非平衡科学

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1.1 □平□とは

□□□□□□□□□□□非平衡(non-equilibrium)□□□□□□定□□□. □□□非平衡□□□□□□□, □□□□□□□□□□□□□(□力学, □□力学, □体力学, □子力学, 力学□...etc.)□数学□□定□□□□□□□□□, □□□□□□□□□力学□□□□□非平衡□□□□□□□定□□□□□□□□.

□□□□□□力学□□□□□, □体□□□□□□□□□作□□□□□□□□□□□□□□□□□□□□□□□□. □□, □刻t□□□$\mathcal{X}$□□□□□□□□□$x \in \{1, \cdots, N\}$□□□□□□□分布□$p_X(x;t)$□表□□□□. □□□□分布□□□□

$$\sum_{x=1}^{N} p_X(x;t) = 1, \tag{1.1}$$

□非□□

$$p_X(x;t) \geq 0, \tag{1.2}$$

□□□□□□□□□. □□□X□□□□□□□x□□□□□□□数□□□. □□□□分布□□□□□□□$\mathcal{X}$□□□□□□□□□□□□□□□□□□□□□□□□□□子□□□□□□□□行□□□□□□. □□□□□□□□□□□□□□□□□□□□□□子□□□□□行□□□□, □□□□□□x□□□□□□□□

$$\frac{\partial}{\partial t} p_X(x;t) = 0, \tag{1.3}$$

□□□□□□□□□□□□□□□□□$\mathcal{X}$□□□□定常□□□□□, □(1.3)□□□□□□□依存□□□□□分布$p_X(x;t) = p_X^{\mathrm{ss}}(x)$□定常分布□□□. □$\mathcal{X}$□□□□□□□□□□□□□□□□□□□□□□□□□□, □□□□□□$t \to \infty$□定常分布□□□□.

□$\mathcal{X}$□□□□□□□□□示□□数□□□□□□□□□□□□□□□□□□□□到□□□定常分布□□□□□□分布□□□□□□. □□□□□定常分布□□□□□□分布□□□□□

□定常□□□平衡□□□□□．例□□，□□度β□□□□□□□□□□□□□□□□□□□□□□□□定常分布□，□$\mathcal{X}$□□□□□□□x□□□□□□□□□$E_X(x)$□□□□

$$p_X^{\mathrm{ss}}(x) = \frac{\exp(-\beta E_X(x))}{\sum_x \exp(-\beta E_X(x))}, \tag{1.4}$$

□□□□□□□□分布□□□□□□．□□□□度β□□□□□□□学□□□□□□μ□□□□子□□□□□□□□□，□X□□□□□□□x□□□□□□□□□$E_X(x)$□□子数$N_X(x)$□□□□定常分布□

$$p_X^{\mathrm{ss}}(x) = \frac{\exp(-\beta(E_X(x) - \mu N_X(x)))}{\sum_x \exp(-\beta(E_X(x) - \mu N_X(x)))}, \tag{1.5}$$

□□□□□□□□□□□□分布□□□□□□．□□□□平衡分布□□例□□□．

□□□□□□□□□□□，□□□□□□□．□□分布□□□□□□□□□□□□

$$\frac{\partial}{\partial t} p_X(x;t) \neq 0, \tag{1.6}$$

□□□□□□非定常□□，分布□□□□□□□□□□

$$\frac{\partial}{\partial t} p_X(x;t) = 0, \tag{1.7}$$

□□□□□□定常□□□□□．□□定常□□□□□□例□□□定常分布□□□□□□分布□□□□□□平衡□□□存□□□．平衡□□□□□□□非平衡□□□□□□□□□，非平衡□□□□□□□□□□□□存□□□．□□□非定常□□□□□．□□□□□定常分布□□□□□□分布□□□□□□□□□□□□□非平衡定常□□□□□．表□□□□□□□□□□□□□．

表1.1　定常□□□非定常□□/平衡□□□非平衡□□

□□	定□	定常/非定常	平衡/非平衡
非平衡非定常□□	$\partial p_X(x;t)/\partial t \neq 0$	非定常	非平衡
非平衡定常□□	$\partial p_X(x;t)/\partial t = 0$□□$p_X^{\mathrm{ss}}(x)$□非□□□□□	定常	非平衡
平衡□□	$\partial p_X(x;t)/\partial t = 0$□□$p_X^{\mathrm{ss}}(x)$□□□□□□	定常	平衡

□□□□力学□□□□□□□□□□□$R(t)$□，□□□□□□x□依存□□□□□$r(x)$□分布$p_X(x;t)$□□□□□□□平□$\langle r \rangle_{p_X}$□□□□

$$R(t) = \langle r \rangle_{p_X} = \sum_x r(x) p_X(x;t), \tag{1.8}$$

□□□□□□．□□□□□□□定常□□□□□□□□

$$\frac{dR(t)}{dt} = \sum_x r(x) \frac{\partial p_X(x;t)}{\partial t} = 0, \tag{1.9}$$

□□□□□□□□□□□□□□□□．□□□□□□□□□□□□□□□□□□□□□□□□□□平衡□□□□□□□□□□□．例□□□□最□□□□□例□□□□□度□□□□□□□□□□□□度勾□□□□□□□□．□□□□，□□□□□□□□□□□□□□□□□□□□□□□□，常□□定□□□□□□□□□□□□平衡□□□□□□．

□□□, 非平衡□科学□□□□□□□□□□□□□□□□□□□□□□□□□□□□. □
□□□非平衡定常□□□科学□, 非定常□□□□□□科学□□□. 前□□静□□非□□□
□□分布□科学□□□, □□□□□分布□□□□□□□□□科学□□□. □□□□□□□□
□□□分布□□□□□□□□□□□□□□□□□力学□□力学□□□□, 初□□□□□□
行□□□□□□□□□.

1.2 □□のダイナミクス

1.2.1 マスター方□式

□□□□□□□□□□□□□□□□□□□, □平衡□□□非平衡□□□□□□□□□□
□□□□□□□□. □□□□□□□方□□□□□□□□□□□□□□□□□□□□□□□
□□察□□□□□□□□□□. □□□察□□□□□□方□□□□, □□分布□□□□□□
□□□□□分布□□□□□□依存□□□□□□□□□□□□□□□

$$\frac{\partial}{\partial t}p_X(x;t)=\sum_{x'=1}^{N}W(x|x';t)p_X(x';t). \tag{1.10}$$

□□□$x\in\{1,\ldots,N\}$, $x'\in\{1,\ldots,N\}$□□□. □□係数$W(x|x';t)$□□移□□□□□□
□□.

$p_X(x;t)$□□□分布□□□□□□□, □□□移□□□$W(x,x')$□□□□□□□□□□□
□□□□. □□□□□□方□□(1.10)□x□対□□□□□□□□□□□□□□□(1.1)□□

$$\sum_{x=1}^{N}\sum_{x'=1}^{N}W(x|x';t)p_X(x';t)=\frac{\partial}{\partial t}\sum_{x=1}^{N}p_X(x;t)=\frac{\partial}{\partial t}1=0, \tag{1.11}$$

□□□□□. □□□□□分布$p_X(x';t)$□対□□□□□□□□□□□□□□□□□□□□□□
□□□□□, 例□□□□□y□□□□

$$p_X(x';t)=\delta_{x'y}=\left\{\begin{array}{ll}1 & (x'=y)\\ 0 & (x'\neq y)\end{array}\right., \tag{1.12}$$

□□□分布□□□□□□□, □(1.11)□□□□□$y\in\{1,\ldots,N\}$□対□□

$$\sum_{x=1}^{N}W(x|y;t)=0, \tag{1.13}$$

□□□□□□□□□□□□□□□□□□□.

□□□□□□方□□(1.10)□□□□□$dt>0$□□□□, □散□□□□□□. □□□□散□
□□□□□□方□□□

$$p_X(x;t+dt)-p_X(x;t)=\sum_{x'=1}^{N}W(x|x';t)p_X(x';t)dt, \tag{1.14}$$

□□□□□□□□□□□□. □□□, □□□非□□□□(1.2)□□

$$p_X(x;t+dt)=\sum_{x'=1}^{N}\left(\delta_{xx'}+W(x|x';t)dt\right)p_X(x';t)\geq 0, \tag{1.15}$$

□□□□□, □□□□□□□□分布$p_X(x';t)$□対□□□□□□□□□□□□□□□□□□□□□□□□□, $p_X(x';t)=\delta_{x'y}$□対□□

$$\delta_{xy}+W(x|y;t)dt\geq 0, \tag{1.16}$$

□□□□□, $x\neq y$□□□□□□□$x\in\{1,\dots,N\}$, $y\in\{1,\dots,N\}$□□□□

$$W(x|y;t)\geq 0, \tag{1.17}$$

□□□□□□□□□□□□□□□.

□移□□□□対□□□□□条□□□□□(1.13)□□(1.17)□□□□□□, □□分布□□□□□□□□移□□□□条□□□□$y\neq x$□

$$W(x|y;t)\geq 0, \tag{1.18}$$

$$W(x|x;t)=-\sum_{x'|x'\neq x}W(x'|x;t)\leq 0, \tag{1.19}$$

□□□条□□□□□□□.

□□□□移□□□□条□□□□□□□□, □□□□方□□□別□表□□□□□□□□□□. □(1.19)□条□□□□□□□□□□方□□(1.10)□

$$\begin{aligned}\frac{\partial}{\partial t}p_X(x;t) &= \sum_{x'|x'\neq x}W(x|x';t)p_X(x';t)+W(x|x;t)p_X(x;t) && (1.20)\\ &= \sum_{x'|x'\neq x}[W(x|x';t)p_X(x';t)-W(x'|x;t)p_X(x;t)] && (1.21)\\ &= \sum_{x'=1}^{N}[W(x|x';t)p_X(x';t)-W(x'|x;t)p_X(x;t)], && (1.22)\end{aligned}$$

□□□□□□□. 最□□行□□$W(x|x;t)p_X(x;t)-W(x|x;t)p_X(x;t)=0$□□, $x'=x$□□寄□□0□□□□□□□□□.

1.2.2 □□の流れ

□□□□方□□□□(1.22)□表□□□□□□便利□□□□□□. □□表□□□□□□

$$J(x|x';t)=W(x|x';t)p_X(x';t)-W(x'|x;t)p_X(x;t), \tag{1.23}$$

□寄□$J(x|x';t)$□x'□□x□□□刻t□□□□□□□□□□□. □□□□□□□□□□□方□□□□(1.22)□表□□

$$\frac{\partial}{\partial t}p_X(x;t)=\sum_{x'=1}^{N}J(x|x';t), \tag{1.24}$$

□□□□. □□□□$p_X(x;t)$□□□□□□□x'□□x□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□. □□□□□□□$J(x|x';t)$□

$$J(x|x';t)=J_+(x|x';t)-J_-(x|x';t), \tag{1.25}$$

□x'□□x□□□□□□

$$J_+(x|x';t)=W(x|x';t)p_X(x';t), \tag{1.26}$$

□x□□x'□□□□□□

$$J_-(x|x';t) = W(x'|x;t)p_X(x;t), \tag{1.27}$$

□□□□□□□□□□□□□□□. □□□□□□$x \neq x'$□常□非□□□$J_+(x|x';t) \geq 0$, $J_-(x|x';t) \geq 0$□□□□□□□□□□□□. □□□□□□□□□□□□□□□□□□□□□□□□, □□□□□□□□□□□□保存則$(\partial/\partial t[\sum_x p_X(x;t)] = 0)$□□□□□□□□, □□□□□□□□□□□□方□□(1.24)□表□, □□□□□□□□□□□□□□表□

$$\frac{\partial}{\partial t} p_X(x;t) = \sum_{x'=1}^{N} [J_+(x|x';t) - J_-(x|x';t)], \tag{1.28}$$

□□□□□□□□□□保存則□□□□□□□□□□□□□□□□□□□□□□□□□□.

