'] O(t) \right\rangle_0}{\langle S_0' O(t)\rangle_0}\right] \int_0^t ds\ h_s \frac{d}{ds}\langle V(s) O(t)\rangle_0
\end{aligned}
$$

Effective temperature

$$
= \beta_{eff}\chi_{\text{Kubo}}
$$

- Generally time-dependent : late time limit is often taken
- Multiplicative correction instead of additive
- Obviously depends on the observable
- Successful in certain scenarios

Ref: Cugliandolo, J Phys A 2011