Introduction to

Stochastic Thermodynamics

Lecture 2

The 22nd KIAS-APCTP Winter School on Statistical Physics

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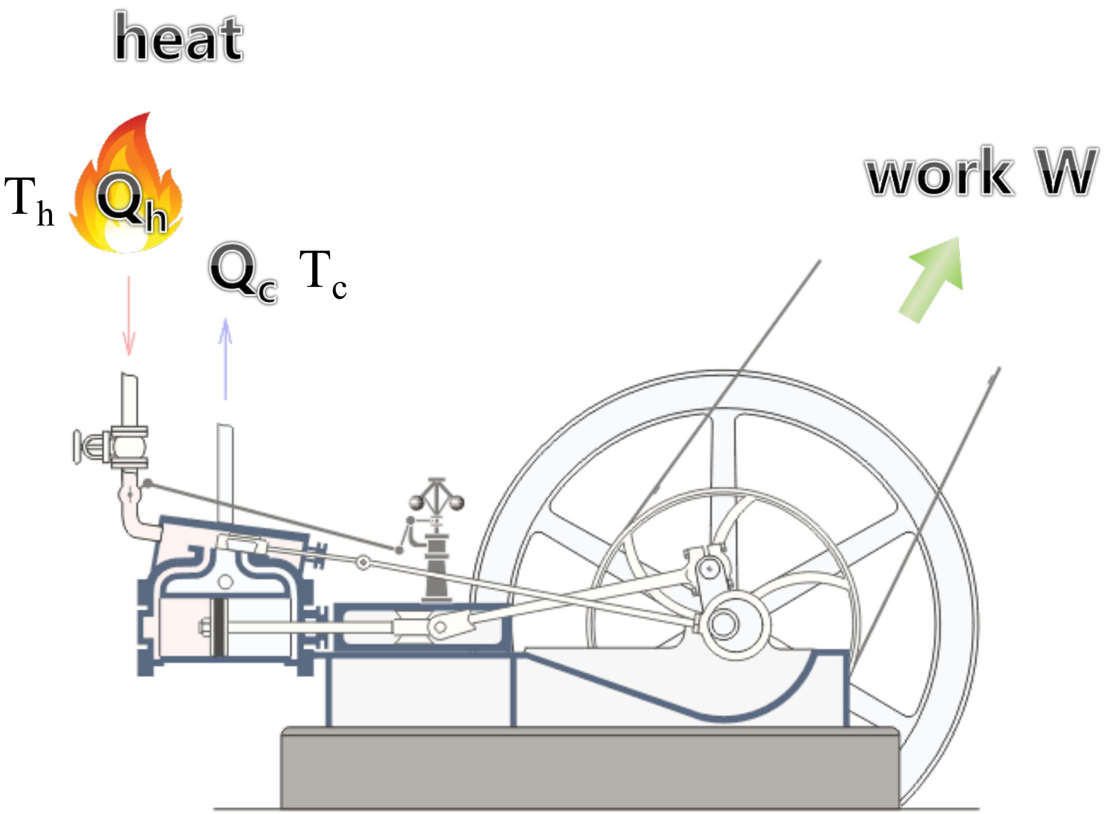
What is Thermodynamics?

a branch of physics that deals with **heat**, **work**, and **temperature**, and **their relation** to **energy**, **entropy**…

Wikipedia: Thermodynamics



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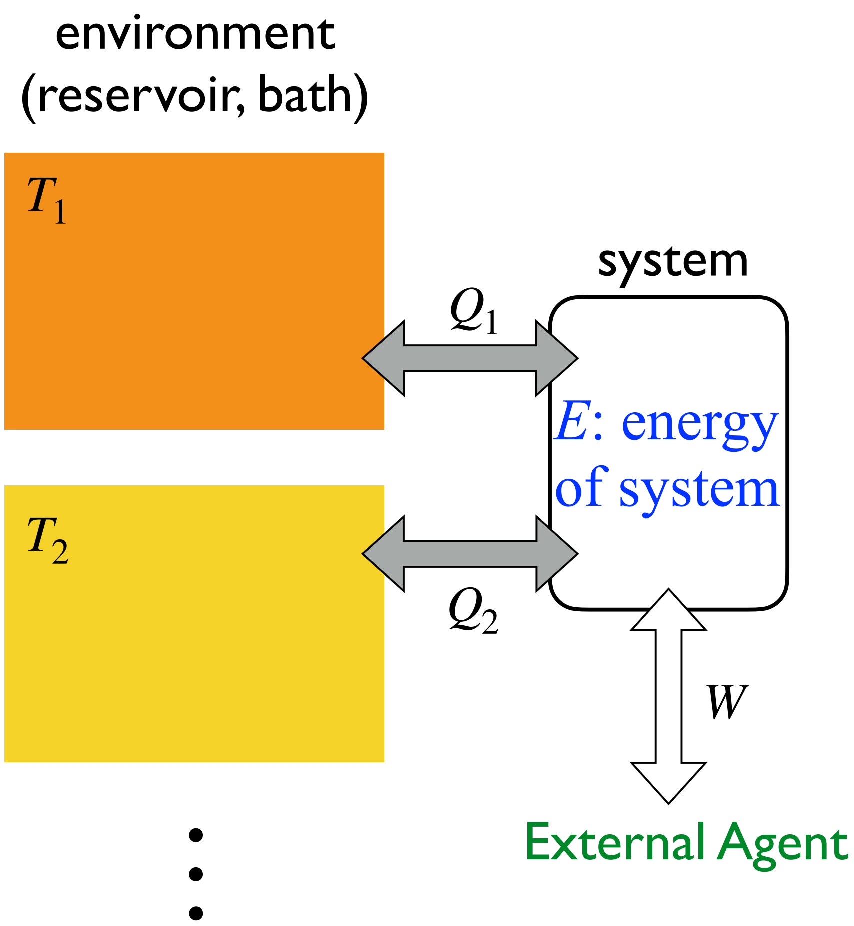


