Linear Stochastic Systems

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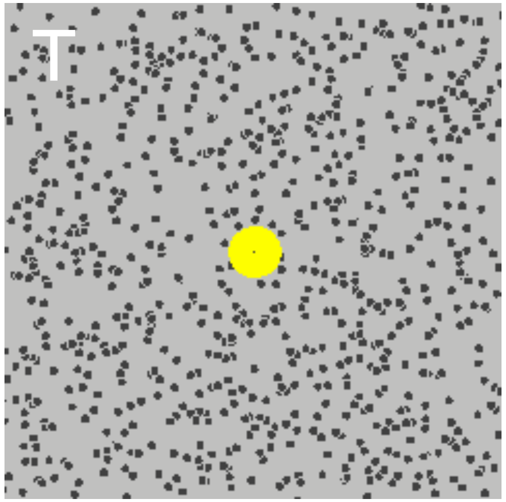
Contents

1-1 Stochastic System Description (1 Dim.)

: Brownian dynamics



Wikipedia

Phenomenological stochastic equation of motion

$$v = \dot{x}$$

$$m\dot{v} = \text{environmental force} = -\gamma v + \xi(t) \qquad \text{(Langevin equation)}$$

frictional force $-\gamma v$: $m\dot{v} = -\gamma v$

$v \to 0$ inconsistent with $\langle v^2 \rangle = \dfrac{k_{\mathrm{B}}T}{m}$

random (fluctuating) force $\xi(t)$

simplest form: Gaussian white noise

$$\langle \xi(t) \rangle = 0 \qquad \langle \xi(t)\xi(t') \rangle = 2D\delta(t - t')$$

1-2 Correlation function (1 Dim.)

: Brownian dynamics

Langevin equation: $m\dot{v} = -\gamma v + \xi(t)$

velocity

Let $v(t) = e^{-\gamma t/m} w(t) \;\; \rightarrow m\dot{v} = \underbrace{-\gamma e^{-\gamma t/m} w(t)}_{-\gamma v(t)} + \underbrace{m e^{-\gamma t/m} \dot{w}(t)}_{\xi(t)} \rightarrow w(t) = \frac{1}{m}\int_0^t ds\; e^{\gamma s/m} \xi(s)$

$$v(t) = e^{-\gamma t/m} v(0) + \frac{1}{m}\int_0^t ds\; e^{-\gamma(t-s)/m} \xi(s)$$

velocity correlation

$$\begin{aligned}
\langle v(t_1) v(t_2) \rangle &= e^{-\gamma(t_1+t_2)/m} v^2(0) + e^{-\gamma t_1/m} \frac{v(0)}{m} \int_0^{t_2} ds\; e^{-\gamma(t_2-s)/m} \langle \xi(s) \rangle \\
&\quad + e^{-\gamma t_2/m} \frac{v(0)}{m} \int_0^{t_1} ds\; e^{-\gamma(t_1-s)/m} \langle \xi(s) \rangle \\
&\quad + \int_0^{t_1} ds\; e^{-\gamma(t_1-s)/m} \int_0^{t_2} ds'\; e^{-\gamma(t_2-s')/m} \underbrace{\langle \xi(s) \xi(s') \rangle}_{= 2D\delta(s-s')} \\
&= \left(v^2(0) - \frac{D}{\gamma m} \right) e^{-\gamma(t_1+t_2)/m} + \frac{D}{\gamma m} e^{-\gamma |t_1 - t_2|/m}
\end{aligned}$$

$(t_1 = t_2 \rightarrow \infty)$ $\langle v^2 \rangle = \dfrac{D}{\gamma m} = \dfrac{k_\mathrm{B} T}{m} \;\; \rightarrow D = \gamma k_\mathrm{B} T$ Einstein relation

1-3 Thermodynamic First Law (1 Dim.)

