Diffusion Dynamics with Linear Drift Force

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I. Introduction

$$\frac{\partial P}{\partial t} = \nabla\cdot(-f + D\cdot\nabla)P(q,t) \qquad q, f \in R^n \quad \Leftrightarrow \quad \dot{q}(t) = f(q,t) + \xi(t)$$

f : drift force, rate function, force in over-damping limit

D : diffusion matrix $\quad \langle \xi_i(t)\xi_j(t')\rangle = 2D_{ij}\delta(t-t')$

Equilibrium: steady state with detailed balance

$$P_{st} \propto e^{-\Phi_{st}}, \quad f = -D\cdot\nabla\Phi_{st}$$

$$\Rightarrow \begin{cases} j_{st} = (f - D\cdot\nabla)P_{st} = 0 \\ P(q'|\,q)e^{-\Phi_{st}(q)} = P(q\,|\,q')e^{-\Phi_{st}(q')} \end{cases}$$

zero steady state current
detailed balance (DB)

Non-equilibrium $\quad D^{-1}\cdot f = -\nabla\Phi + g, \quad g:$ non-conservative

$$\Rightarrow \quad j_{st} \neq 0$$

breaking of detailed balance

$D^{-1}\cdot f$:(generalized) force $\qquad g$: NEQ-drving force

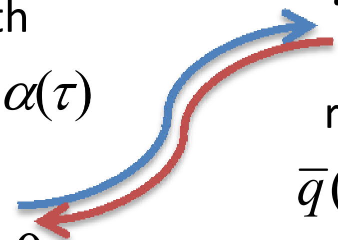
(i) non-conservative force
(ii) non-identical and correlated noise $\quad D \neq cI$
(iii) time-dependent parameter $\quad \Phi(q, \alpha(t))$

I. Introduction

path

$q(\tau),\ \alpha(\tau)$

$\tau = t$



$\tau = 0$

reversed path

$\bar{q}(\tau) = q(t-\tau)$

$\bar{\alpha}(\tau) = \alpha(t-\tau)$

For Brownian dynamics, $q = (x, p)$

$\bar{x}(\tau) = x(t-\tau)$

$\bar{p}(\tau) = -p(t-\tau)$

$\bar{\alpha}(\tau) = \alpha(t-\tau)$

Conditional probability $\Pi[q;\alpha]$ for path q vs $\Pi[q;\alpha]$ for reversed path $\bar{q}$

$$\frac{\Pi[q]}{\Pi[\bar{q}]} = \exp\left(\int_0^t d\tau\ \dot{q}^T \cdot D^{-1} \cdot f\right)$$

$$= \exp\left(-\int_0^t d\tau\, \dot{q}^T \cdot (\nabla\Phi - g)\right)$$

$$\Pi[q]/\Pi[\bar{q}] = e^{-\Delta\Phi} \text{ (DB)}$$

$$= \exp\left(-\int_0^t d\tau\left(\frac{d\Phi}{dt} - \dot{q}^T \cdot g - \frac{\partial\Phi}{\partial t}\right)\right)$$

Potential (Energy) $\Phi(q,\alpha)$

$$= \exp(-\Delta\Phi + W)$$

Work production $W = \int_0^t d\tau\left(\dot{q}^T \cdot g + \frac{\partial\Phi}{\partial t}\right)$

$$= \exp(-Q)$$

Heat production: $\Delta\Phi = W + Q$ 1st law

Inverse temperature : $D \to \beta^{-1} D$, measure for overall strength of noise

II. Linear Drift Force

Linear drift force:
- almost exactly solvable case
- showing all natures of non-equilibrium