1.3 定常状態と平□状態

1.3.1 定常状態における□□の流れ

□□□□□□□□□□□□方□□□表□(1.24)□□□□, 定常□□□□□□□□□□□□□□□□察□□□□□. □□非定常□□□条□□(1.6)□□□□□□$J(x|x';t)$□□□□

$$\sum_{x'=1}^{N} J(x|x';t) \neq 0, \tag{1.29}$$

□□□□□□□□□. □□□□, □□x□別□□□x'□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□. □方□定常□□□条□□(1.7)□

$$\sum_{x'=1}^{N} J(x|x';t) = 0, \tag{1.30}$$

□□□□□□□□□x□対□□別□□□x'□□□□□□□□□□□□□□□□□□□□□□□□□□□.

□□□移□□□□□□□依存□□□□□□□□□, 定常□□□条□□(1.30)□□□□□分布$p_X(x;t)$□□□□依存□□□. □□□□□□, □移□□□□□□□依存□□□□□定常分布□□□□依存□□□□□. □□□依存□□□□移□□□□$W(x|x')$□□□□定常分布$p_X^{\rm ss}(x)$□

$$\sum_{x'=1}^{N} W(x|x')p_X^{\rm ss}(x') = 0, \tag{1.31}$$

$$\sum_{x'=1}^{N} p_X^{\rm ss}(x') = 1, \tag{1.32}$$

□□□□□方□□□□□□□□, □□□数□□□□□□□□□□□□□□, □□□□□□□□□□□□□□□□□□. □□, 定常□□□□□□□□□□定常分布$p_X^{\rm ss}(x)$□□□□

$$J^{\rm ss}(x|x') = W(x|x')p_X^{\rm ss}(x') - W(x'|x)p_X^{\rm ss}(x), \tag{1.33}$$

□□□□□□定常□□□□□□□対□□条□

$$\sum_{x'} J^{\rm ss}(x|x') = 0, \tag{1.34}$$

□□定常□□□□□□□□□□□□対□□□束条□□□□□□□□□□□.□□定常□□□□□□□条□□,□□□□□□□□Kirchhoff□□□□則□□□□□□□□条□□□□□□□□□□□□□□定常□□□□□□□□□□□□□□□□数学□□□□□□□□□□,□□□□□□□□□定常□□□□□□□□□□□□□□□□[1].□□□□□□□□□□□□□□,□□□□□□□□□□□□□□□□□力学□□察□□□□□□□□□割□果□□.

1.3.2 平□状態における□□の流れ

平衡□□□定□□定常分布□□□□□□分布□□□□□□□□□□□□□□□□,□□□□□□□□□□□□□□□,□□□□□□条□□平衡□□□定□□□□□□□□□□□□□□.□□定□□□□□□□□条□□□□□□□□□□□□,□□□□□□□□□定□□□□□.

□移□□□□□□□依存□□□□□,□□□□□□条□□

$$J^{\mathrm{ss}}(x|x') = 0, \tag{1.35}$$

□□□□$x \in \{1,\ldots,N\}$, $x' \in \{1,\ldots,N\}$□□□□□□□□□□□□□.□□□定常□□□□□□,□□□□□□□□□□□□□□存□□□□□□□□□□□.□□□□□□□□条□□□□□平衡□□□□□,定常□□□条□□(1.34)□□動□□□□□□□□□□□□□.□□□□□□□□□□条□□

$$W(x|x')p_X^{\mathrm{ss}}(x') = W(x'|x)p_X^{\mathrm{ss}}(x), \tag{1.36}$$

□□□□□□,定常□□□□□□□

$$J_+^{\mathrm{ss}}(x|x') = W(x|x')p_X^{\mathrm{ss}}(x'), \tag{1.37}$$

□□□□

$$J_-^{\mathrm{ss}}(x|x') = W(x'|x)p_X^{\mathrm{ss}}(x), \tag{1.38}$$

□□□□□□□条□

$$J_+^{\mathrm{ss}}(x|x') = J_-^{\mathrm{ss}}(x|x'), \tag{1.39}$$

□□□□□□□□□□□□.

□□□□□□□□,□□□□□□□□条□□□□□□,□□□数x, x'□□□,例□□□子□□度□□□□□□□□対□□□□□分□□□□□□□□□□□□.□□□□度□□□□□□□□□□,□□□□□□条□□修□□□□□[2].

□□□□□□□□□□□条□□□□平衡分布□定□□,定常分布□□□□□□分布□□□□□□□□平衡分布□定□□整□□□保□□□□,□移□□□□対□□□□□□□条□□□□,□□□□□□□□条□□□□□□条□□存□□□.例□□□□度β□□□□□□□□□□□□□□□,定常分布□□□□□□分布(1.4)□□□□□□□□□条□□□□□□□条□(1.36)□□

$$\frac{W(x'|x)}{W(x|x')} = \exp(\beta(E_X(x) - E_X(x'))), \tag{1.40}$$

□□□□移□□□□□□束□□□□□□□□□□.□□□束条□□□□□□□□□□条□□□□.□□□□方□□□平衡□□□□□□□□□□□□□□□□□□□□□□□□□

□□□□□□□□□□□, □□□□□□移□□□□□□□□束条□□□□□□□, □□□□□□□□□□□低□□□□□□□□行□□□□□□□□□□□□移□□□□□□□□□□□□□□□□□. □□□□□□□$E_X(x)$□□散□□□□□□□

$$W(x'|x) = 0 \Leftrightarrow W(x|x') = 0, \tag{1.41}$$

□□□条□□□□□□□□, □□条□□□定□□□□□□□□□□□□. □□条□□□□□□□□$\mathcal{X}$□□□□□作□□□□□x'□□□□x□□□□□有□□□□□□□□□□□□□x□□□□x'□□□□□□□□□□□有□□□□□□□□□□□□□□□□□対□□□□□. □□□□□□□□□□条□□, □□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□例□□文□ [3]□□□□□□.

□□□□□□□□条□(1.36)□□□□□□□□□□□□□□□□□□□, □□□□□□□□条□□□□, □$\mathcal{X}$□□□□□□□□□□□□□□□□□□□□□□$\Delta s^{\mathrm{bath}}(x'|x)$□□□□,

$$\frac{W(x'|x)}{W(x|x')} = \exp(\Delta s^{\mathrm{bath}}(x'|x)), \tag{1.42}$$

□□□□□□□□. □□□□□□□□□□□□□□□□□□□$\Delta s^{\mathrm{bath}}(x'|x)$□□□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□. 実□, 定常□□□□□□□□□条□□□□□□□□$\Delta s^{\mathrm{bath}}(x'|x) = \beta(E_X(x) - E_X(x'))$□□□□□□□□□□□□□$\phi_X(x) = \beta E_X(x)$□□分□$\Delta s^{\mathrm{bath}}(x'|x) = \phi_X(x) - \phi_X(x')$□□□□□, □□□□□□条□□□□□□□非平衡定常□□□□□□□, □□□□□□□□分□□□□□□□□□□□□□□□□□□□□□□□□. □□□□□□□□□□□□□□□□常□$\phi_X(x) = -\ln p_X^{\mathrm{ss}}(x)$□□□□□□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□□□□□分□□□□.

例□□□□□□□□条□□□□□□□例□□□□, □数□□□□□□□□□□□□□□□□. □□□□□□□□□□移□□□□□□□□□□□□□□□□□□□□□□□□□□. □□x'□□□□x□□移□□□□□□□□□□□□度□$\beta_{x'|x}(= \beta_{x|x'})$□□□. □□□□□□□□□□□条□(1.42)□$\Delta s^{\mathrm{bath}}(x'|x) = \beta_{x'|x}(E_X(x) - E_X(x'))$□□□□□□□□□□□. □□□□, 例□□□□□□□□□□x, x', x''□対□□□□□□□□条□(1.36)□

$$\exp[\beta_{x'|x}(E_X(x) - E_X(x'))] = \frac{p_X^{\mathrm{ss}}(x)}{p_X^{\mathrm{ss}}(x')} \tag{1.43}$$

$$\exp[\beta_{x''|x'}(E_X(x') - E_X(x''))] = \frac{p_X^{\mathrm{ss}}(x')}{p_X^{\mathrm{ss}}(x'')} \tag{1.44}$$

$$\exp[\beta_{x|x''}(E_X(x'') - E_X(x))] = \frac{p_X^{\mathrm{ss}}(x'')}{p_X^{\mathrm{ss}}(x)}, \tag{1.45}$$

□□□□, □□□□□□□□条□□

$$\begin{aligned}(\beta_{x'|x} - \beta_{x|x''})E_X(x) + (\beta_{x''|x'} - \beta_{x'|x})E_X(x')\\ +(\beta_{x|x''} - \beta_{x''|x'})E_X(x'') = 0,\end{aligned} \tag{1.46}$$

□□□□□□, $\beta_{x'|x} = \beta_{x''|x'} = \beta_{x|x''}$□□□□□□□□□□□□□□. □□□□□□□□□□□□□□□$\mathcal{X}$□□□□□□□$E_X(x)$□□□□□□度□依存□□□□□□□□□□.□□□□$\mathcal{X}$□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□.

□□□□□□□□□□□□□, □□x'□□□□x□□□移□□数□□□□□□行□□□□□□□□□□□□□□□□□□□□□□□□□□□□. □□□□□□□ν□□□□□□

$$W(x'|x) = \sum_{\nu} W^{(\nu)}(x'|x) \tag{1.47}$$

□□□□□□□□ν□□□□□移□□□□□寄□$W^{(\nu)}(x'|x)$□□□□□□□□□□. □□□□, □□□□□□□□条□□, □□ν□□□□□□□□□□□□□□$\Delta s^{\mathrm{bath}(\nu)}(x'|x)$□□□□

$$\frac{W^{(\nu)}(x'|x)}{W^{(\nu)}(x|x')} = \exp(\Delta s^{\mathrm{bath}(\nu)}(x'|x)), \tag{1.48}$$

□□□□□□□□. □□□□□□□□□□□□□条□(1.48)□□□□□□□, □□□□□□□□□□条□(1.36)□□□□□□.

□2□

□□□□

序□□□□□□□□□□□□□方□□□□□□□□□□, □□□□□□□力学□□□□平衡□非平衡□□□□□□行□□□□□□□. 本□□□□□□□□□□方□□□□□□□□□□定□□□□□□□□□□□□□□□. □□□□□分方□□□□□□□□Langevin方□□□, □□□□方□□□□□□□□□□□□□.