: Brownian dynamics

Langevin equation: $m\dot{v} = -\frac{\partial}{\partial x}U(x,\lambda_t) + f_{\text{nc}} - \gamma v + \xi(t)$

$$\boxed{m\dot{v}\circ vdt} = -\boxed{\frac{\partial}{\partial x}U(x,\lambda_t)\circ vdt} + f_{\text{nc}}\circ vdt + (-\gamma v + \xi(t))\circ vdt$$

$$\boxed{\frac{m}{2}(v_{t+dt}^2 - v_t^2)} \qquad dU = \boxed{\partial_x U \dot{x} dt} + \partial_\lambda U \dot{\lambda} dt$$

Stratonovich multiplication

$$\left(\circ v = \times \frac{v_{t+dt} + v_t}{2}\right)$$

$$\underbrace{dU + \frac{m}{2}(v_{t+dt}^2 - v_t^2)}_{dE} = \underbrace{\frac{\partial}{\partial \lambda}U\dot{\lambda}dt + f_{\text{nc}}\circ vdt}_{dW} + \underbrace{(-\gamma v + \xi(t))\circ vdt}_{dQ}$$

dE : energy change

dW : work

dQ : heat

integral form

$$E(t) - E(0) = \int_0^t \frac{\partial}{\partial \lambda}U\dot{\lambda}dt + \int_0^t f_{\text{nc}} vdt + \int_0^t (-\gamma v + \xi(t))\circ vdt$$

1-4 Overdamped Systems (1 Dim.)

:Thermodynamic first law

Langevin equation: $m\dot{v} = -\frac{\partial}{\partial x}U(x,\lambda_t) + f_{\mathrm{nc}} - \gamma v + \xi(t)$

Reynolds number: $Re = \frac{F_{\mathrm{inertia}} = m\dot{v}}{F_{\mathrm{viscous}} = \gamma v}$

Re of cell or sub-cellular motion is small.

ex) typical bacterium: *Re* ~ 10^{-4}
typical molecular motor: *Re* ~ 10^{-8}

inertia term neglected: overdamped Langevin equation

$$\gamma\dot{x} = -\frac{\partial}{\partial x}U(x,\lambda_t) + f_{\mathrm{nc}} + \xi(t)$$

thermodynamic first law

$$\underbrace{\longrightarrow dU}_{dE\text{ : energy change}} = \underbrace{\frac{\partial}{\partial\lambda}U\dot{\lambda}dt + f_{\mathrm{nc}}\circ dx}_{dW\text{ : work}} + \underbrace{(-\gamma\dot{x}+\xi(t))\circ dx}_{dQ\text{ : heat}}$$