$$f = -F \cdot q \qquad D^{-1} \cdot f = -(D^{-1}F) \cdot q$$

Symmetric + asymmetric

$$D^{-1}F = G^s + G^a$$

Equilibrium

$$G^a = 0, \qquad \Phi_{st} = -\frac{1}{2} q^T \cdot D^{-1} F \cdot q$$

$$D^{-1}F = F^T D^{-1} \Rightarrow FD - DF^T = 0$$ condition for DB

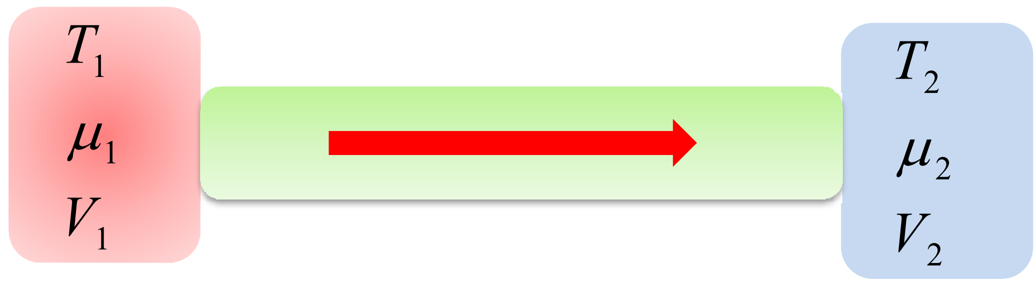
Non-equilibrium

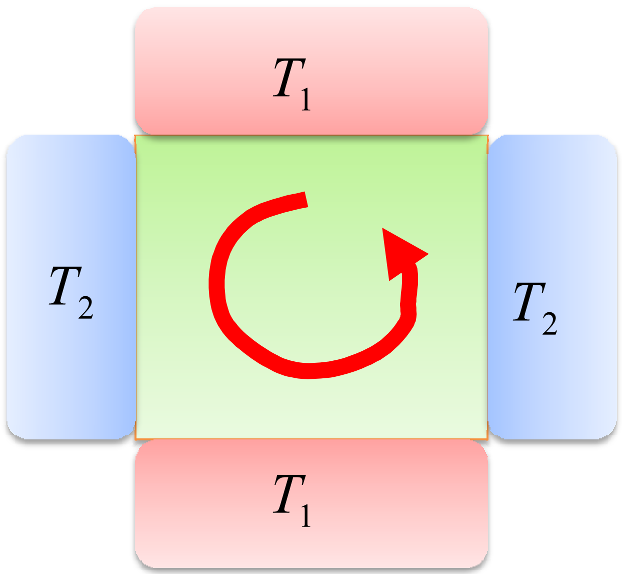
Steady state (Kwon-Ao-Thouless, PNAS, 2005)

$$\Phi_{st} = -\frac{1}{2} q^T \cdot (D+Q)^{-1} F \cdot q, \qquad Q:$$ anti-symmetric matrix

$$FQ + QF^T = FD - DF^T$$ breaking of DB

$$J_{st} \propto -Q \cdot \nabla \Phi_{st} e^{-\Phi_{st}}$$ circulation current around equi-probability surface





$$D \propto \begin{pmatrix} T_1 & 0 \\ 0 & T_2 \end{pmatrix} \xrightarrow{\text{coord transf}} \begin{pmatrix} d_1 & c \\ c & d_2 \end{pmatrix}$$

f : non-conservative $\rightarrow F \neq F^T$

$$FD \neq F^T D$$ NEQ

$$FQ + QF = FD - DF^T$$ anit-symm matrix

$$J \propto -Q \cdot \nabla\Phi \, e^{-\Phi}$$ circulation

II. Linear Drift Force

Non-equilibrium

$$G = D^{-1}F = G^{s} + G^{a}$$

$$G^{s} = \frac{1}{2}\left(D^{-1}F + F^{T}D^{-1}\right) + \delta G^{s}, \quad G^{a} = \frac{1}{2}\left(D^{-1}F - F^{T}D^{-1}\right) - \delta G^{s}$$

Energy : $\Phi = \frac{1}{2} q^{T} \cdot G^{s} \cdot q$

NEQ-drving force : $g = -G^{a} \cdot q$

Non-equilibrium work production

$$W[q] = -\int_0^t d\tau \; \dot{q} \cdot G^{a} \cdot q \qquad (\dot{\alpha} = 0, \;\; \partial\Phi / \partial t = 0)$$

Need to find

$$P(q,t) = \int dq_0 P(q,t : q_0, t = 0) P_{in}(q_0)$$

$$P_{in}(q_0) = |\det(2\pi (G^{s})^{-1})|^{-1/2} \; e^{-q^{T} \cdot G^{s} \cdot q / 2}$$ Initial equilibrium pdf

III. Path Integral Formalism

Generating functional

$$Z[q(t);l;\lambda] = \int D[q]\exp\left(S[q] - \lambda W[q] + \int_0^t d\tau\, l(\tau)^T \cdot q(\tau) \right)$$