2.1 □□の□性□

□□□□□□□□□□□□□□□□□□. □□□数$\boldsymbol{X} = \{X_1, \dots, X_n\}$□□□□□□□□数□□□$\boldsymbol{x} = \{x_1, \dots, x_n\} \in \{1, \cdots, N\}^n$ □□□□□□□分布□$p_{X_1,\dots,X_n}(x_1, \dots, x_n) = p_{\boldsymbol{X}}(\boldsymbol{x})$□□□□. □□□□□□□分布□□□□

$$\sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) = 1, \tag{2.1}$$

□非□□

$$p_{\boldsymbol{X}}(\boldsymbol{x}) \geq 0, \tag{2.2}$$

□□□□□□□.

2.1.1 周辺化

□□□□□□分布$p_{\boldsymbol{X}}(\boldsymbol{x})$□□, $m(< n)$□□□□□数□□$\boldsymbol{X}_1 = \{X_1, \dots, X_m\} \subset \boldsymbol{X}$□□□□□□$\boldsymbol{x}_1 = \{x_1, \dots, x_m\}$□□□□□□□分布$p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)$□□□□□□□□□. □□□作□□□□□□□. □体□□□X_m□□□□□□数$\boldsymbol{X}_2 = \{X_{m+1}, \dots, X_n\}$□□□□□□□□$\boldsymbol{x}_2 = \{x_{m+1}, \dots, x_n\}$□□□□□□□□□□□

$$p_{\boldsymbol{X}_1}(\boldsymbol{x}_1) = \sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1, \boldsymbol{x}_2), \tag{2.3}$$

□□□□□分布$p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)$□□□□□□□□□□, □□□□□□□分布□□□□□□□□□□□□非□□□条□□□□□□□□□□□□□□□□□□□□□. □□□□□□□□

$$\sum_{\boldsymbol{x}_1} p_{\boldsymbol{X}_1}(\boldsymbol{x}_1) = \sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) = 1, \tag{2.4}$$

非□□□□□□□

$$p_{\boldsymbol{X}_1}(\boldsymbol{x}_1) = \sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}}(\boldsymbol{x}) \geq 0, \tag{2.5}$$

□□□□□□□□□□.

2.1.2 条件付き□□分布

□□□□□□□数□□$\boldsymbol{X}_1 = \{X_1, \dots, X_m\}$□□□$\boldsymbol{x}_1 = \{x_1, \dots, x_m\}$□□□条□□□□□□□□数□□$\boldsymbol{X}_2 = \{X_{m+1}, \dots, X_n\}$□□□$\boldsymbol{x}_2 = \{x_{m+1}, \dots, x_n\}$□□□条□□□□□分布□□□□□□定□□□□□□□□□.

$$\begin{aligned} p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1) &= p_{X_{m+1},\dots,X_n|X_1,\dots,X_m}(x_{m+1}, \dots, x_n|x_1, \dots, x_m) \\ &= \frac{p_{\boldsymbol{X}}(\boldsymbol{x})}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)} = \frac{p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1, \boldsymbol{x}_2)}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)}. \end{aligned} \tag{2.6}$$

□□□□条□□□□□分布□□□□□□□□□□□□,□□□□□□□□□□□非□□□条□□□□□□□□□□□□□□□.□□□□□□□□

$$\sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1) = \frac{\sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}}(\boldsymbol{x})}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)} = \frac{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)} = 1, \tag{2.7}$$

非□□□□□□□

$$p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1) = \frac{p_{\boldsymbol{X}}(\boldsymbol{x})}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)} \geq 0, \tag{2.8}$$

□□□□□□□□□□.□□□□条□□□□□分布□定□□□□□□□□□□□□□□□, Bayes□□□□□□□□□□□.$n = 2$□□□

$$p_{X_1|X_2}(x_1|x_2) = \frac{p_{X_2|X_1}(x_2|x_1) p_{X_1}(x_1)}{p_{X_2}(x_2)} = \frac{p_{X_2|X_1}(x_2|x_1) p_{X_1}(x_1)}{\sum_{x_1} p_{X_2|X_1}(x_2|x_1) p_{X_1}(x_1)}, \tag{2.9}$$

□□□, X_2□□□□□□□□□□□□□□□□□X_1□□□□□□□□□□□□□察□□□□□□□. $p_{X_1|X_2}(x_1|x_2)$□□□□□, $p_{X_1}(x_1)$□□前□□□位□□□□□□□, □度□数$p_{X_2|X_1}(x_2|x_1)$□□□□□前□□□□□□□□□□新□□□□□□□□□□□□□□□. Bayes□定□文□□□□度□□数□□定□□□□□□□□□.

□□, 条□□□□□分布□対□□□□□□□□□□□.□□□□□□□数□□□$m < l < n$□□□□□□□$\boldsymbol{X}_1 = \{X_1, \dots, X_m\}$, $\boldsymbol{X}_2 = \{X_{m+1}, \dots, X_l\}$, $\boldsymbol{X}_3 = \{X_{l+1}, \dots, X_n\}$□□□□□分割□□□□□, 対□□□□□□□□□□$\boldsymbol{x}_1 = \{x_1, \dots, x_m\}$, $\boldsymbol{x}_2 = \{x_{m+1}, \dots, x_l\}$, $\boldsymbol{x}_3 = \{x_{l+1}, \dots, x_n\}$□□□□. □□□, $\boldsymbol{x}_2$□対□□□□□□□,

$$\begin{aligned} \sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}_2,\boldsymbol{X}_3|\boldsymbol{X}_1}(\boldsymbol{x}_2, \boldsymbol{x}_3|\boldsymbol{x}_1) &= \frac{\sum_{\boldsymbol{x}_2} p_{\boldsymbol{X}}(\boldsymbol{x})}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)} \\ &= \frac{p_{\boldsymbol{X}_1,\boldsymbol{X}_3}(\boldsymbol{x}_1, \boldsymbol{x}_3)}{p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)} = p_{\boldsymbol{X}_3|\boldsymbol{X}_1}(\boldsymbol{x}_3|\boldsymbol{x}_1), \end{aligned} \tag{2.10}$$

□□□□□□□数□□$\boldsymbol{X}_1$□条□□□□□□□□数□□$\boldsymbol{X}_3$□□□条□□□□□分布□□□□□, □□□数□□$\boldsymbol{X}_2$□□□□□□□□□□□.

□□条□□□□□分布□定□(2.6)□使□□□□, □□□chain rule□□□□□□□□□□□□分布□条□□□□□分布□□□□分□□□分□□□□□□□. □□chain rule□

$$p_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{k=2}^{n} p_{X_k|X_1,\dots,X_{k-1}}(x_k|x_1, \dots, x_{k-1}) p_{X_1}(x_1), \tag{2.11}$$

□□□□□, 定□(2.6)□□□□

$$
\begin{aligned}
p_{\boldsymbol{X}}(\boldsymbol{x}) &= p_{\boldsymbol{X}}(\boldsymbol{x}) \prod_{k=1}^{n-1} \frac{p_{X_1,\ldots,X_k}(x_1,\ldots,x_k)}{p_{X_1,\ldots,X_k}(x_1,\ldots,x_k)} \\
&= \prod_{k=2}^{n} \frac{p_{X_1,\ldots,X_k}(x_1,\ldots,x_k)}{p_{X_1,\ldots,X_{k-1}}(x_1,\ldots,x_{k-1})} p_{X_1}(x_1) \\
&= \prod_{k=2}^{n} p_{X_k|X_1,\ldots,X_{k-1}}(x_k|x_1,\ldots,x_{k-1}) p_{X_1}(x_1), \qquad (2.12)
\end{aligned}
$$

□□□□□□□□□□.

2.1.3 □□変数□の独□性

□□□□□数□□$\boldsymbol{X}_1 = \{X_1,\ldots,X_m\}$□$\boldsymbol{X}_2 = \{X_{m+1},\ldots,X_n\}$□□□□□□□□□□□$\boldsymbol{x}_1 = \{x_1,\ldots,x_m\}$□$\boldsymbol{x}_2 = \{x_{m+1},\ldots,x_n\}$□対□□

$$
p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2) = p_{\boldsymbol{X}_1}(\boldsymbol{x}_1) p_{\boldsymbol{X}_2}(\boldsymbol{x}_2), \qquad (2.13)
$$

□□□□□□, $\boldsymbol{X}_1$□$\boldsymbol{X}_2$□□□□□□□□□. □□□□□□条□□□□□分布□定□(2.6)□□□□

$$
p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1) = p_{\boldsymbol{X}_2}(\boldsymbol{x}_2), \qquad (2.14)
$$

□□□□□□□□□□□□□□. □□□条□□□□□分布□□□□□□□数□□$\{X_1,\ldots,X_m\}$□依存□□存□□□□□□□□□□□□. □□□□□□条□□□□□分布$p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1)$□□□$\boldsymbol{x}_1$□依存□□□□数□□□□□□□分布$p_{\boldsymbol{X}_2}(\boldsymbol{x}_2)$□□□□□□□□□□□□□□□□□□.

□□□条□□□□□□□□□□□□□□□□□□. □□□数□□$\boldsymbol{X}_1 = \{X_1,\ldots,X_m\}$, $\boldsymbol{X}_2 = \{X_{m+1},\ldots,X_l\}$, $\boldsymbol{X}_3 = \{X_{l+1},\ldots,X_n\}$□□□□□対□□□□□$\boldsymbol{x}_1 = \{x_1,\ldots,x_m\}$, $\boldsymbol{x}_2 = \{x_{m+1},\ldots,x_l\}$, $\boldsymbol{x}_3 = \{x_{l+1},\ldots,x_n\}$□対□□

$$
p_{\boldsymbol{X}_2,\boldsymbol{X}_3|\boldsymbol{X}_1}(\boldsymbol{x}_2,\boldsymbol{x}_3|\boldsymbol{x}_1) = p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1) p_{\boldsymbol{X}_3|\boldsymbol{X}_1}(\boldsymbol{x}_3|\boldsymbol{x}_1), \qquad (2.15)
$$

□□□□□□, $\boldsymbol{X}_2$□$\boldsymbol{X}_3$□$\boldsymbol{X}_1$□□□□□□□□□□□. 条□□□□□分布□定□□(2.6)□□□□□□□□□□□□□

$$
p_{\boldsymbol{X}_3|\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_3|\boldsymbol{x}_2,\boldsymbol{x}_1) = p_{\boldsymbol{X}_3|\boldsymbol{X}_1}(\boldsymbol{x}_3|\boldsymbol{x}_1), \qquad (2.16)
$$

□□□□□□□□□.