heat: energy transfer btw system and bath

work: energy transfer btw system and E.A.

→ open system

Relation for energy

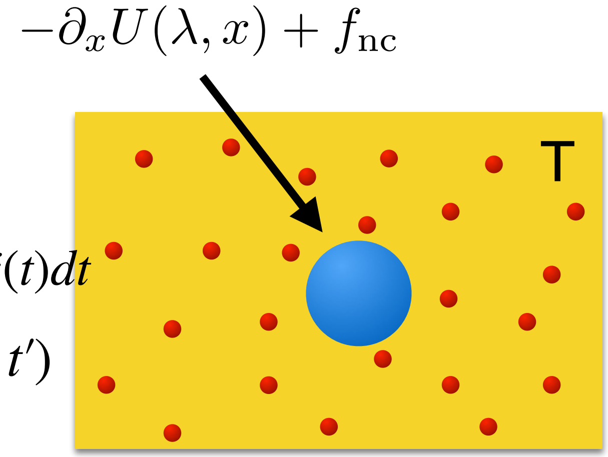
$$1^{\text{st}}: \quad \Delta E = Q_1 + Q_2 + W$$

Relation for entropy

$$2^{\text{nd}}: \quad \Delta S_{\text{tot}} \geq 0$$

Heat & Work

1. Underdamped Langevin equation



$$x(t+dt) - x(t) = v(t)dt$$

$$m\left(v(t+dt) - v(t)\right) = -\partial_x U(\lambda(t), x(t))dt + f_{\rm nc}(t)dt - \gamma v(t)dt + \sigma\xi(t)dt$$

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \delta(t-t')$$

$$\underbrace{v(t) \circ m\left(v(t+dt) - v(t)\right)}_{=dK} = \underbrace{-v(t) \circ \partial_x U(\lambda(t), x(t))dt}_{=-dU + \partial_\lambda U \dot{\lambda} dt} + \underbrace{v(t) \circ f_{\rm nc}(t)dt}_{=f_{\rm nc}(t)v(t)dt} + v(t) \circ \left(-\gamma v(t) + \sigma\xi(t)\right) dt$$

$$\underbrace{dK + dU}_{=dE} = \underbrace{\partial_\lambda U \dot{\lambda} dt + f_{\rm nc}(t)v(t)dt}_{=dW} + \underbrace{v(t) \circ \left(-\gamma v(t) + \xi(t)\right) dt}_{=dQ}$$: 1st law

Work : $dW_c = \partial_\lambda U \dot{\lambda} dt$: work done by conservative force or Jarzynski work

$dW_{\rm nc} = f_{\rm nc} v dt$: work done by nonconservative force

$dW = dW_c + dW_{\rm nc}$: work done by external force

Heat : $dQ = v(t) \circ \left(-\gamma v(t) + \xi(t)\right) dt$: work done by heat-bath force (must be Stratonovich)