Action

$$S[q] = -\frac{1}{4}\int_0^t d\tau\, (q + Fq)^T \cdot D^{-1} \cdot (q + Fq)$$

Probability

$$P(q;t) = Z[q; l = 0; \lambda = 0] = |\det(2\pi A^{-1}(t))|^{-1/2}\, e^{-1/2 q^T \cdot A(t) \cdot q}$$

Expectation value

$$\langle F[q] \rangle = F\left[\frac{\delta}{\delta l}\right] \hat{Z}[l] \Big|_{l \to 0}$$

exactly solvable

$$\hat{Z}[l] = \int dq(t) Z[q(t); l; \lambda = 0] = \exp\left(\frac{1}{2} \iint d\tau d\tau'\, l(\tau)^T \cdot \Gamma(\tau, \tau') \cdot l(\tau') \right)$$

III. Path Integral Formalism

Probability distribution function for work production

$$P[W] = \int \frac{d\lambda}{2\pi} e^{iW\lambda + \ln \varsigma(i\lambda)}$$

Only solvable Perturbatively in λ

$$\varsigma(\lambda) = \left\langle e^{-\lambda W} \right\rangle = \int dq(t) Z[q(t); l = 0; \lambda] = \exp\left(-\frac{1}{2} \int_0^t d\tau \, \mathrm{Tr} A^{-1}(\tau; \lambda) \Lambda(\lambda) \right)$$

with

$$\Lambda(\lambda) = \frac{1}{2}\left(F^T D^{-1} F - \widetilde{F}^T D^{-1} \widetilde{F} \right), \quad \widetilde{F} = F - 2\lambda G^a$$

III. Path Integral Formalism

Discretization $q(0) = q_0, q_1, \ldots, q_{N-1}, q_N = q(t) \qquad \Delta t = t/N$

Path integral -> Gaussian integrals over $\{q_i\}$

$$A^{-1}(t) = F^{-1}\left(D+Q-e^{-Ft}(D+Q)e^{-F^T t}\right)+e^{-Ft}A^{-1}(0)e^{-F^T t} \Rightarrow P(q,t) \propto e^{-1/2\, q^T \cdot A(t) \cdot q}$$

$$\xrightarrow[t\to\infty]{} F^{-1}(D+Q)$$

Steady state (Kwon-Ao-Thouless,PNAS, 2005)

$$\left\langle q(t)^T \cdot q(t')\right\rangle = \Gamma(t,t') = \begin{cases} e^{-F(t-t')}A^{-1}(t'), & t > t' \\ A^{-1}(t')e^{-F^T(t'-t)}, & t' > t \end{cases}$$

$$\Phi_{st} = \frac{1}{2} q^T \cdot (D+Q)^{-1} F \cdot q$$

Expectation value of work production

$$\left\langle W\right\rangle = -\int_0^t d\tau \,\mathrm{Tr} A^{-1}(\tau) G^a F \xrightarrow[t\to\infty]{} -t\mathrm{Tr} FQD^{-1} > 0$$

Entropy production rate

$$\left\langle \Delta\Phi\right\rangle = \left\langle W\right\rangle + \left\langle Q\right\rangle \xrightarrow[t\to\infty]{} \left\langle W\right\rangle \approx -\left\langle Q\right\rangle = t\left\langle \sigma\right\rangle$$

$$\Delta S_{tot} = \Delta S_{sys} + \Delta S_{res}, \quad \Delta S_{sys} = -\Delta \ln P \to \text{finite}, \quad \Delta S_{res} = -Q \approx W$$

$$\left\langle \sigma\right\rangle = -\mathrm{Tr} FQD^{-1}$$

rate of entropy piled up in the reservoir,
approximate total entropy production rate

IV. Example

Diffusion in 2 dimensions

$$q^T = (x, y)$$

$$F = \begin{pmatrix} k_1 & \kappa_1 \\ \kappa_2 & k_2 \end{pmatrix} \qquad D = \begin{pmatrix} \alpha & \varepsilon \\ \varepsilon & \gamma \end{pmatrix}$$

$$FQ + QF^T = FD - DF^T$$

$$\Rightarrow Q = \frac{\hat{q}}{k_1 + k_2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad \hat{q} = \varepsilon(k_1 - k_2) + \gamma\kappa_1 - \alpha\kappa_2$$