□□条□□□□□□□□□□□$\boldsymbol{X}_3 = X_k$, $\{X_1,\ldots,X_{k-1}\} = \boldsymbol{X}_1 \cup \boldsymbol{X}_2$□□□. □□$\boldsymbol{X}_1$□$\{X_1,\ldots,X_{k-1}\}$□□分□□□□□. □□□分□□$\boldsymbol{X}_1$□$X_k$□□□□□□□□□□□$\mathrm{Pa}(X_k)$□□□表□□□□□$\boldsymbol{X}_1 = \mathrm{Pa}(X_k) \subset \{X_1,\ldots,X_{k-1}\}$□表□□□. □□□□□(2.16)□□□

$$
p_{X_k|X_1,\ldots,X_{k-1}}(x_k|x_1,\ldots,x_{k-1}) = p_{X_k|\mathrm{Pa}(X_k)}(x_k|\mathrm{pa}(x_k)), \qquad (2.17)
$$

□□□□□□□□□. □□□$\mathrm{pa}(x_k)$□□□□数□□$\mathrm{Pa}(X_k)$□対□□□□□

$$
\mathrm{pa}(x_k) = \{x_l | X_l \in \mathrm{Pa}(X_k)\} \subset \{x_1,\ldots,x_{k-1}\}, \qquad (2.18)
$$

□表□．□□□，□□条□□□□□□□，X_k□□□□条□□□□□□X_k□□□□□□□□Pa(X_k)□□□□数□□□条□□□□□□□□□□□□□□□□□□□□□□．□□□□chain rule (2.11)□□□□□□□□非常□□□□□□□□□□□□□□□□□□□□，

$$p_{\boldsymbol{X}}(\boldsymbol{x})=\prod_{k=2}^{n}p_{X_k|\mathrm{Pa}(X_k)}(x_k|\mathrm{pa}(x_k))p_{X_1}(x_1). \tag{2.19}$$

□□□□□chain rule□表□□，□□□数□□依存□□表□□□□□有□□□□，□□Pa(X_k)□□体□□□□方□□□□X_k□□□□□□□□有□非□□□□□(DAG)□表□□□□□□□□□□□□□□□□□□[4]□□□□□．□□□□□□□□□□□□□□□□□依存□□□□□□□□□□□□有□□□□□□□□，例□□□□□□□□□□□作□□□□□□□□□□□□□□．

2.1.4 状態が□□の場合

□□□□□□□□□□散□□$x_k \in \{1,\dots,N\}$□対□□□□□行□□□□□□，□□□$x_k\in\mathsf{R}$□□□□□分布□□□□□□□□□□□□□□□□定□□□□．□□□□□□□数$\boldsymbol{X}=\{X_1,\dots,X_n\}$□□□□□□□□数□□□$\boldsymbol{x}=\{x_1,\dots,x_n\}\in\mathsf{R}^n$ □□□□□□□分布□$P_{X_1,\dots,X_n}(x_1,\dots,x_n)=P_{\boldsymbol{X}}(\boldsymbol{x})$□□□□

$$\int d\boldsymbol{x}P_{\boldsymbol{X}}(\boldsymbol{x})=1, \tag{2.20}$$

□非□□

$$P_{\boldsymbol{X}}(\boldsymbol{x})\geq 0, \tag{2.21}$$

□□□□，□□□□

$$\int d\boldsymbol{x}_1P_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2)=P_{\boldsymbol{X}_2}(\boldsymbol{x}_2), \tag{2.22}$$

□□□□，□□□□□□□□□定□□□□□□□．□□□$\boldsymbol{X}_1=\{X_1,\dots,X_m\}$, $\boldsymbol{x}_1=\{x_1,\dots,x_m\}$, $\boldsymbol{X}_2=\{X_{m+1},\dots,X_n\}$, $\boldsymbol{x}_2=\{x_{m+1},\dots,x_n\}$□□□□□．□□，□□□□□□□□□□□□□□散□□$x_k\in\{1,\dots,N\}$□対□□□□□行□□□□□□，□□□□$x_k\in\mathsf{R}$□□$\sum_{x=1}^{N}$□$\int dx$□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□．

2.2 Markov□鎖

□□□，□□□□条□□□□□分布□□□□□□□数□□$\{X_1,\dots,X_m\}$□依存□□□□□□□□□□数□□Pa(X_k)□表□□□条□□□□□□□□□□□□□□□□□□□□□，□□□□Pa(X_k) $=X_{k-1}$□□□□□□□□□□□□□□□□□．□□□□条□□□□□分布□

$$p_{X_k|X_1,\dots,X_{k-1}}(x_k|x_1,\dots,x_{k-1})=p_{X_k|X_{k-1}}(x_k|x_{k-1}), \tag{2.23}$$

□□□□□□□□□□□□□□．□□□□□□□□数X_k□□前□□□□数X_{k-1}□□□依存□，□□□前□□□□数□□$\{X_{k-2},\dots,X_1\}$□□□依存□□□□□□□□□□□□□□．□

□□□, □□□chain rule□

$$p_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{k=2}^{n} p_{X_k|X_{k-1}}(x_k|x_{k-1}) p_{X_1}(x_1). \tag{2.24}$$

□□□□□□□□Markov□□□□□, $X_1 \to X_2 \to X_3 \to \cdots X_n$□□□□□□□□.

□□□□3□$i < j < k$□□□□□□□□□

$$p_{X_i,X_j,X_k}(x_i, x_j, x_k) = p_{X_k|X_j}(x_k|x_j) p_{X_j|X_i}(x_j|x_i) p_{X_i}(x_i), \tag{2.25}$$

□□□□□□□□□□□示□□. $\boldsymbol{X}_1 = \{X_1, \ldots, X_{i-1}\}$, $\boldsymbol{X}_2 = \{X_{i+1}, \ldots, X_{j-1}\}$, $\boldsymbol{X}_3 = \{X_{j+1}, \ldots, X_{k-1}\}$□□, 対□□□□□□$\boldsymbol{x}_1 = \{x_1, \ldots, x_{i-1}\}$, $\boldsymbol{x}_2 = \{x_{i+1}, \ldots, x_{j-1}\}$, $\boldsymbol{x}_3 = \{x_{j+1}, \ldots, x_{k-1}\}$□□□□. □□□□

$$\begin{aligned}
& p_{\boldsymbol{X}_3,X_k|X_i,X_j}(\boldsymbol{x}_3, x_k|x_i, x_j) \\
&= \frac{\sum_{\boldsymbol{x}_1,\boldsymbol{x}_2} p_{\boldsymbol{X}_3,X_k|\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_3, x_k|\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j) p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)}{\sum_{\boldsymbol{x}_1,\boldsymbol{x}_2} p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)} \\
&= \frac{\prod_{k'=j+1}^{k} p_{X_{k'}|X_{k'-1}}(x_{k'}|x_{k'-1}) \sum_{\boldsymbol{x}_1,\boldsymbol{x}_2} p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)}{\sum_{\boldsymbol{x}_1,\boldsymbol{x}_2} p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)} \\
&= \prod_{k'=j+1}^{k} p_{X_{k'}|X_{k'-1}}(x_{k'}|x_{k'-1}) \\
&= \frac{\prod_{k'=j+1}^{k} p_{X_{k'}|X_{k'-1}}(x_{k'}|x_{k'-1}) \sum_{\boldsymbol{x}_1,x_i,\boldsymbol{x}_2} p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)}{\sum_{\boldsymbol{x}_1,x_i,\boldsymbol{x}_2} p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)} \\
&= \frac{\sum_{\boldsymbol{x}_1,x_i,\boldsymbol{x}_2} p_{\boldsymbol{X}_3,X_k|\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_3, x_k|\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j) p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)}{\sum_{\boldsymbol{x}_1,x_i,\boldsymbol{x}_2} p_{\boldsymbol{X}_1,X_i,\boldsymbol{X}_2,X_j}(\boldsymbol{x}_1, x_i, \boldsymbol{x}_2, x_j)} \\
&= p_{\boldsymbol{X}_3,X_k|X_j}(\boldsymbol{x}_3, x_k|x_j),
\end{aligned} \tag{2.26}$$

□□□□□□□□□□□□, $\boldsymbol{X}_3$□対□□□□□□□□□□

$$\begin{aligned}
p_{X_k|X_i,X_j}(x_k|x_i, x_j) &= \sum_{\boldsymbol{x}_3} p_{\boldsymbol{X}_3,X_k|X_i,X_j}(\boldsymbol{x}_3, x_k|x_i, x_j) \\
&= \sum_{\boldsymbol{x}_3} p_{\boldsymbol{X}_3,X_k|X_j}(\boldsymbol{x}_3, x_k|x_j) = p_{X_k|X_j}(x_k|x_j),
\end{aligned} \tag{2.27}$$

□X_k□X_i□X_j□□□□□条□□□□□□□□□□□□□□□. □□条□□□□□□□, □体□対□□$p_{X_i,X_j}(x_i, x_j)$□□□□□

$$p_{X_k|X_i,X_j}(x_k|x_i, x_j) p_{X_i,X_j}(x_i, x_j) = p_{X_k|X_j}(x_k|x_j) p_{X_i,X_j}(x_i, x_j) \tag{2.28}$$

$$p_{X_i,X_j,X_k}(x_i, x_j, x_k) = p_{X_k|X_j}(x_k|x_j) p_{X_j|X_i}(x_j|x_i) p_{X_i}(x_i), \tag{2.29}$$

□□(2.25)□$X_i \to X_j \to X_k$□□□Markov□□□□□□□□□□□□□.

2.3 Chapman-Kolmogorov方□式

2.3.1 Markov□□

□□□□□□□□□□□□□数X_k□□□□□□□□□何□□□□□□□□□. □□□□分布$p_{\boldsymbol{X}}(\boldsymbol{x})$□□□□□□□□□□□□□□□□□□□□□□□□, □□□□□□□□□□□

□□□察□□□□□□□.□, □□□数□X_k□□刻t_k□□$\mathcal{X}$□□□x_k□表□□□□数□□□□□□□□□.□□□, □□□□$t_1 < t_2 < ... < t_n$□□□□□□□.□□□, 条□□□□□分布

$$p_{X_k|X_1,\dots,X_{k-1}}(x_k|x_1,\dots,x_{k-1}), \tag{2.30}$$

□□刻t_k□□□□□$x_1,\dots,x_{k-1}$□□□□□□□□刻□□□x_k□□定□□□□□□□□□□□□□□□□□.□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□数X_t□□□□□□□□方□□□□□□□□□.

□□□□□□□Markov□□

$$p_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{k=2}^{n} p_{X_k|X_{k-1}}(x_k|x_{k-1}) p_{X_1}(x_1), \tag{2.31}$$

□□□□□□□□□□□, □□□□□□□Markov□□□□□.

2.3.2 Chapman-Kolmogorov方□式

Markov□□□□□□□, Markov□□□□□□$t_i < t_j < t_k$□对□□

$$p_{X_i,X_j,X_k}(x_i,x_j,x_k) = p_{X_k|X_j}(x_k|x_j) p_{X_j|X_i}(x_j|x_i) p_{X_i}(x_i), \tag{2.32}$$

□□□□□.□□□□x_j□□□□□, □□□$p_{X_i}(x_i)$□□□□□□

$$p_{X_k|X_i}(x_k|x_i) = \sum_{x_j} p_{X_k|X_j}(x_k|x_j) p_{X_j|X_i}(x_j|x_i) \tag{2.33}$$

□□□□□.□□□□Chapman-Kolmogorov方□□□□□. □刻□依存□□□□□□□, $p_{X_k|X_j}(x_k|x_j) = p(x_3;t_3|x_2;t_2)$, $p_{X_j|X_i}(x_j|x_i) = p(x_2;t_2|x_1;t_1)$, $p_{X_k|X_i}(x_k|x_i) = p(x_3;t_3|x_1;t_1)$□□□□□□□□□□

$$p(x_3;t_3|x_1;t_1) = \sum_{x_2} p(x_3;t_3|x_2;t_2) p(x_2;t_2|x_1;t_1), \tag{2.34}$$

□□□.□□□$p(x;t|y;s)$□□刻$s(<t)$□□□y□□□□□□条□□□□□□刻t□□□x□□□□□□□□□□□□□□.□□$p(x;t|y;s)$□□数□□□□□□察□□□□□□$\mathcal{X}$□□□□□□□□□□□□□□□□□□□□□□□□, Chapman-Kolmogorov方□□□Markov□□□□□□$p(x;t|y;s)$□□□□条□□表□□□□.