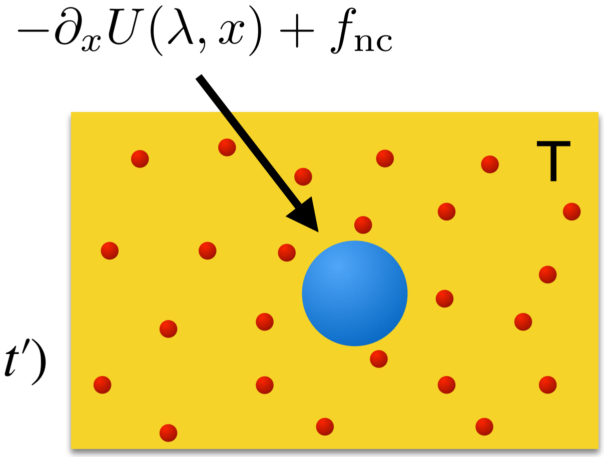
Heat & Work

2. Overdamped Langevin equation

overdamped limit $(m/\gamma \to 0)$

$$\dot{x} = v, \quad m\dot{v} = -\partial_x U(\lambda, x) + f_{\rm nc} - \gamma v + \sigma\xi$$

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \delta(t - t')$$



$$\Longrightarrow \quad \gamma\dot{x} = -\partial_x U(\lambda, x) + f_{\rm nc} + \sigma\xi$$

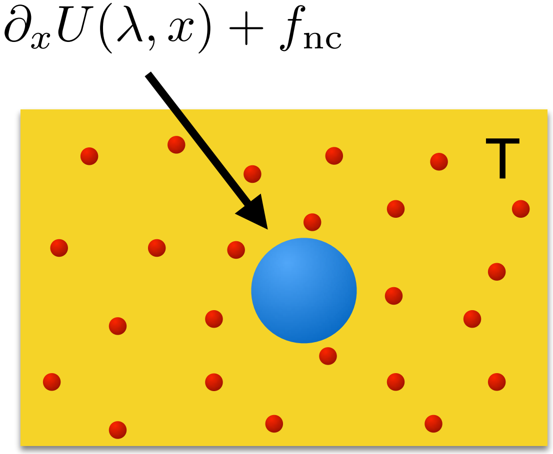
$$\gamma\left(x(t+dt) - x(t)\right) = -\partial_x U(\lambda(t), x(t))dt + f_{\rm nc}(t)dt + \sigma\xi(t)dt$$

Heat & Work

2. Overdamped Langevin equation

overdamped limit $(m/\gamma \to 0)$

$$\gamma\left(x(t+dt)-x(t)\right) = -\partial_x U(\lambda(t),x(t))dt + f_{\rm nc}(t)dt + \sigma\xi(t)dt$$



$$\langle \xi(t)\rangle = 0, \quad \langle \xi(t)\xi(t')\rangle = \delta(t-t')$$

$$\dot{x}(t)\circ\gamma\left(x(t+dt)-x(t)\right) = -\dot{x}(t)\circ\partial_x U(\lambda(t),x(t))dt + \dot{x}(t)\circ f_{\rm nc}(t)dt + \dot{x}(t)\circ\sigma\xi(t)dt$$

$$= -\partial_x U(\lambda(t),x(t))\circ dx(t)$$

Note on stochastic calculus

$$dU = \partial_\lambda U d\lambda + \partial_x U \circ dx$$

expansion w.r.t x should be Stratonovich!

$$\Rightarrow -\partial_x U \circ dx = -dU + \partial_\lambda U d\lambda$$

Heat & Work

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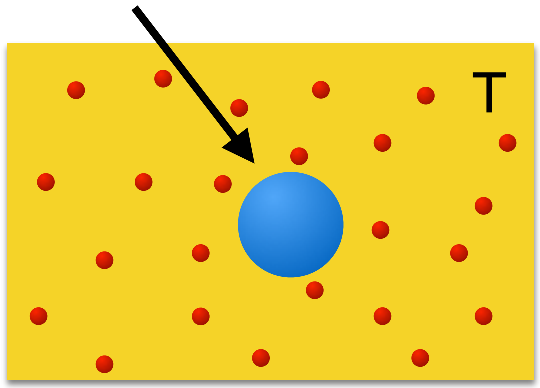
overdamped limit $(m/\gamma \to 0)$



$$\gamma \left(x(t+dt) - x(t) \right) = -\,\partial_x U(\lambda(t), x(t))dt + f_{\rm nc}(t)dt + \sigma\xi(t)dt$$

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \delta(t-t')$$

$$\dot{x}(t) \circ \gamma \left(x(t+dt) - x(t) \right) = -\dot{x}(t) \circ \partial_x U(\lambda(t), x(t))dt + \dot{x}(t) \circ f_{\rm nc}(t)dt + \dot{x}(t) \circ \sigma\xi(t)dt$$

$$= -\,dU + \partial_\lambda U \dot{\lambda} dt$$

$$dU = \partial_\lambda U \dot{\lambda} dt + f_{\rm nc}(t) \circ \dot{x}(t)dt + \left(-\gamma\dot{x}(t) + \sigma\xi(t) \right) \circ \dot{x}(t)dt$$: 1st law

$= dE$ $\quad$ $= dW$ $\quad$ $= dQ$

Work : $dW_{\rm c} = \partial_\lambda U \dot{\lambda} dt$: work done by conservative force or Jarzynski work