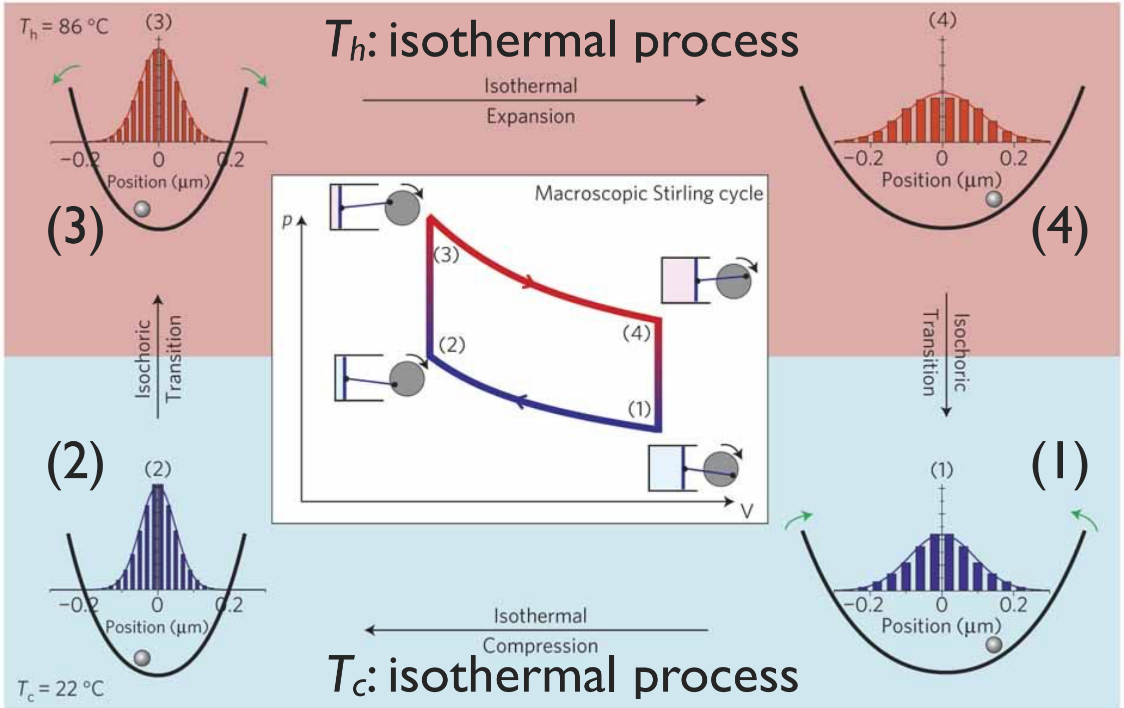
integral form

$$E(t) - E(0) = \int_0^t \frac{\partial}{\partial\lambda}U\dot{\lambda}dt + \int_0^t f_{\mathrm{nc}}\circ dx + \int_0^t (-\gamma\dot{x}+\xi(t))\circ dx$$

1-5 Engine Examples (1 Dim.)

: Stochastic Stirling heat engine

Blickle and Bechinger, Nat. Phys. 8, 143 (2012)



large stiffness k_{max}
(small volume)

small stiffness k_{min}
(large volume)

$$\langle W_{(1)\to(2)}\rangle = \int_{t_{(1)}}^{t_{(2)}} \frac{\partial}{\partial k}\left(\frac{1}{2}k\langle x^2\rangle\right)\frac{dk}{dt}dt$$

$$= \frac{1}{2}\int_{k_{\min}}^{k_{\max}} \langle x^2\rangle dk$$

quasi-static process $\langle x^2\rangle = \frac{T}{k}$

$$= \frac{T_c}{2}\ln\frac{k_{\max}}{k_{\min}}$$

integral form $E(t) - E(0) = \int_0^t \frac{\partial}{\partial\lambda}U\dot{\lambda}dt + \int_0^t f_{\rm nc}\circ dx + \int_0^t(-\gamma\dot{x} + \xi(t))\circ dx$

1-5 Engine Examples (1 Dim.)

: Stochastic Stirling heat engine

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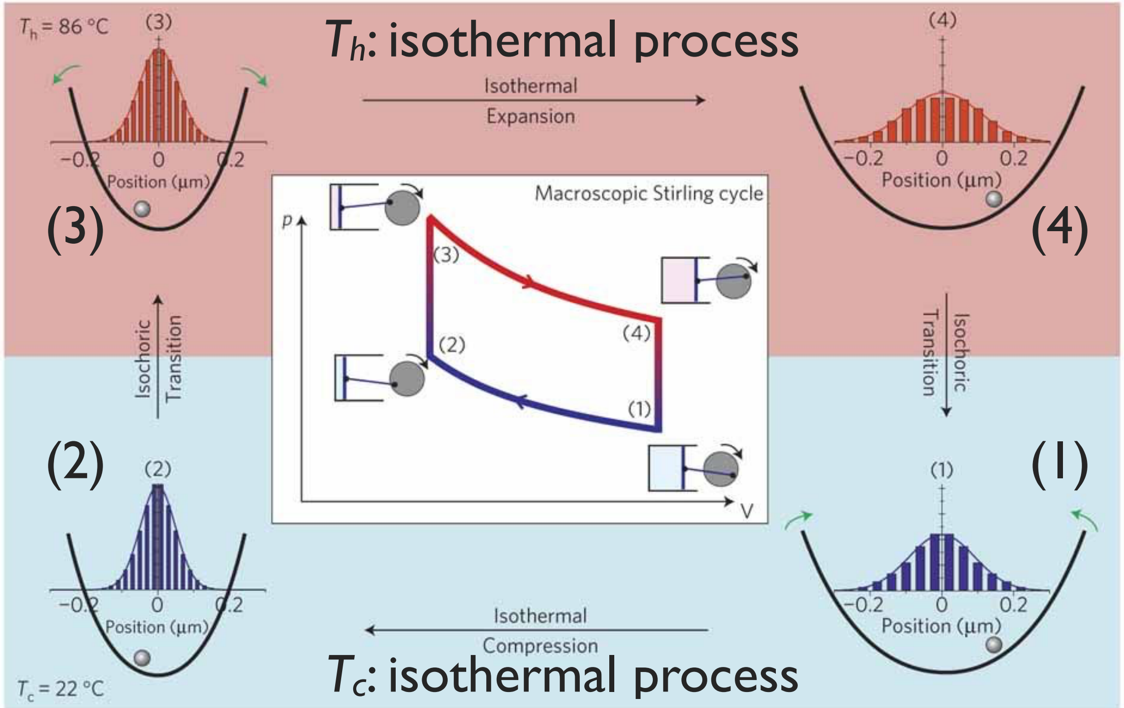