□□x_k□□□□$x_k \in \mathsf{R}$□□□, $P_{X_k|X_j}(x_k|x_j) = P(x_3;t_3|x_2;t_2)$, $P_{X_j|X_i}(x_j|x_i) = P(x_2;t_2|x_1;t_1)$, $P_{X_k|X_i}(x_k|x_i) = P(x_3;t_3|x_1;t_1)$□□□□, Chapman-Kolmogorov方□□□

$$P(x_3;t_3|x_1;t_1) = \int dx_2 P(x_3;t_3|x_2;t_2) P(x_2;t_2|x_1;t_1), \tag{2.35}$$

□□□□□□□□□□□.□□□□$P(x;t|y;s)$□□定□□□分方□□□□□□□□□□□□□.

2.4 マスター方□式

2.4.1 □散状態の場合

Chapman-Kolmogorov方□□□□分方□□□□□□□□□□□□□, □□□分方□□□対□□□□分方□□□□□□□□□□□□□. 実□□□□分方□□□□□□□□方□□□□□□□□□□□□□□□□□□□. □□□□□□□散□□□□□察□□.

□□□□□□$dt > 0$□□□□□□. □□□t_2□$t_1 < t_2 < t_3$□□□□□□□□□□, $t_2 = t_3 - dt$□□□□. □□□, Chapman-Kolmogorov方□□(2.34)□□□□□□

$$p(x_3; t_3|x_2; t_2) = p(x_3; t_2 + dt|x_2; t_2), \tag{2.36}$$

□□□□□□□□□. □□□数□対□□

$$\lim_{dt\to 0} p(x_3; t_2 + dt|x_2; t_2) = \delta_{x_3,x_2}, \tag{2.37}$$

□□□□□□□□□□□. □□□□□$dt \to 0$□□□□, □刻t_2□□□□□□x_2□□□□, □刻$t_2 + dt$□□□□□□$x_3 = x_2$□□□□□□1□, □□□□□□□$x_3 \neq x_2$□0□□□□□□□□□□□□□□□□□□□.

□□dt□有□□□□, dt□□□□□□□□□係数□$W(x_3|x_2; t_2)$□□□□. □□□ dt□□□□□□□□□□□

$$p(x_3; t_2 + dt|x_2; t_2) = \delta_{x_3,x_2} + W(x_3|x_2; t_2)dt + O(dt^2). \tag{2.38}$$

□□□□□□□□□□□□□□. □□□$O(dt^2)$□dt^2□□□□□□□□表□□□□□□□□□□□. $p(x_3; t_2 + dt|x_2; t_2)$□非□□□□□□□□□□$x_3 \neq x_2$□

$$W(x_3|x_2; t_2) \geq 0, \tag{2.39}$$

□, □□□□□□条□

$$\sum_{x_3} p(x_3; t_2 + dt|x_2; t_2) = 1, \tag{2.40}$$

□□□□□□□□

$$\sum_{x_3} W(x_3|x_2; t_2) = 0, \tag{2.41}$$

$$W(x_2|x_2; t_2) = -\sum_{x_3|x_3\neq x_2} W(x_3|x_2; t_2) \leq 0, \tag{2.42}$$

□条□□□□□□□□.

□□dt□□□□□□□□□□(2.38)□表□□Chapman-Kolmogorov方□□(2.34)□□□□□□□,

$$\begin{aligned} p(x_3; t_2 + dt|x_1; t_1) &= \sum_{x_2} [\delta_{x_3,x_2} + W(x_3|x_2; t_2)dt] p(x_2; t_2|x_1; t_1) \\ &= p(x_3; t_2|x_1; t_1) + dt \sum_{x_2} W(x_3|x_2; t_2) p(x_2; t_2|x_1; t_1), \end{aligned} \tag{2.43}$$

□□,

$$
\begin{aligned}
&\frac{p(x_3;t_2+dt|x_1;t_1)-p(x_3;t_2|x_1;t_1)}{dt}\\
&=\sum_{x_2} W(x_3|x_2;t_2)p(x_2;t_2|x_1;t_1)\\
&=\sum_{x_2|x_2\neq x_3}[W(x_3|x_2;t_2)p(x_2;t_2|x_1;t_1)-W(x_2|x_3;t_2)p(x_3;t_2|x_1;t_1)]\\
&=\sum_{x_2}[W(x_3|x_2;t_2)p(x_2;t_2|x_1;t_1)-W(x_2|x_3;t_2)p(x_3;t_2|x_1;t_1)] \qquad (2.44)
\end{aligned}
$$

□□□□□. □□□条□□□□□分布□対□□□□□方□□□□□□□□□□□.□□□□$p_{X_i}(x_i)=p_X(x_1;t_1)$□表□□□□□□, □(2.44)□□□□$p_{X_i}(x_i)=p_X(x_1;t_1)$□□□□$x_i$□□□□□□□□□□□□行□□□□□□□. □□□□, □□□□□□□分布$p_X(x;t)=\sum_{x_1}p(x;t|x_1;t_1)p_X(x_1;t_1)$□対□□□,

$$
\begin{aligned}
&\frac{p_X(x_3;t_2+dt)-p_X(x_3;t_2)}{dt}\\
&=\sum_{x_2} W(x_3|x_2;t_2)p_X(x_2;t_2)\\
&=\sum_{x_2}[W(x_3|x_2;t_2)p_X(x_2;t_2)-W(x_2|x_3;t_2)p_X(x_3;t_2)], \qquad (2.45)
\end{aligned}
$$

□□□□□□□, $x_2=x'$, $x_3=x$, $t_2=t$□□□表□□□□□□$dt\to 0$□□□□□察□□□,

$$
\begin{aligned}
\frac{\partial}{\partial t}p_X(x;t) &= \sum_{x'} W(x|x';t)p_X(x';t)\\
&=\sum_{x'}[W(x|x';t)p_X(x';t)-W(x'|x;t)p_X(x;t)], \qquad (2.46)
\end{aligned}
$$

□□□□□.□□□□1□□□察□□□□□□方□□□□□□□□, 係数□□□□□□$W(x|x';t)$□□刻t□□x'□□x□□□移□□□□□□□□.□

2.4.2 □□状態の場合

□□□□□□□□□$x\in$ R□□□□□□□□□□□□方□□□□察□□□. □□□$x_2=x_3$□□□□□分布$P(x_3;t_2+dt|x_2;t_2)$□□□□□□□□□数$\delta(x_3-x_2)$□□□□□□□□□□□□□□□□干□□□□□□□□□. □□□□□□□

$$\lim_{dt\to 0}P(x_3;t_2+dt|x_2;t_2)=\delta(x_3-x_2) \qquad (2.47)$$

□□□□dt□□□□□□□□□□

$$P(x_3;t_2+dt|x_2;t_2)=[1+\mathsf{W}(x_2;t_2)dt]\delta(x_3-x_2)+W(x_3|x_2;t_2)dt \qquad (2.48)$$

□□□□$\mathsf{W}(x_2;t_2)$□□□□□□□□□□□□□□□□□. □□□$x_2=x_3$□□□□□□□□□$W(x_3|x_2;t_2)$□□□係数□□□□□□□, $x_2=x_3$□□□dt□□□□□寄□□□□□□□□□□□□□□□□□□□□□. □□□非□□□□$x_3\neq x_2$□

$$W(x_3|x_2;t_2)\geq 0, \qquad (2.49)$$

□□□, □□□□□□ $\int dx_3 P(x_3;t_2+dt|x_2;t_2)=1$□□,

$$\mathsf{W}(x_2;t_2) = -\int dx' W(x'|x_2;t_2) \tag{2.50}$$

□□□□□. □□□□□□□□□□□Chapman-Kolmogorov方□□(2.35)□□(2.48)□□□□□□

$$\begin{aligned}
&\frac{P(x_3,t_2+dt|x_1;t_1)-P(x_3;t_2|x_1;t_1)}{dt} \\
&= \mathsf{W}(x_3;t_2)P(x_3;t_2|x_1;t_1) + \int dx_2 W(x_3|x_2;t_2)P(x_2;t_2|x_1;t_1) \\
&= \int dx' [W(x_3|x';t_2)P(x',t_2|x_1;t_1) - W(x'|x_3;t_2)P(x_3;t_2|x_1;t_1)],
\end{aligned} \tag{2.51}$$

□□□□□. □□□ $P_{X_i}(x_i)=P_X(x_1;t_1)$, $x_3=x$, $t_2=t$□□□表□□□□□, $P_{X_i}(x_i)=P_X(x_1;t_1)$□□□□□□□ $P_X(x;t)=\int dx_1 P(x;t|x_1;t_1)P_X(x_1;t_1)$□□□□□□□□□□ $dt\to 0$□□□□□察□□□,

$$\frac{\partial}{\partial t}P_X(x;t) = \int dx' \left[W(x|x';t)P_X(x';t) - W(x'|x;t)P_X(x;t)\right], \tag{2.52}$$

□□□□□□□対□□□□□□方□□□□□□□. □□□ $W(x|x';t)$□□刻t□□x'□□x□□□移□□□□□□□□.

□□□□□□□□□□散□□□□□□□□□, Chapman-Kolmogorov方□□□□□□□□方□□□□□□□□.□□□□□$\mathcal{X}$□□□□□□□□□□Markov□□□□□, □□□□方□□□□察□□□□□□□□□□□□□□□□□□, 1□□□□□□Markov□□□□□□□□. 実□□□前□□□□□□依存□□□□□□□□□□□□□□□Markov□□□□定□, □□□□□□$\mathcal{X}$□□分□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□, 広□□□□□□□□□□□□1□□□□□□□□. □□□, □□□□□□$\mathcal{X}$□□□□□□□依存□□□□□□□□□□□□□□□□□, □□□□□非Markov□□□□□□□□□□□□□□方□□□□□□□□□□□□□□. □□□□□□□□□□□□□□非Markov□□□□□□□□□□□, Chapman-Kolmogorov方□□□□□□□□chain rule□□□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□分布□□□□□□□□□□□□□□□□□□□□.