$dW_{\rm nc} = f_{\rm nc} \circ \dot{x}dt$: work done by nonconservative force (must be Stratonovich)

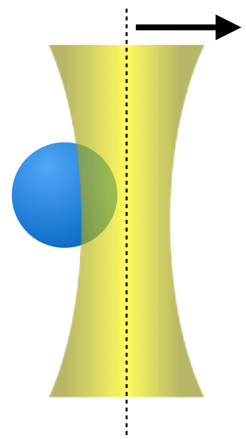
$dW = dW_{\rm c} + dW_{\rm nc}$: work done by external force

Heat : $dQ = \left(-\gamma\dot{x}(t) + \xi(t) \right) \circ \dot{x}(t)dt$: work done by heat-bath force (must be Stratonovich)

Heat & Work

Examples of heat and work calculation

1) optical tweezers experiment (overdamped)



$$\gamma \dot{x} = -k(x - \lambda(t)) + \xi, \qquad U\left(\lambda(t), x(t)\right) = \frac{k}{2}\left(x(t) - \lambda(t)\right)^2$$

work (Jarzynski work)

$$dW_c = \frac{\partial U}{\partial \lambda}\dot{\lambda}dt = -k\left(x(t) - \lambda(t)\right) a dt$$

$$\Rightarrow W_c = -ka\int_0^\tau \left(x(t) - at\right) dt = -kadt\sum_{i=0}^{N}\left(x(t_i) - at_i\right)$$

experiment (or simulation)

heat

$$dQ = \left(-\gamma \dot{x}(t) + \xi(t)\right) \circ \dot{x}(t)dt = k\left(x(t) - \lambda(t)\right) \circ dx(t)$$

$$= kx(t) \circ dx(t) - \lambda(t) \circ dx(t) = \frac{k}{2}\left[x(t+dt)^2 - x(t)^2\right] - \lambda(t)\left[x(t+dt) - x(t)\right]$$

$$\Rightarrow Q = \frac{k}{2}\sum_{i=0}^{N}\left[\left(x(t_{i+1})^2 - x(t_i)^2\right) - \lambda(t_i)\left(x(t_{i+1}) - x(t_i)\right)\right]$$

$$= \frac{k}{2}\left(x(t_N)^2 - x(t_0)^2\right) - \frac{k}{2}\sum_{i=0}^{N}\lambda(t_i)\left(x(t_{i+1}) - x(t_i)\right)$$

experiment (or simulation)

Heat & Work

Examples of heat and work calculation

2) 2-dimensional Brownian gyrator (overdamped)

$$\gamma \dot{x} = -kx + \epsilon y + \xi_x$$
$$\gamma \dot{y} = -ky - \epsilon x + \xi_y$$

conservative ($-kx$, $-ky$)   non-conservative ($+\epsilon y$, $-\epsilon x$)

$$\langle \xi_a(t)\xi_b(t')\rangle = 2\gamma k_{\mathrm{B}} T_a \delta_{ab}\delta(t-t')$$

work
$$dW_{\mathrm{c}} = \frac{\partial U}{\partial \lambda}\dot{\lambda}dt = 0$$

$$dW_{\mathrm{nc},x} = \epsilon y(t) \circ dx(t) = \epsilon y(t)\big(x(t+dt) - x(t)\big)$$

$$dW_{\mathrm{nc},y} = -\epsilon x(t) \circ dy(t) = \epsilon x(t)\big(y(t+dt) - y(t)\big)$$

heat
$$dQ_x = \big(-\gamma \dot{x}(t) + \xi_x(t)\big) \circ dx(t) = \big(kx(t) - \epsilon y(t)\big) \circ dx(t)$$
$$= \frac{k}{2}\left(x(t+dt)^2 - x(t)^2\right) - \epsilon y(t)\big(x(t+dt) - x(t)\big)$$

$$dQ_y = \Big(-\gamma \dot{y}(t) + \xi_y(t)\Big) \circ dy(t) = \big(ky(t) + \epsilon x(t)\big) \circ dy(t)$$
$$= \frac{k}{2}\left(y(t+dt)^2 - y(t)^2\right) + \epsilon x(t)\big(y(t+dt) - y(t)\big)$$

Heat & Work

Overdamped Langevin dynamics $\gamma \dot{x} = -\partial_x U(\lambda, x) + f_{\text{nc}} + \sigma \xi$

1. work : $dW_{\text{c}} = \partial_\lambda U \dot{\lambda} dt \qquad dW_{\text{nc}} = f_{\text{nc}} \circ \dot{x} dt \qquad dW = dW_{\text{c}} + dW_{\text{nc}}$