large stiffness k_{max}
(small volume)

small stiffness k_{min}
(large volume)

$$\langle W_{(1)\to(2)}\rangle = \frac{T_c}{2}\ln\frac{k_{\max}}{k_{\min}}$$

$$\langle W_{(3)\to(4)}\rangle = \frac{T_h}{2}\ln\frac{k_{\min}}{k_{\max}}$$

$$\langle W_{(2)\to(3)}\rangle = \langle W_{(4)\to(1)}\rangle = 0$$

$$\langle Q_{(1)\to(2)}\rangle = \cancel{\langle \Delta E_{(1)\to(2)}\rangle} - \langle W_{(1)\to(2)}\rangle$$

$$\langle Q_{(3)\to(4)}\rangle = \cancel{\langle \Delta E_{(3)\to(4)}\rangle} - \langle W_{(3)\to(4)}\rangle$$

$$\langle Q_{(2)\to(3)}\rangle = \langle \Delta E_{(2)\to(3)}\rangle = \frac{1}{2}(T_h - T_c)$$

$$\langle Q_{(4)\to(1)}\rangle = \langle \Delta E_{(4)\to(1)}\rangle = \frac{1}{2}(T_c - T_h)$$

efficiency: $\eta = \dfrac{-\langle W_{(3)\to(4)}\rangle - \langle W_{(1)\to(2)}\rangle}{\langle Q_{(2)\to(3)}\rangle + \langle Q_{(3)\to(4)}\rangle} = \dfrac{\eta_C}{1+\eta_C/\ln(k_{\max}/k_{\min})} < \eta_C = 1 - \dfrac{T_c}{T_h}$

Check this equality.

2-1 Multidimensional Stochastic Systems

: Description and thermodynamic first law

Langevin equation: $\gamma \dot{\boldsymbol{x}} = -\nabla_{\boldsymbol{x}} U(\boldsymbol{x}, \lambda_t) + \boldsymbol{F}^{\mathrm{nc}} + \boldsymbol{\xi}$

$$\boldsymbol{x} = (x_1, \cdots, x_N)^{\mathsf{T}} \qquad \boldsymbol{F}^{\mathrm{nc}} = (f_1^{\mathrm{nc}}, \cdots, f_N^{\mathrm{nc}})^{\mathsf{T}}$$

$$\boldsymbol{\xi} = (\xi_1, \cdots, \xi_N)^{\mathsf{T}} \quad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(t')\rangle = 2\mathrm{D}\delta(t - t')$$

D: *N*x*N* symmetric positive definite matrix

thermodynamic first law: $dU = \frac{\partial U}{\partial \lambda}\dot{\lambda}dt + \boldsymbol{F}^{\mathrm{nc}} \circ \dot{\boldsymbol{x}}dt + (-\gamma\dot{\boldsymbol{x}} + \boldsymbol{\xi}) \circ \dot{\boldsymbol{x}}dt$

integral form: $E(t) - E(0) = \int_0^t \frac{\partial U}{\partial \lambda}\dot{\lambda}dt + \int_0^t \boldsymbol{F}^{\mathrm{nc}} \circ \dot{\boldsymbol{x}}dt + \int_0^t (-\gamma\dot{\boldsymbol{x}} + \boldsymbol{\xi}) \circ \dot{\boldsymbol{x}}dt$