2.5 Fokker-Planck方□式

2.5.1 Kramers-Moyal展□

□□□□□□□□□□□□□□□□□□方□□□□□□□□察□□□□. □□□□□□$x\in\mathsf{R}(x'\in\mathsf{R})$□対□□□□□□方□□(2.52)□, $r=x-x'$□□□□数□□□□□, $W(x|x';t)=w(r|x';t)$□□□□□□分□□□□□移□□□□表□□□□□□,

$$\begin{aligned}
\partial_t P_X(x;t) &= \int dr \left[W(x|x-r;t)P_X(x-r;t) - W(x-r|x;t)P_X(x;t)\right] \\
&= \int dr \left[w(r|x-r;t)P_X(x-r;t) - w(-r|x;t)P_X(x;t)\right],
\end{aligned} \tag{2.53}$$

□□□□□□□□□□□．□□□$w(r|x-r;t)P_X(x-r;t)$□対□□□□□□□Taylor□□□□□□□，

$$w(r|x-r;t)P_X(x-r;t) = \sum_{k=0}^{\infty} \frac{(-r)^k}{k!}(\partial_x)^k [w(r|x;t)P_X(x;t)]. \tag{2.54}$$

□□Taylor□□□□□□□方□□(2.53)□□□□□□

$$\begin{aligned} \partial_t P(x,t) &= \sum_{k=1}^{\infty} \frac{(-1)^k}{k!}(\partial_x)^k \left[\left[\int drr^k w(r|x;t) \right] P_X(x;t) \right] \\ &\quad + \int dr \left[w(r|x;t)P_X(x;t) - w(-r|x;t)P_X(x;t) \right] \\ &= \sum_{k=1}^{\infty} \frac{(-1)^k}{k!}(\partial_x)^k \left[\left[\int drr^k w(r|x;t) \right] P_X(x;t) \right], \end{aligned} \tag{2.55}$$

□□□□□□□□□□□．□□□，$k=0$□□□分□□□$\int drw(r|x;t) = \int drw(-r|x;t)$□□□□□□□□□．□□□，□□□□□□□□□□方□□□

$$\partial_t P_X(x;t) = \sum_{k=1}^{\infty} \frac{(-1)^k}{k!}(\partial_x)^k [A^{(k)}(x;t)P_X(x;t)], \tag{2.56}$$

$$A^{(k)}(x;t) = \int drr^k w(r|x;t). \tag{2.57}$$

□□□□□分方□□□□□□□□□□□□．□□□□□Kramers-Moyal□□□□□□□□□．

2.5.2 Fokker-Planck方□式

□□□□□□□例□□□Kramers-Moyal□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□．□□□□

$$\partial_t P_X(x;t) = -\partial_x [A^{(1)}(x;t)P_X(x;t)] + \frac{1}{2}(\partial_x)^2 [A^{(2)}(x;t)P_X(x;t)], \tag{2.58}$$

□□□□□□□□．□□□(2.58)□Fokker-Planck方□□□□□□□□□．

□□Fokker-Planck方□□□□□□□□□□□□□□□□定□，Taylor□□□□□□□□切□□□□□□□□□□□□□□□□□□．例□□，□□□$|r|$□□$w(r|x';t)$□有□□□□□□，□分□□□$|r|$□□$w(r|x';t) \simeq 0$□□□□□□□□□□□□□□□移□□□□□□□□□□□□□□切□□□□□□□□□□．

□□Fokker-Planck方□□(2.58)□□□□□□□□□□□□□□□□□□□□□□□□□．

$$\partial_t P_X(x;t) = -\partial_x [\nu_X(x;t)P_X(x;t)] = -\partial_x [j_X(x;t)], \tag{2.59}$$

$$j_X(x;t) = A^{(1)}(x;t)P_X(x;t) - \frac{1}{2}\partial_x [A^{(2)}(x;t)P_X(x;t)]. \tag{2.60}$$

□□□□□□□□□□□□，$\nu_X(x;t)$□□度□□□□□，$j(x,t)$□□□□□□□□□□□□□□□．定常□□□条□□$j(x,t)$□□□□□

$$-\partial_x [j_X(x;t)] = 0, \tag{2.61}$$

□□□□□□□□□. □□□□前□□散□□$x \in \{1,\dots,N\}$, $x' \in \{1,\dots,N\}$□□□□□
定常□□□条□

$$\sum_{x'=1}^{N} J(x|x';t) = 0, \tag{2.62}$$

□対□□□□□□□□□□□□□□. □□□□分□□子∂_x□□分□□□dx□対□□

$$-\partial_x[j_X(x;t)] = \frac{j_X(x,t)}{dx} - \frac{j_X(x+dx,t)}{dx} + O(dx), \tag{2.63}$$

□□□□□□, □$j_X(x,t)/dx$□□$-j_X(x+dx,t)/dx$□□□□□□□□□□□□□□, □散□
□□□□□□$\sum_{x'=1}^{N}$□対□□□□□□□□□. □□□□□□□□□□□平衡□□□条□□,

$$j_X(x;t) = 0, \tag{2.64}$$

□□□□x□□□□□□□□□□□□□□□□□.

□□□□□定常□□□$j_X(x;t) = \text{const.}$□□□□定□□□□□□□□□存□□□□□□
□□□□□□□. □方□平衡□□□$j_X(x;t) = 0$□□□□□□存□□□□□□□□□□□
□□□.

2.5.3 多次元のFokker-Planck方□式

□□x□$x = \boldsymbol{y} = \{y_1,\dots,y_d\} \in \mathsf{R}^d$□□□□$d$□□□□□□□□□□□□□, □□□
□Fokker-Planck方□□□□□□□□□□□□, □□□□方□□□□□□数□Taylor□□□
□□□Kramers-Moyal□□□□□□□□, Fokker-Planck方□□□□□□□□□, □□□□□
□□Fokker-Planck方□□□□□□□□□□□.

$$\partial_t P_{\boldsymbol{Y}}(\boldsymbol{y};t) = -\sum_i \partial_{y_i}[j_{Y_i}(\boldsymbol{y};t)], \tag{2.65}$$

$$j_{Y_i}(\boldsymbol{y};t) = A_i^{(1)}(\boldsymbol{y};t)P_{\boldsymbol{Y}}(\boldsymbol{y};t) - \sum_j \frac{1}{2}\partial_{y_j}[A_{ij}^{(2)}(\boldsymbol{y};t)P_{\boldsymbol{Y}}(\boldsymbol{y};t)]. \tag{2.66}$$

定常□□□条□□□□□□

$$\sum_i \partial_{y_i}[j_{Y_i}(\boldsymbol{y};t)] = 0, \tag{2.67}$$

□□□□□, 平衡□条□□□□□i, $\boldsymbol{y}$□

$$j_{Y_i}(\boldsymbol{y};t) = 0, \tag{2.68}$$

□□□□□□. 定常□□□1□□□□□□□□□□□□□□□($j_X(x;t) = \text{const.}$)□□□□
□□□□□□, 2□□□□□□□□□$\sum_i$□□□□□□□□, 例□□Y_1Y_2面□□□□□□□
□□□□□□□□□□□□□□定常条□□□□□□□□□.

2.5.4 移流拡散方□式

Fokker-Planck方□□(2.58)□, 例□□□□□□□□□Brown□動□□□□子□□散□
□□□□□□□使□□□□□□□. □□□□$A^{(1)}(x;t)$□□□□□移□□, $A^{(2)}(x;t)$□□□
□□□散□□□□□□□□□□□. □□□□□度□β, □□□□動度□μ□□. □□□□

□□□□子□□□□□□□$U_X(x)$□□動□□□移□□散□□□□□□□□,移□□□□□□□□□力$-\partial_x U_X(x)$□□動□□□,□散□□□度β^{-1}□□例□□□□□

$$A^{(1)}(x;t) = -\mu\partial_x U_X(x), \tag{2.69}$$
$$A^{(2)}(x;t) = 2\mu\beta^{-1}. \tag{2.70}$$

□□□□□□, Fokker-Planck方□□□□□□□□移□□散方□□□□□□□□□□□□□□□□□.

$$\partial_t P_X(x;t) = \mu\partial_x[(\partial_x U_X(x))P_X(x;t)] + \mu\beta^{-1}(\partial_x)^2[P_X(x;t)]. \tag{2.71}$$

□□□□□□□動度μ□□□係数□□数□□□□□□例係数□□□.

□□□□□□□□□□□□□, □□□□□平衡分布□□察□□□□□□□□□□□□□□□□□□□□. □□□□□□□表□(2.59)□□□□□(2.71)□

$$j_X(x;t) = -\mu\partial_x U_X(x)P_X(x;t) - \mu\beta^{-1}\partial_x[P_X(x;t)], \tag{2.72}$$
$$\nu_X(x;t) = -\mu\partial_x[U_X(x) + \beta^{-1}\ln P_X(x;t)]. \tag{2.73}$$

□□□□□□□□□. 平衡□条□□$j_X(x;t) = 0$, □□□□$\nu_X(x;t) = 0$□□□□□□, $\nu_X(x;t) = 0$□□□□定常分布$P_X^{\mathrm{ss}}(x)$□

$$U_X(x) + \beta^{-1}\ln P_X^{\mathrm{ss}}(x) = \mathrm{const.}, \tag{2.74}$$

□□,

$$P_X^{\mathrm{ss}}(x) = \frac{\exp(-\beta U_X(x))}{\int dx \exp(-\beta U_X(x))}, \tag{2.75}$$

□□□□□□□□分布□□□□□□□□□□□□□□.

2.6 Onsager-Machlup□数

Fokker-Planck方□□□□□分布□□□□□□□□□□□□□□方□□□□□□□□□□□□□□□□□. □□□□□刻t□□□y□□□条□□□□□□□□□dt□□□刻$t+dt$□□□x□□□条□□□□□分布$P(x;t+dt|y;t)$□□□□□□□□□□□□□.

□, Fokker-Planck方□□(2.58)□□□□□□□□□□□□.

$$\begin{aligned}\partial_t P_X(x;t) &= -\partial_x[A^{(1)}(x;t)P_X(x;t)] + \frac{1}{2}\partial_x^2[A^{(2)}(x;t)P_X(x;t)] \\ &= \mathcal{L}_{\mathrm{FP}}P_X(x;t),\end{aligned} \tag{2.76}$$
$$\mathcal{L}_{\mathrm{FP}} = -\partial_x A^{(1)}(x;t) + \frac{1}{2}\partial_x^2 A^{(2)}(x;t). \tag{2.77}$$

□□$\mathcal{L}$□Fokker-Planck□□子□□□□□□□. Chapman-Kolmogorov方□□□□□□□□方□□□□□□□□□□□□□□□□□□□□, 条□□□□□分布□□□□□□□□方□□□□□□□□□□□□□□□□. □□□条□□□□□分布$P(x;t|y;s)$□対□□Fokker-Planck方□□□

$$\partial_t P(x;t|y;s) = \mathcal{L}_{\mathrm{FP}}P(x;t|y;s), \tag{2.78}$$

□□□.