2. heat : $dQ = \big(-\gamma \dot{x}(t) + \sigma \xi(t)\big) \circ \dot{x}(t) dt$

Underdamped Langevin dynamics $\dot{x} = v, \quad m\dot{v} = -\partial_x U(\lambda, x) + f_{\text{nc}} - \gamma v + \sigma \xi$

1. work : $dW_{\text{c}} = \partial_\lambda U \dot{\lambda} dt \qquad dW_{\text{nc}} = f_{\text{nc}} v dt \qquad dW = dW_{\text{c}} + dW_{\text{nc}}$

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Heat & Work

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2. heat : $dQ = \left(-\gamma \dot{x}(t) + \sigma\xi(t)\right) \circ \dot{x}(t) dt$

Mean value of work & heat

dynamics : $\dot{z} = f(z(t)) + \sigma\xi$

$$\partial_t P(z,t) = -\partial_z J(z,t) \qquad J(z,t) = \left[f\left(z(t)\right) - \frac{1}{2}\partial_z \sigma^2\right] P(z,t)$$

$$\langle g(z(t)) \circ \dot{z}(t) \rangle = \left\langle \left[g(z(t)) + \frac{1}{2}(\partial_z g)\dot{z} dt\right] \dot{z}(t) \right\rangle$$

$$= \langle g(z(t)) f(z(t)) \rangle + \langle g(z(t)) \sigma\xi(t) \rangle + \frac{1}{2}\left\langle (\partial_z g)\dot{z}^2 \right\rangle dt \qquad = \frac{1}{2}\left\langle (\partial_z g)\sigma^2 \xi^2(t) \right\rangle dt = \left\langle (\partial_z g)\sigma^2/2 \right\rangle$$

$$= \int dz g(z) f(z) P(z,t) + \int dz (\partial_z g(z)) \frac{\sigma^2}{2} P(z,t) \qquad = -\int dz g(z) \partial_z \frac{\sigma^2}{2} P(z,t)$$

$$= \int dz g(z) \left[f(z) - \frac{1}{2}\partial_z \sigma^2\right] P(z,t)$$

$$= \int dz g(z) J(z,t)$$

Heat & Work

Overdamped Langevin dynamics $\gamma \dot{x} = -\partial_x U(\lambda, x) + f_{\rm nc} + \sigma\xi$

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$$\langle g(z(t)) \circ \dot{z}(t) \rangle = \int dz g(z) J(z,t)$$

1. work : $\langle \dot{W}_{\rm nc} \rangle = \langle f_{\rm nc} \circ \dot{x} \rangle = \int dx f_{\rm nc} J(x,t)$

2. heat : $\langle \dot{Q} \rangle = \left\langle \left(-\gamma \dot{x}(t) + \sigma\xi(t)\right) \circ \dot{x}(t) \right\rangle = \left\langle \left(\partial_x U(\lambda,x) - f_{\rm nc}\right) \circ \dot{x}(t) \right\rangle$

$$= \int dx \left(\partial_x U(\lambda,x) - f_{\rm nc}\right) J(x,t)$$

Stochastic Trajectory

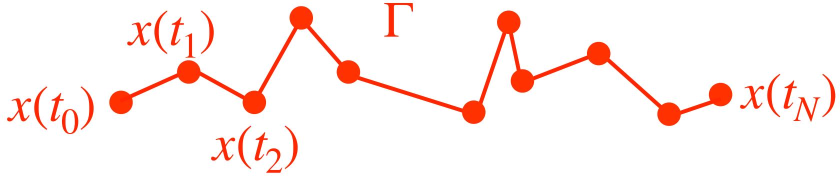
Overdamped Langevin dynamics

$$\gamma\left(x(t+dt)-x(t)\right)=f(x(t))dt+\sigma dW(t) \qquad \sigma^2=2\gamma k_B T$$

$$\langle dW(t)\rangle=0,\quad \langle dW(t)dW(t')\rangle=\begin{cases}0 & (t\neq t')\\ dt & (t=t')\end{cases}$$

Schematic of a stochastic system

$$t_n\equiv n dt \quad (t_N=\tau)$$



1) Probability for observing the transition $x(t_n)\to x(t_n+dt)$

probability for observing Gaussian random variable z: $P(z)dz=\dfrac{1}{\sqrt{2s^2\pi}}e^{-\frac{z^2}{2s^2}}dz$

probability for observing Gaussian noise $dW(t_n)$:

$$d(dW(t_n))=\frac{\gamma}{\sigma}dx(t_n+dt)$$

$$P(dW(t_n))d(dW(t_n))=\frac{1}{\sqrt{2s^2\pi}}e^{-\frac{dW(t_n)^2}{2s^2}}d(dW(t_n)) \qquad (s^2=dt)$$