$t \to \infty$ limit

$$\langle \sigma \rangle = t^{-1}\langle W \rangle = \frac{\hat{q}^2}{\det D \cdot \mathrm{Tr}\, F} > 0$$

2nd law of thermodynamics
Valid for general stochastic process

$$\langle \sigma^2 \rangle_c = t^{-2}\langle W^2 \rangle = t^{-1}\frac{\left(2\det F + (\mathrm{Tr}\, F)^2\right)\hat{q}^2}{2\det D \cdot \det A \cdot \mathrm{Tr}\, \mathrm{F}}$$

$$\langle W^n \rangle_c \propto t, \quad \langle \sigma^n \rangle_c \propto t^{-n+1}$$

V. Summary and Future

1. Non-equilibrium is caused by
   (i) non-identical/correlated noise $D \neq cI$
   (ii) non-conservative force $f \neq -\nabla V$
   $\Rightarrow \quad D^{-1} \cdot f \neq -\nabla \Phi$

2. FT can be applied for general stochastic systems.

$$D^{-1} \cdot f = -\nabla \Phi + g$$

force $D^{-1} \cdot f$ non-conservative force g

energy Φ work $W = \int_0^t d\tau \, \dot{q} \cdot g$ heat $\Delta \Phi - W$

3. Linear drift force as an analytically solvable case

$$f = -F \cdot q \Rightarrow \quad D^{-1} \cdot F = G^s + G^a$$

$$\Phi = q^T \cdot G^s \cdot q / 2, \quad \dot{W} = -\dot{q}^T \cdot G^a \cdot q$$

$$t^{-1} \langle W \rangle \xrightarrow[t \to \infty]{} \langle \sigma \rangle > 0, \quad t^{-2} \langle \mathrm{W}^2 \rangle_c \xrightarrow[t \to \infty]{} \langle \sigma^2 \rangle_c \sim O(t^{-1})$$

V. Summary and Future

4. Future interests

4.1 Modification of FT in the presence of irreversible force

$$\dot{p} = -\gamma \cdot p/m + f(x,t) + g(x,p) + \xi, \quad g(\bar{x},\bar{p}) = -g(x,p)$$

- Irreversible force might be unavoidable in impure materials
- Simple case in 1-dim: temperature-cooling (Kim and Qian, PRL,2004;PRE, 2007)

$$g(x,p) = -\alpha \cdot p/m \;\Rightarrow\; \gamma^{\text{eff}} = \gamma + \alpha, \quad \beta^{\text{eff}} = (1+\alpha/\gamma)\beta$$

- In high dimensions with α : matrix for anisotropic media
  - no simple temperature-cooling
  - non-Maxwell distribution for velocity
  - modification of FT

4.2 Simulation study for discrete variables such as Ising spins with updating rule

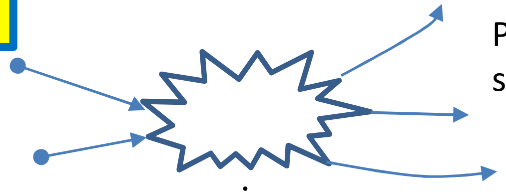
$$\frac{\Pi(A \to B)}{\Pi(B \to A)} = e^{-\beta \Delta Q}$$

ΔQ: Heat production for transition $A \to B$

V. Future Topics

4.3 Neural network with asymmetric synaptic coupling

$$\sigma_i = \mathrm{sgn}\Big(\sum_j J_{ij}\sigma_j - h_i\Big) \quad \text{for} \quad J_{ij} \neq J_{ji}$$



$$J_{ij}^s = 1/2(J_{ij} + J_{ji}) \;\Rightarrow\; H = -\sum_{(i,j)} J_{ij}^s \sigma_i \sigma_j$$

$$J_{ij}^a = 1/2(J_{ij} - J_{ji}) \;\Rightarrow\; \Delta W = \sum_{i,j} J_{ij}^a (\Delta\sigma_i)\sigma_j$$

cf
$$\begin{cases} \Phi = 1/2 q^T \cdot G^s \cdot q \\ W = -\int_0^t d\tau\, \dot{q}^T \cdot G^a \cdot q \end{cases}$$

4.4 Modelling of experiments

Ex: additive colored (memory-dependent) noise (in granular exp)
-> higher dimension with white noise