□□Fokker-Planck方□□□□$P(x;t+dt|y;t)$□□析□□表□□□□□□□□□□□□□. □□, □□□dt□对□□$O(dt^2)$□□□□□

$$P(x;t+dt|y;t) = (1+dt\mathcal{L}_{\rm FP})P(x;t|y;t), \tag{2.79}$$

□□□□□. □□□Chapman-Kolomogorov方□□□□master方□□□□□□□□□使□□□定□□□ $P(x;t|y;t)=\delta(x-y)$ □使□□, □□

$$P(x;t+dt|y;t) = \left[1+dt\mathcal{L}_{\rm FP}\right]\delta(x-y), \tag{2.80}$$

□实行□□. □□□□□□□□数$\delta(x-y)$□□□□□, $A^{(1)}(x;t)\delta(x-y)=A^{(1)}(y;t)\delta(x-y)$□$A^{(2)}(x;t)\delta(x-y)=A^{(2)}(y;t)\delta(x-y)$□□□□□□□, $\mathcal{L}_{\rm FP}$□x□依存□□y□□□□□□□□□□,

$$\begin{aligned} P(x;t+dt|y;t) &= \left[1+dt\mathcal{L}_{\rm FP}\right]\delta(x-y) \\ &= \left[1+dt\left[-\partial_x A^{(1)}(y;t)+\frac{1}{2}(\partial_x)^2A^{(2)}(y;t)\right]\right]\delta(x-y) \end{aligned} \tag{2.81}$$

□□□□. □□□□□□□数$\delta(x-y)$□Fourier□□□□□□表□

$$P(x;t|y;t) = \delta(x-y) = \int\frac{ds}{2\pi}\exp\left[is(x-y)\right], \tag{2.82}$$

□利□□□□,

$$\begin{aligned} &P(x;t+dt|y;t) \\ &= \left[1+dt\left[-\partial_x A^{(1)}(y;t)+\frac{1}{2}(\partial_x)^2A^{(2)}(y;t)\right]\right]\int\frac{ds}{2\pi}\exp\left[is(x-y)\right] \\ &= \int\frac{ds}{2\pi}\left[1+dt\left[-isA^{(1)}(y;t)-\frac{1}{2}s^2A^{(2)}(y;t)\right]\right]\exp\left[is(x-y)\right], \end{aligned} \tag{2.83}$$

□□□□, □□□$O(dt^2)$□□□□□

$$\begin{aligned} &1+dt\left[-isA^{(1)}(y;t)-\frac{1}{2}s^2A^{(2)}(y;t)\right] \\ &= \exp\left[\left[-isA^{(1)}(y;t)-\frac{1}{2}s^2A^{(2)}(y;t)\right]dt\right], \end{aligned} \tag{2.84}$$

□□□□□□□□□利□□□, □□□□分□实行□□□

$$\begin{aligned} &P(x;t+dt|y;t) \\ &= \int\frac{ds}{2\pi}\exp\left[\left[-isA^{(1)}(y;t)-\frac{1}{2}s^2A^{(2)}(y;t)\right]dt+is(x-y)\right] \\ &= \int\frac{ds}{2\pi}\exp\left[-\frac{dt}{2}A^{(2)}(y;t)\left[s+i\frac{A^{(1)}(y;t)-\frac{x-y}{dt}}{A^{(2)}(y;t)}\right]^2-\frac{\left[\frac{x-y}{dt}-A^{(1)}(y;t)\right]^2}{2A^{(2)}(y;t)}dt\right] \\ &= \frac{1}{\sqrt{2\pi A^{(2)}(y;t)dt}}\exp\left[-\frac{\left[\frac{x-y}{dt}-A^{(1)}(y;t)\right]^2}{2A^{(2)}(y;t)}dt\right], \end{aligned} \tag{2.85}$$

□□□. □□□, $x=x_{i+1}$, $y=x_i$, $\dot{x}_i=(x_{i+1}-x_i)/dt$□表□□□□□□□, □□定□□□□Onsager-Machlup□数$L_{\rm OM}(x_i,\dot{x}_i;t)$□□□□

$$\begin{aligned} L_{\rm OM}(x_i,\dot{x}_i;t) &= \frac{\left[\dot{x}_i-A^{(1)}(x_i;t)\right]^2}{2A^{(2)}(x_i;t)}, \\ P(x_{i+1};t+dt|x_i;t) &= \frac{1}{\sqrt{2\pi A^{(2)}(x_i;t)dt}}\exp\left[-L_{\rm OM}\left(x_i,\dot{x}_i;t\right)dt\right], \end{aligned} \tag{2.86}$$

□□□□条□□□□□分布□表□□□□□□□□□□.

□□□□□□□□数□□□□使□□□Fokker-Planck□□子$\mathcal{L}_{\mathrm{FP}}$□$x$□依存□□□□□□□□□□□行□□□，□□分$\partial_x A^{(1)}(x;t)$, $\partial_x A^{(2)}(x;t)$, $(\partial_x)^2 A^{(2)}(x;t)$□□□□余分□□□□□□□□[5]. □□□条□□□□□分布□表□□□□□□□□. □□余分□□□実□x_i□x_{i+1}□□数□□□□□□□□□□□□□□□□□□□□□□, dt□1□□□□□□□□(2.86)□□□□□□□.

□□Fokker-Planck方□□□Markov□□□□□□□□□□□, □□□□□□□□□□□Onsgaer-Machlup□数□□□□□□□□□□□□. dt□□□□□□刻$t = idt$□□□□□数□X_i, □□□x_i□□□□□, □□□□□□数$\boldsymbol{X} = \{X_1, \ldots, X_n\}$□□□□□□□□□$\boldsymbol{x} = \{x_1, \ldots, x_n\}$□□□□□分布$P_{\boldsymbol{X}}(\boldsymbol{x})$□, Onsager-Machlup□数□□□□

$$
\begin{aligned}
P_{\boldsymbol{X}}(\boldsymbol{x}) &= \prod_{i=1}^{n-1} P(x_{i+1};(i+1)dt|x_i;idt)P_{\mathrm{X}_1}(x_1) \\
&= \frac{P_{\mathrm{X}_1}(x_1)\exp\left[-\sum_{i=1}^{n-1} L_{\mathrm{OM}}(x_i,\dot{x}_i;idt)dt\right]}{(2\pi dt)^{\frac{n-1}{2}}\prod_{i=1}^{n-1}\sqrt{A^{(2)}(x_i;idt)}},
\end{aligned}
\tag{2.87}
$$

□□□□□□□□□.□□□□$\dot{x}_i = (x_{i+1} - i_k)/dt$□□□.

2.7 Langevin方□式

2.7.1 Wiener□□

□□□□□Wiener□□□□□□□□□□□□□□□□, Fokker-Planck方□□□□□□Onsager-Machlup□数□□□条□□□□□分布□表□□□□察□□□. Wiener□□$\mathcal{B}_t$□

- $\mathcal{B}_0 = 0$.
- $\mathcal{B}_t$□(□□□□□実□)□□.
- □分$\mathcal{B}_{t+\Delta t} - \mathcal{B}_t$□平□0, 分散$\Delta t$□□□□分布□□□.
- □分$\mathcal{B}_{t+\Delta t} - \mathcal{B}_t$□, □□□□□□□分□□□□□□.

□□□□□□□□□□□□□数学□□定□□□□.

□□Wiener□□□□□□表□□(2.86)□□□□□□□□. □□□□□Wiener□□□□分$d\mathcal{B}_t = \mathcal{B}_{t+dt} - \mathcal{B}_t$□□□□. □□□Wiener□□□□□□□平□0, 分散dt□□□□分布

$$
\mathrm{Prob}(d\mathcal{B}_t) = \frac{1}{\sqrt{2\pi dt}}\exp\left(-\frac{(d\mathcal{B}_t)^2}{2dt}\right), \tag{2.88}
$$

□□□, □□□□□□□□分□対□□□□, □□□□

$$
\mathrm{Prob}(d\mathcal{B}_{dt}, \ldots, d\mathcal{B}_{(n-1)dt}) = \prod_{i=1}^{n-1}\mathrm{Prob}(d\mathcal{B}_{idt}) \tag{2.89}
$$

□□□. □□□□, $d\mathcal{B}_{idt}$□x_{i+1}□□□□数□□

$$
d\mathcal{B}_{idt} = \frac{1}{\sqrt{A^{(2)}(x_i;idt)}}\left[x_{i+1} - x_i - A^{(1)}(x_i;idt)dt\right], \tag{2.90}
$$

□□□□□□□□. □□□□数□□□□x_{i+1}□対□□□□Prob(x_{i+1})□,

$$
\begin{aligned}
\mathrm{Prob}(x_{i+1}) &= \left|\frac{\partial[d\mathcal{B}_{idt}]}{\partial[x_{i+1}]}\right| \mathrm{Prob}(d\mathcal{B}_{idt}) \\
&= \frac{1}{\sqrt{2\pi A^{(2)}(x_i;idt)dt}} \exp\left[-\frac{\left[\frac{x_{k+1}-x_k}{dt} - A^{(1)}(x_i;idt)\right]^2}{2A^{(2)}(x_i;idt)}dt\right], \quad (2.91)
\end{aligned}
$$

□□□□□□. □□□$|\partial[d\mathcal{B}_{idt}]/\partial[x_{i+1}]|$□□□□□□□□□□. □□□, Prob$(x_{i+1}) = P(x_{i+1};(i+1)dt|x_i;idt)$□□□□□, Onsager-Machlup□数□□□□表□□(2.86)□, □数□□□(2.90)□□□□□, Wiener□□□□分$d\mathcal{B}_{idt}$□□□□□□□□□□□□□□□□. □□, □分□□□□□□(2.89)□, □数□□□(2.90)□□□□□□□□□□□□□□□表□(2.87)□□□□□□□□□□□□. □□□□, □分□□□□□□(2.89)□, □数□□□□□□$\boldsymbol{x} = \{x_1, \ldots, x_n\}$□□□□□□□□Markov□□□□□□□□保□□□.

2.7.2 Langevin方□式

Wiener□□□□□□□数□□□(2.90)□□□□□□□

$$\frac{x_{i+1}-x_i}{dt} = A^{(1)}(x_i;idt) + \sqrt{A^{(2)}(x_i;idt)}\frac{d\mathcal{B}_{idt}}{dt}, \quad (2.92)$$

□□□□□□□□□. □□□$t = idt$, $x(t+dt) = x_{i+1}$, $x(t) = x_i$□□□表□□□□□□□,

$$\frac{x(t+dt)-x(t)}{dt} = A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)}\frac{d\mathcal{B}_t}{dt}, \quad (2.93)$$

□□□. □□□$dt \to 0$□□□□,

$$\lim_{dt\to 0} \frac{x(t+dt)-x(t)}{dt} = \dot{x}(t), \quad (2.94)$$

$$\lim_{dt\to 0} \sqrt{A^{(2)}(x(t);t)}\frac{d\mathcal{B}_t}{dt} = \sqrt{A^{(2)}(x(t);t)} \cdot \xi(t), \quad (2.95)$$

□□□□□□□□□□□□, Langevin方□□

$$\dot{x}(t) = A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)} \cdot \xi(t), \quad (2.96)$$

□□□□□□□□□. □□Langevin方□□□□分方□□

$$\dot{x}(t) = A^{(1)}(x(t);t), \quad (2.97)$$

□□□□□□□□□□□□□□□□□□□□□□□□□$\xi(t)$□□例□□□$\sqrt{A^{(2)}(x(t);t)} \cdot \xi(t)$□新□□加□□□□□□□□□□□□□, □□□分方□□□□□□□□□.