$$=\frac{1}{\sqrt{2\pi dt}}\exp\left[-\frac{1}{2\sigma^2 dt}\left\{\gamma\left(x(t_n+dt)-x(t_n)\right)-f(x(t_n))dt\right\}_{\bullet}^2\right]\frac{\gamma}{\sigma}dx(t_n+dt)$$

$$x(t_n+dt)-x(t_n)=\dot{x}(t_n)dt$$

Ito

$$=\frac{1}{\sqrt{4\pi k_B T dt/\gamma}}\exp\left[-\frac{dt}{4k_B T/\gamma}\left\{\dot{x}(t_n)-f(x(t_n))/\gamma\right\}_{\bullet}^2\right]dx(t_n+dt)$$

$$=P\left(x(t_n+dt)\,|\,x(t_n)\right)dx(t_n+dt)$$

Stochastic Trajectory

Overdamped Langevin dynamics

$$\gamma\left(x(t+dt)-x(t)\right)=f(x(t))dt+\sigma dW(t) \qquad \sigma^2=2\gamma k_B T$$

$$\langle dW(t)\rangle=0,\quad \langle dW(t)dW(t')\rangle=\begin{cases}0 & (t\neq t')\\ dt & (t=t')\end{cases}$$

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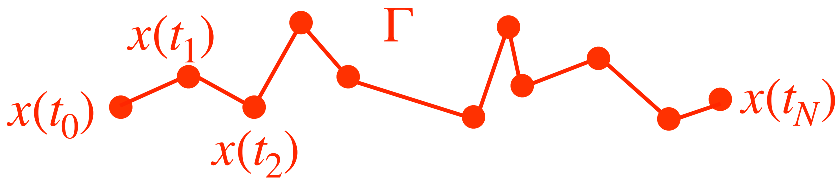

1) Probability for observing the transition $x(t_n) \rightarrow x(t_n+dt)$

$$P\left(x(t_n+dt)\,|\,x(t_n)\right)dx(t_n+dt)=\frac{1}{\sqrt{4\pi k_\mathrm{B}Tdt/\gamma}}\exp\left[-\frac{dt}{4k_\mathrm{B}T/\gamma}\left\{\dot{x}(t_n)-f(x(t_n))/\gamma\right\}^2\right]dx(t_n+dt)$$

Onsager-Machlup function

2) Conditional probability for observing Γ starting from $x(t_0)$

$$\mathscr{P}\left(\Gamma\,|\,x(t_0)\right)=\prod_{n=1}^{N}P\left(x(t_n)\,|\,x(t_{n-1})\right)dx(t_n)$$

$$=\prod_{n=1}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_\mathrm{B}Tdt/\gamma}}\right)\exp\left[-\frac{dt}{4k_\mathrm{B}T/\gamma}\sum_{n=0}^{N-1}\left\{\dot{x}(t_n)-f(x(t_n))/\gamma\right\}^2\right]$$

Stochastic Trajectory

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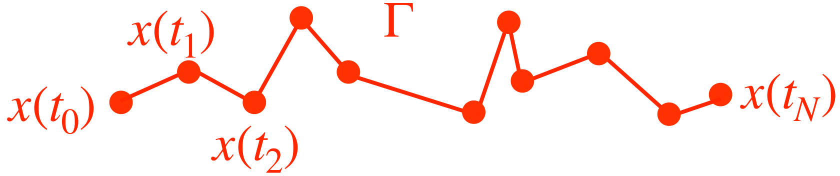

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$$=\prod_{n=1}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[-\frac{dt}{4k_B T/\gamma}\sum_{n=0}^{N-1}\left\{\dot{x}(t_n)-f(x(t_n))/\gamma\right\}^2\right]$$

3) probability for observing Γ

$$\mathscr{P}(\Gamma)=\mathscr{P}\left(\Gamma\,|\,x(t_0)\right)p_0(x(t_0))dx(t_0)$$

initial distribution

$$=\prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[-\frac{1}{4k_B T/\gamma}\int_0^{\tau}dt\left\{\dot{x}(t)-f(x(t))/\gamma\right\}^2\right]p_0(x(t_0))$$

Stochastic Trajectory

Overdamped Langevin dynamics

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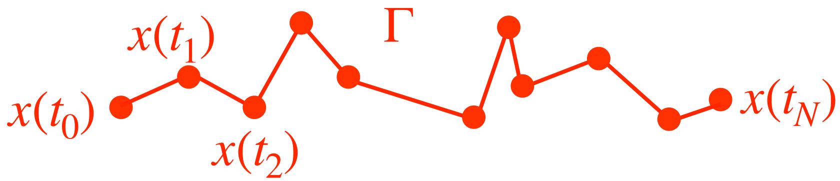