2-2 Multidimensional Linear Stochastic Systems

: Linear system and stability condition

Langevin equation: $\gamma\dot{\boldsymbol{x}} = -\nabla_{\boldsymbol{x}} U(\boldsymbol{x}, \lambda_t) + \boldsymbol{F}^{\mathrm{nc}} + \boldsymbol{\xi}$

$$\boldsymbol{x} = (x_1, \cdots, x_N)^{\mathsf{T}} \qquad \boldsymbol{F}^{\mathrm{nc}} = (f_1^{\mathrm{nc}}, \cdots, f_N^{\mathrm{nc}})^{\mathsf{T}}$$

$$\boldsymbol{\xi} = (\xi_1, \cdots, \xi_N)^{\mathsf{T}} \quad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(t')\rangle = 2\mathsf{D}\delta(t - t')$$

D: *N*x*N* symmetric positive definite matrix

Linear potential: $-\nabla_{\boldsymbol{x}} U(\boldsymbol{x}, \lambda_t) = -\mathsf{K}\boldsymbol{x}$ (K: *N*x*N* matrix)

Linear non-conservative force: $\boldsymbol{F}^{\mathrm{nc}} = \mathsf{F}\boldsymbol{x}$ (F: *N*x*N* matrix)

$\rightarrow \dot{\boldsymbol{x}} = -\mathsf{A}\boldsymbol{x} + \boldsymbol{\Xi}$ $\quad (\boldsymbol{\Xi} = \boldsymbol{\xi}/\gamma)$: multidimensional Ornstein-Uhlenbeck process

Formal solution: $\boldsymbol{x}(t) = e^{-\mathsf{A}t}\boldsymbol{w}(t) \rightarrow \boldsymbol{x}(t) = e^{-\mathsf{A}t}\boldsymbol{x}(0) + \int_0^t ds\ e^{-\mathsf{A}(t-s)}\boldsymbol{\Xi}$

stability condition: $\mathsf{SAS}^{-1} = \mathsf{A}_{\mathrm{d}} \rightarrow e^{-\mathsf{A}t} = \mathsf{S}^{-1}e^{-\mathsf{A}_{\mathrm{d}}t}\mathsf{S}$

if an eigenvalue of A is negative, $\boldsymbol{x}(t)$ diverges.

all eigenvalues of A should be positive for convergence in long time limit.

2-3 Correlation function

Langevin equation:

$\rightarrow \dot{\boldsymbol{x}} = -\mathsf{A}\boldsymbol{x} + \boldsymbol{\Xi} \qquad (\boldsymbol{\Xi} = \boldsymbol{\xi}/\gamma)$: multidimensional Ornstein-Uhlenbeck process

Formal solution: $\boldsymbol{x}(t) = e^{-\mathsf{A}t}\boldsymbol{w}(t) \rightarrow \boldsymbol{x}(t) = e^{-\mathsf{A}t}\boldsymbol{x}(0) + \int_0^t ds\; e^{-\mathsf{A}(t-s)}\boldsymbol{\Xi}$

Define $\mathsf{B}^t \equiv e^{-\mathsf{A}t} \rightarrow x_i(t) = \sum_j \mathsf{B}^t_{ij} x_j(0) + \int_0^t ds \sum_j \mathsf{B}^{t-s}_{ij} \Xi_j(s)$