3) probability for observing Γ

$$\mathscr{P}(\Gamma)=\prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_{\mathrm{B}}Tdt/\gamma}}\right)\exp\left[-\frac{1}{4k_{\mathrm{B}}T/\gamma}\int_0^\tau dt\,\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\bullet}^2\right]p_0(x(t_0))$$

Note on stochastic calculus

$$\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\odot_a}^2=\dot{x}(t)^2+\frac{f(x(t))^2}{\gamma^2}-\frac{2}{\gamma}f(x(t))\odot_a\dot{x}(t)$$

$$f(x(t))\odot_a\dot{x}(t)=\left[(1-a)f(x(t+dt))+af(x(t))\right]\dot{x}(t)=\left[f(x(t))+(1-a)\partial_x f(x)\dot{x}(t)dt\right]\dot{x}(t)$$

$$=f(x(t))\dot{x}+(1-a)\partial_x f(x)\dot{x}(t)^2dt=f(x(t))\dot{x}+(1-a)\frac{2k_{\mathrm{B}}T}{\gamma}\partial_x f(x)$$

$$=\dot{x}(t)^2+\frac{f(x(t))^2}{\gamma^2}-\frac{2}{\gamma}f(x(t))\dot{x}(t)-(1-a)\frac{4k_{\mathrm{B}}T}{\gamma^2}\partial_x f(x)$$

$$=\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\bullet}^2-(1-a)\frac{4k_{\mathrm{B}}T}{\gamma^2}\partial_x f(x)$$

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Schematic of a stochastic system

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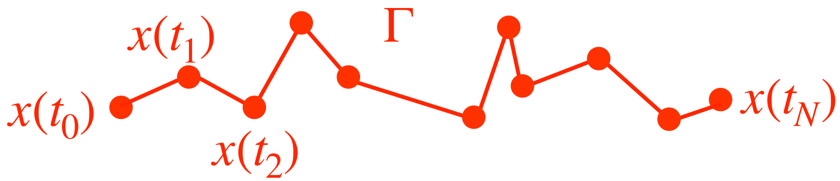

3) probability for observing Γ

$$\mathscr{P}(\Gamma)=\prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[-\frac{1}{4k_B T/\gamma}\int_0^{\tau}dt\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\bullet}^{2}\right]p_0(x(t_0))$$

$$\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\odot_a}^{2}=\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\bullet}^{2}-(1-a)\frac{4k_B T}{\gamma^2}\partial_x f(x)$$

$$=\prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[\int_0^{\tau}dt\left(-\frac{1}{4k_B T/\gamma}\left\{\dot{x}(t)-f(x(t))/\gamma\right\}_{\odot_a}^{2}-\frac{(1-a)}{\gamma}\partial_x f(x)\right)\right]p_0(x(0))$$

Stochastic Trajectory

Overdamped Langevin dynamics

3) probability for observing Γ

$$\mathscr{P}(\Gamma) = \prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[\int_0^\tau dt\left(-\frac{1}{4k_B T/\gamma}\left\{\dot{x}(t)-f(x(t))/\gamma\right\}^2_{\odot_a}-\frac{(1-a)}{\gamma}\partial_x f(x)\right)\right]p_0(x(0))$$

$= \mathscr{P}(\Gamma\,|\,x(0))$

$$P(\Gamma\,|\,x(0)) = \prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[\int_0^\tau dt\left(-\frac{1}{4k_B T/\gamma}\left\{\dot{x}(t)-f(x(t),t)/\gamma\right\}^2_{\circ}-\frac{1}{2\gamma}\partial_x f(x)\right)\right]$$

$a = 1/2$

Stochastic Trajectory

Heat & path probabilities

$$\Gamma$$

$$x(t_0 = 0) \quad x(t_1) \quad \cdots \quad x(t_n) \quad \cdots \quad x(t_{N-1}) \quad x(t_N = \tau)$$

$$\rightarrow \tilde{x}(t) = x(\tau - t)$$

$$\tilde{x}(t_N = \tau) \quad \tilde{x}(t_{N-1}) \cdots \tilde{x}(\tau - t_n) \cdots \tilde{x}(t_1) \quad \tilde{x}(0)$$

$$\tilde{\Gamma}$$

time-forward path probability

$$P(\Gamma \mid x(0)) = \prod_{n=0}^{N} \left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}} \right) \exp \left[\int_0^\tau dt \left(-\frac{1}{4k_B T/\gamma} \left\{ \dot{x}(t) - f(x(t), t)/\gamma \right\}_\circ^2 - \frac{1}{2\gamma} \partial_x f(x) \right) \right]$$

$a = 1/2$

time-reversal path probability

$$\tilde{P}(\tilde{\Gamma} \mid x(\tau)) = \prod_{n=0}^{N} \left(\frac{d\tilde{x}(t_n)}{\sqrt{4\pi k_B dt T/\gamma}} \right) \exp \left[\int_0^\tau dt \left(-\frac{1}{4k_B T/\gamma} \left\{ \dot{\tilde{x}}(t) - f(\tilde{x}(t), \tau - t)/\gamma \right\}_\circ^2 - \frac{1}{2\gamma} \partial_{\tilde{x}} f(\tilde{x}) \right) \right]$$

$t' \equiv \tau - t$

$$\rightarrow \tilde{x}(t) = x(t'), \quad \dot{\tilde{x}}(t) = \frac{d}{dt}\tilde{x}(t) = \frac{d}{dt}x(\tau - t) = -\frac{d}{dt'}x(t') = -\dot{x}(t')$$

$$= \prod_{n=0}^{N} \left(\frac{dx(t'_n)}{\sqrt{4\pi k_B dt T/\gamma}} \right) \exp \left[\int_\tau^0 -dt' \left(-\frac{1}{4k_B T/\gamma} \left\{ -\dot{x}(t') - f(x(t'), t')/\gamma \right\}_\circ^2 - \frac{1}{2\gamma} \partial_x f(x) \right) \right]$$

$t' \rightarrow t$

$$= \prod_{n=0}^{N} \left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}} \right) \exp \left[\int_0^\tau dt \left(-\frac{1}{4k_B T/\gamma} \left\{ -\dot{x}(t) - f(x(t), t)/\gamma \right\}_\circ^2 - \frac{1}{2\gamma} \partial_x f(x) \right) \right]$$

Stochastic Trajectory

Heat & path probabilities

$$\Gamma$$
$$x(t_0=0)\quad x(t_1)\quad \cdots\; x(t_n)\quad \cdots\; x(t_{N-1})\quad x(t_N=\tau)$$
$$\rightarrow \tilde{x}(t) = x(\tau - t)$$
$$\tilde{x}(t_N=\tau)\quad \tilde{x}(t_{N-1})\;\cdots\; \tilde{x}(\tau - t_n)\;\cdots\; \tilde{x}(t_1)\quad \tilde{x}(0)$$
$$\tilde{\Gamma}$$

time-forward path probability

$$P(\Gamma\,|\,x(0)) = \prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[\int_0^\tau dt\left(-\frac{1}{4k_B T/\gamma}\left\{\dot{x}(t) - f(x(t),t)/\gamma\right\}_\circ^2 - \frac{1}{2\gamma}\partial_x f(x)\right)\right]$$

$a = 1/2$

time-reversal path probability

$$\tilde{P}(\tilde{\Gamma}\,|\,x(\tau)) = \prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}}\right)\exp\left[\int_0^\tau dt\left(-\frac{1}{4k_B T/\gamma}\left\{-\dot{x}(t) - f(x(t),t)/\gamma\right\}_\circ^2 - \frac{1}{2\gamma}\partial_x f(x)\right)\right]$$

$$\ln\frac{\mathscr{P}(\Gamma\,|\,x(0))}{\tilde{\mathscr{P}}(\tilde{\Gamma}\,|\,\tilde{x}(\tau))} =$$

Stochastic Trajectory

Summary (overdamped Langevin dynamics)

probability for observing Γ

$$\mathscr{P}(\Gamma) = \prod_{n=0}^{N} \left(\frac{dx(t_n)}{\sqrt{4\pi k_B T dt/\gamma}} \right) \exp\left[\int_0^\tau dt \left(-\frac{1}{4k_B T/\gamma} \left\{ \dot{x}(t) - f(x(t))/\gamma \right\}^2_{\odot_a} - \frac{(1-a)}{\gamma} \partial_x f(x) \right) \right] p_0(x(0))$$

$$\ln \frac{\mathscr{P}(\Gamma \,|\, x(0))}{\tilde{\mathscr{P}}(\tilde{\Gamma} \,|\, \tilde{x}(\tau))} = -\frac{Q}{k_B T}$$

Summary (underdamped Langevin dynamics)

probability for observing Γ

$$\mathscr{P}(\Gamma) = \prod_{n=0}^{N} \frac{dv(t_n) dx(t_n)}{\sqrt{4\pi k_B T dt/m^2}} \delta\left(\dot{x}(t_n) - v(t_n) \right)$$

$$\times \exp\left[\int_0^\tau dt \left(-\frac{\left\{ \dot{v}(t) + \gamma v(t)/m - f(t)/m \right\}^2_{\odot_a}}{4k_B T/m^2} - \frac{(1-a)}{m} \left\{ \partial_v f(t) - \gamma \right\} \right) \right] p_0(x(0), v(0))$$