Correlation function $\langle x_i(t') x_j(t) \rangle$

$$= \left\langle \left(\sum_k \mathsf{B}^{t'}_{ik} x_k(0) + \int_0^{t'} ds \sum_k \mathsf{B}^{t'-s}_{ik} \Xi_k(s) \right) \left(\sum_l \mathsf{B}^t_{jl} x_l(0) + \int_0^t ds' \sum_l \mathsf{B}^{t-s'}_{jl} \Xi_l(s') \right) \right\rangle$$

$$= \sum_{k,l} \mathsf{B}^{t'}_{ik} \mathsf{B}^t_{jl} x_k(0) x_l(0) + \sum_{k,l} \mathsf{B}^{t'}_{ik} \int_0^t ds \mathsf{B}^{t-s}_{jl} x_k(0) \langle \Xi_l(s) \rangle$$

$$+ \sum_{k,l} \mathsf{B}^t_{jl} \int_0^{t'} ds' \mathsf{B}^{t'-s'}_{ik} x_l(0) \langle \Xi_k(s') \rangle + \int_0^{t'} ds' \int_0^t ds \sum_{kl} \mathsf{B}^{t'-s'}_{ik} \mathsf{B}^{t-s}_{jl} \langle \Xi_k(s') \Xi_l(s) \rangle$$

$$= \sum_{k,l} \mathsf{B}^{t'}_{ik} \mathsf{B}^t_{jl} x_k(0) x_l(0) + \frac{2T}{\gamma} \int_0^{\min(t,t')} ds \sum_{kl} \mathsf{B}^{t'-s}_{ik} \mathsf{B}^{t-s}_{jl}$$

2-4 Covariance Matrix and Steady-State Distribution

: Covariance matrix (equal-time correlation function in a steady state)

Langevin equation:

$$\rightarrow \dot{\boldsymbol{x}} = -\mathsf{A}\boldsymbol{x} + \boldsymbol{\Xi} \qquad (\boldsymbol{\Xi} = \boldsymbol{\xi}/\gamma) \qquad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(t') \rangle = 2\mathsf{D}\delta(t-t')$$

Define $\mathsf{C} = \langle \boldsymbol{x}\boldsymbol{x}^{\mathsf{T}} \rangle_s = \begin{pmatrix} \langle x_1 x_1 \rangle_s & \dots & \langle x_1 x_N \rangle_s \\ \vdots & \ddots & \vdots \\ \langle x_N x_1 \rangle_s & \dots & \langle x_N x_N \rangle_s \end{pmatrix}$

$$\frac{d\mathsf{C}}{dt} = -\mathsf{AC} - \mathsf{CA}^{\mathsf{T}} + 2\mathsf{D}/\gamma^2 + O(dt) = 0 \quad \rightarrow \mathsf{AC} + \mathsf{CA}^{\mathsf{T}} = 2\mathsf{D}/\gamma^2$$

symmetric: $(N^2+N)/2$ linear equations

Derive $\mathsf{AC} + \mathsf{CA}^{\mathsf{T}} = 2\mathsf{D}/\gamma^2$

Steady state distribution

$$P_s(\boldsymbol{x}) = \frac{1}{\sqrt{\det(2\pi\mathsf{C})}} \exp\left(-\frac{1}{2}\boldsymbol{x}^{\mathsf{T}}\mathsf{C}^{-1}\boldsymbol{x}\right)$$

Kwon, Ao, Thouless, PNAS 102, 13029 (2005)

Kwon, Noh, Park, PRE 83, 061145 (2011)

→ Any moments can be calculated. $\langle x_i^n x_j^m \rangle_s$

2-5 Example: Linear Stochastic Engine

: Model

nonconservative force

$$\gamma \dot{x}_1 = \boxed{-kx_1} + \boxed{\epsilon x_2} + \xi_1 \qquad T_1$$

$$\gamma \dot{x}_2 = \boxed{-kx_2} + \boxed{\delta x_1} + \xi_2 \qquad T_2$$

potential force

$$\langle \xi_i(t)\xi_j(t')\rangle = 2\gamma T_i \delta_{ij}\delta(t-t')$$

$$T_1 > T_2$$

relevant system: Brownian gyrator

Filliger *et al.*, PRL 99, 230602 (2007)

Chiang *et al.*, PRE 96, 032123 (2017)

Work, heat energy

$$\underbrace{k\langle x_1 \circ \dot{x}_1\rangle_s}_{\dot{E}_1} = \underbrace{\epsilon\langle x_2 \circ \dot{x}_1\rangle_s}_{\dot{W}_1} + \underbrace{\langle(-\gamma\dot{x}_1 + \xi_1)\circ \dot{x}_1\rangle_s}_{\dot{Q}_1} = 0 \;\rightarrow \dot{Q}_1 = -\dot{W}_1 = -\epsilon\langle x_2 \circ \dot{x}_1\rangle_s$$

$$\underbrace{k\langle x_2 \circ \dot{x}_2\rangle_s}_{\dot{E}_2} = \underbrace{\delta\langle x_1 \circ \dot{x}_2\rangle_s}_{\dot{W}_2} + \underbrace{\langle(-\gamma\dot{x}_2 + \xi_2)\circ \dot{x}_2\rangle_s}_{\dot{Q}_2} = 0 \;\rightarrow \dot{Q}_2 = -\dot{W}_2 = \delta\langle x_2 \circ \dot{x}_1\rangle_s$$

$$\frac{d}{dt}\langle x_i^2\rangle_s = 2\langle x_i \circ \dot{x}_i\rangle_s = 0$$

$$\frac{d}{dt}\langle x_1 x_2\rangle_s = \langle x_1 \circ \dot{x}_2\rangle_s + \langle \dot{x}_1 \circ x_2\rangle_s = 0 \;\rightarrow \langle x_1 \circ \dot{x}_2\rangle_s = -\langle \dot{x}_1 \circ x_2\rangle_s$$

Efficiency

$$\eta = \frac{-\dot{W}}{\dot{Q}_1} = 1 - \frac{\delta}{\epsilon}$$

total work

$$-\dot{W} = -\dot{W}_1 - \dot{W}_2 = (-\epsilon + \delta)\langle x_2 \circ \dot{x}_1\rangle_s$$

2-5 Example: Linear Stochastic Engine

: Model

nonconservative force

$$\gamma \dot{x}_1 = -kx_1 + \epsilon x_2 + \xi_1 \qquad T_1$$

$$\gamma \dot{x}_2 = -kx_2 + \delta x_1 + \xi_2 \qquad T_2$$

potential force

$$\rightarrow \dot{\boldsymbol{x}} = -\mathsf{A}\boldsymbol{x} + \boldsymbol{\Xi}$$

$$\boldsymbol{x} = (x_1, x_2)^{\mathsf{T}} \qquad \mathsf{A} = \frac{1}{\gamma}\begin{pmatrix} k & -\epsilon \\ -\delta & k \end{pmatrix}$$

Efficiency

$$\eta = \frac{-\dot{W}}{\dot{Q}_1} = 1 - \frac{\delta}{\epsilon} \qquad -\dot{W} = -\dot{W}_1 - \dot{W}_2 = (-\epsilon + \delta)\langle x_2 \circ \dot{x}_1 \rangle_s$$

1) Stability condition: all eigenvalues of A should be positive

$$k + \sqrt{\epsilon\delta},\ k - \sqrt{\epsilon\delta} > 0 \ \rightarrow \ \delta\epsilon < k^2$$

2) Work extraction: $-\dot{W} > 0$

$$0 < -\dot{W} = (-\epsilon + \delta)\langle x_2 \circ \dot{x}_1 \rangle_s = (-\epsilon + \delta)(-k\langle x_2 \circ x_1 \rangle_2 + \epsilon\langle x_2 \circ x_2 \rangle_s + \langle x_2 \circ \xi_1 \rangle_s)/\gamma$$

$$\mathsf{C} = \begin{pmatrix} \langle x_1 \circ x_1 \rangle_s & \langle x_1 \circ x_2 \rangle_s \\ \langle x_2 \circ x_1 \rangle_s & \langle x_2 \circ x_2 \rangle_s \end{pmatrix} \rightarrow \mathsf{AC} + \mathsf{CA}^{\mathsf{T}} = 2\mathsf{D}/\gamma^2 \qquad -\dot{W} = \frac{(\epsilon - \delta)(T_1\delta - T_2\epsilon)}{2k\gamma}$$

Derive $-\dot{W} = \dfrac{(\epsilon - \delta)(T_1\delta - T_2\epsilon)}{2k\gamma}$

2-5 Example: Linear Stochastic Engine

: Model

nonconservative force

$$\gamma \dot{x}_1 = -kx_1 + \epsilon x_2 + \xi_1 \qquad T_1$$

$$\gamma \dot{x}_2 = -kx_2 + \delta x_1 + \xi_2 \qquad T_2$$

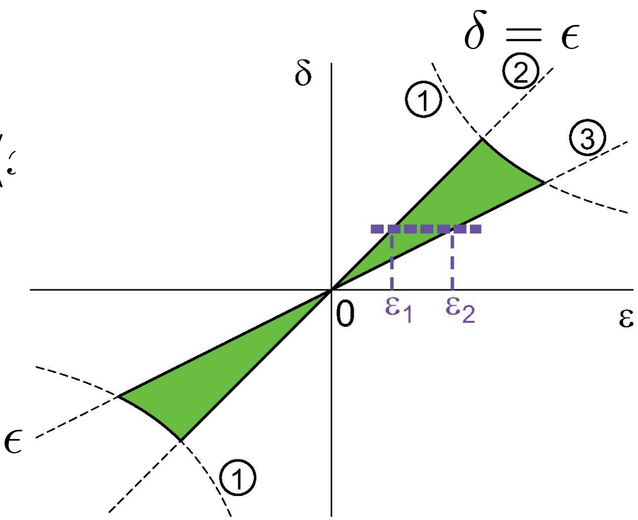
potential force

$$\rightarrow \dot{\boldsymbol{x}} = -\mathsf{A}\boldsymbol{x} + \boldsymbol{\Xi}$$

$$\boldsymbol{x} = (x_1, x_2)^{\mathsf{T}} \qquad \mathsf{A} = \frac{1}{\gamma}\begin{pmatrix} k & -\epsilon \\ -\delta & k \end{pmatrix}$$

Efficiency

$$\eta = \frac{-\dot{W}}{\dot{Q}_1} = 1 - \frac{\delta}{\epsilon} \qquad -\dot{W} = -\dot{W}_1 - \dot{W}_2 = (-\epsilon + \delta)\langle$$



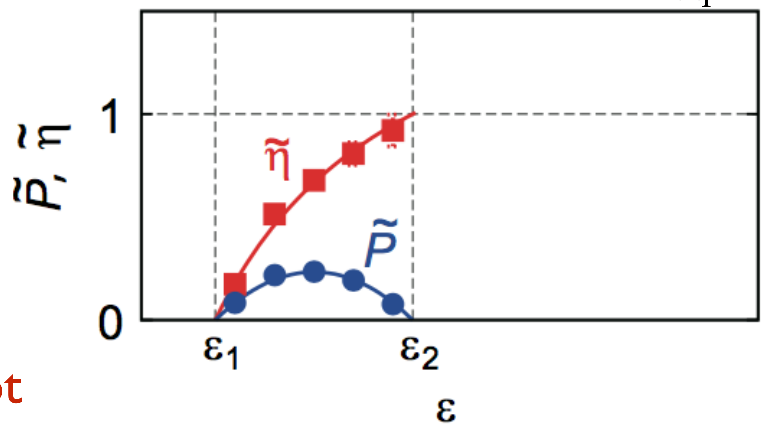
1) Stability condition: all eigenvalues of A should be positive

$$k + \sqrt{\epsilon\delta},\ k - \sqrt{\epsilon\delta} > 0 \ \rightarrow\ \delta\epsilon < k^2 \quad ①$$

2) Work extraction: $-\dot{W} > 0$

$$-\dot{W} = \frac{\underset{②}{(\epsilon - \delta)}\underset{③}{(T_1\delta - T_2\epsilon)}}{2k\gamma} > 0$$

$$\tilde{\eta} \equiv \eta/\eta_{\mathrm{C}} \qquad \tilde{P} \equiv \langle \dot{W} \rangle_{\mathrm{s}} / P_{\mathrm{eq}}^{\max}$$



maximum efficiency: Carnot

power-efficiency tradeoff relation: power vanishes at Carnot