□□□□□$\xi(t)$□対□□□□則□, Wiener□□$\mathcal{B}_t$□定□□□□□□□□□□□□□□□□□□. □□$d\mathcal{B}_t$□□□□分布□□□□□□□□$\xi(t) = \lim_{dt\to 0} d\mathcal{B}_t/dt$□□□□分布□□□. □□□, □□□□□□則□平□□□分散□□□□□□□□□□. □□Wiener□□□□□□$\boldsymbol{\mathcal{B}} = \{\mathcal{B}_t | t \in \mathsf{R}\}$□対□□期□□$\langle\cdots\rangle$□□□□□, 平□□□□分散□□□□□

$$\left\langle \frac{d\mathcal{B}_t}{dt} \right\rangle = \frac{\langle d\mathcal{B}_t \rangle}{dt} = 0, \quad (2.98)$$

$$\left\langle \frac{d\mathcal{B}_t}{dt}\frac{d\mathcal{B}_{t'}}{dt} \right\rangle = \frac{\langle d\mathcal{B}_t d\mathcal{B}_{t'} \rangle}{dt^2} = \begin{cases} 0 & (t \geq t'+dt, t \leq t'-dt), \\ \frac{dt-(t-t')}{dt^2} & (t' \leq t \leq t'+dt), \\ \frac{dt-(t'-t)}{dt^2} & (t'-dt \leq t \leq t'), \end{cases} \tag{2.99}$$

□□, $dt \to 0$□□□□□□□□□

$$\langle \xi(t) \rangle = \lim_{dt\to 0} \left\langle \frac{d\mathcal{B}_t}{dt}(t) \right\rangle = 0, \tag{2.100}$$

$$\langle \xi(t)\xi(t') \rangle = \lim_{dt\to 0} \left\langle \frac{d\mathcal{B}_t}{dt}\frac{d\mathcal{B}_{t'}}{dt} \right\rangle = \delta(t-t'), \tag{2.101}$$

□□□□□. □□□$\langle d\mathcal{B}_t d\mathcal{B}_{t'} \rangle / dt^2$□$t=t'$□□□□□□底□$2dt$, □□$1/dt$□□□□□□□□□□, $dt \to 0$□□□□□□□□数$\delta(t-t')$□□□□□□□□□. □□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□, □□則□□□□□□分布□□□□□□□□□□$\xi(t)$□□□□□□□□□□□□□□□□□□□□□□.

2.7.3 Ito-Stratonovich□□

□□□□□□□□Langevin方□□□□□□□□□,

$$\lim_{dt\to 0} \sqrt{A^{(2)}(x_i; idt)}\frac{d\mathcal{B}_{idt}}{dt} \tag{2.102}$$

□□□□□□□□□□□. □□□□,

$$\lim_{dt\to 0} \sqrt{A^{(2)}(x_{i+1}; idt)}\frac{d\mathcal{B}_{idt}}{dt} \tag{2.103}$$

□

$$\lim_{dt\to 0} \frac{\sqrt{A^{(2)}(x_{i+1}; idt)} + \sqrt{A^{(2)}(x_i; idt)}}{2}\frac{d\mathcal{B}_{idt}}{dt} \tag{2.104}$$

□□□□□□□□□□□□方□□□□□□, □□□果□□□□□□□□. 実□□□□□□□□□□□□果□□□□□□□, □□□□別□□□□□□□. □□□□□, $\sqrt{A^{(2)}(x_{i+1}, idt)}$□Taylor□□□□□, □(2.92)□□□□□□,

$$\begin{aligned} &\sqrt{A^{(2)}(x_{i+1}; idt)} \\ &= \sqrt{A^{(2)}(x_i; idt)} + (x_{i+1}-x_i)\partial_{x_i}\sqrt{A^{(2)}(x_i; idt)} + O((x_{i+1}-x_i)^2) \\ &= \sqrt{A^{(2)}(x_i; idt)} + d\mathcal{B}_t\sqrt{A^{(2)}(x_i; idt)}\partial_{x_i}\sqrt{A^{(2)}(x_i; idt)} + O(dt), \end{aligned} \tag{2.105}$$

□$d\mathcal{B}_t$□□例□□□□□□□□. $d\mathcal{B}_t$□分散□dt□□例□□□□□□□□□□, $d\mathcal{B}_t$□□□□□$O(dt^{1/2})$□□□□□□□□□□. □□□$O((x_{i+1}-x_i)^2)$□$O((d\mathcal{B}_t)^2)$□□□□□, $O(dt)$□□□□□□□□□□□□□□□□□□□□□.

□□□$d\mathcal{B}_t$□$d\mathcal{B}_t/dt$□□□□□□$O(1)$□□□. □□ $d\mathcal{B}_t$□□□分布□分散dt□□□□分布□□□□□, dt□□□□□□$d\mathcal{B}_t$□□□分布□鋭□□□□□□分布□□□□□□, $d\mathcal{B}_t^2$□□□□□□□□1□dt□□□□□□□□□, $dt \to 0$□□□□$d\mathcal{B}_t^2/dt \to 1$□□□□□□□□. □□□, □□□□□□□□□□□□

$$\lim_{dt\to 0} \sqrt{A^{(2)}(x_i; idt)}\frac{d\mathcal{B}_{idt}}{dt} = \sqrt{A^{(2)}(x(t); idt)} \cdot \xi(t), \tag{2.106}$$

$$\begin{aligned}&\lim_{dt\to0}\sqrt{A^{(2)}(x_{i+1};idt)}\frac{d\mathcal{B}_{idt}}{dt}\\&=\sqrt{A^{(2)}(x_i;idt)}\partial_{x_i}\sqrt{A^{(2)}(x_i;idt)}+\sqrt{A^{(2)}(x(t);idt)}\cdot\xi(t),\end{aligned}\tag{2.107}$$

$$\begin{aligned}&\lim_{dt\to0}\frac{\sqrt{A^{(2)}(x_{i+1};idt)}+\sqrt{A^{(2)}(x_i;idt)}}{2}\frac{d\mathcal{B}_{idt}}{dt}\\&=\frac{1}{2}\sqrt{A^{(2)}(x_i;idt)}\partial_{x_i}\sqrt{A^{(2)}(x_i;idt)}+\sqrt{A^{(2)}(x(t);idt)}\cdot\xi(t),\end{aligned}\tag{2.108}$$

□□□□□□.

□□□□□□□□□

$$\lim_{dt\to0}\frac{\sqrt{A^{(2)}(x_{i+1};idt)}+\sqrt{A^{(2)}(x_i;idt)}}{2}\frac{d\mathcal{B}_{idt}}{dt}=\sqrt{A^{(2)}(x(t);t)}\circ\xi(t),\tag{2.109}$$

□□□□□○□□□□表□□□□□□□□□□□□□, ·□○□□□□□散□□□方□□定□□□□□□□. ·□Ito□, ○□Stratonovich□□□□.

Ito□□Stratonovich□□, □□□□□数$f(x)$□$d\mathcal{B}_{idt}/dt$□□□□□□□□□□定□□□□.

$$\lim_{dt\to0}f(x_i)\frac{d\mathcal{B}_{idt}}{dt}=f(x)\cdot\xi(t),\tag{2.110}$$

$$\lim_{dt\to0}\frac{f(x_i)+f(x_{i+1})}{2}\frac{d\mathcal{B}_{idt}}{dt}=f(x)\circ\xi(t).\tag{2.111}$$

Ito□□Stratonovich□□□□□係□, Langevin方□□(2.92)□□□

$$f(x)\circ\xi(t)=\frac{1}{2}\sqrt{A^{(2)}(x(t);t)}\partial_x f(x)+f(x)\cdot\xi(t),\tag{2.112}$$

□□□□□□□□□. □□$f(x)$□x□$(x_i+x_{i+1})/2$□□□□□□□□□□□□□ $dt\to0$□□□□Stratonovich□□□□□□□□□□□□□.

$$\lim_{dt\to0}f\left(\frac{x_i+x_{i+1}}{2}\right)\frac{d\mathcal{B}_{idt}}{dt}=f(x)\circ\xi(t).\tag{2.113}$$

□□□□示□□□□□□□□□□$f(x_{i+1})$□□□□$f((x_i+x_{i+1})/2)$□□□□Taylor□□□□□□□□□□□□.

□□□□Taylor□□□□□□□□Ito□□□□□□□□$O(dt^{3/2})$□□□寄□□□□□□□□□

$$\begin{aligned}dt^2&=0,&(2.114)\\dt\,d\mathcal{B}_t&=0,&(2.115)\\(d\mathcal{B}_t)^2&=dt,&(2.116)\end{aligned}$$

□□□表□□□□□□, □□□便利□□□.

□□□□, □□□□□□□□□□□□□$\xi(t)$□$\sqrt{A^{(2)}(x(t);t)}$□□□□$x(t)$□依存□□係数□□□□□Langevin方□□□□□□□□□□□, Ito□□Langevin方□□

$$\dot{x}(t)=A^{(1)}(x(t);t)+\sqrt{A^{(2)}(x(t);t)}\cdot\xi(t),\tag{2.117}$$

□Stratonovich□ □Langevin方□ □

$$\dot{x}(t) = A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)} \circ \xi(t), \tag{2.118}$$

□ □ □別□ □ □ □ □ □ □ □. □ □Stratonovich□ □Langevin方□ □ □Ito□ □Langevin方□ □ □ □ □ □ □ □ □ □,

$$\dot{x}(t) = A^{*(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)} \cdot \xi(t), \tag{2.119}$$

$$A^{*(1)}(x(t);t) = A^{(1)}(x(t);t) + \frac{1}{2}\sqrt{A^{(2)}(x(t);t)}\partial_{x(t)}\sqrt{A^{(2)}(x(t);t)}, \tag{2.120}$$

□ □ □ □ □ □, Ito□ □ □ □ □ □ □ □ □ □Taylor□ □ □ $O(dt^{1/2}) = O(d\mathcal{B}_t)$□ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □. □体□ □ □

$$\begin{aligned}
\dot{x}(t) &= A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)} \circ \xi(t) \\
&= A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t) + \frac{\dot{x}(t)dt}{2};t)}\frac{d\mathcal{B}_t}{dt} \\
&= A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)}\frac{d\mathcal{B}_t}{dt} + \frac{\dot{x}(t)dt}{2}\left(\partial_{x(t)}\sqrt{A^{(2)}(x(t);t)}\right)\frac{d\mathcal{B}_t}{dt} + O(d\mathcal{B}_t) \\
&= A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)} \cdot \xi(t) \\
&\quad + \frac{\sqrt{A^{(2)}(x(t) + \frac{\dot{x}(t)dt}{2};t)}}{2}\left(\partial_{x(t)}\sqrt{A^{(2)}(x(t);t)}\right) + O(d\mathcal{B}_t) \\
&= A^{(1)}(x(t);t) + \sqrt{A^{(2)}(x(t);t)} \cdot \xi(t) \\
&\quad + \frac{1}{2}\sqrt{A^{(2)}(x(t);t)}\left(\partial_{x(t)}\sqrt{A^{(2)}(x(t);t)}\right) + O(d\mathcal{B}_t),
\end{aligned} \tag{2.121}$$

□ □ □ □Taylor□ □ □$\dot{x}(t)$□ □ □ □繰□ □ □ □, Ito□ □. □ □ □行□ □Taylor□ □ □ □ □ □ □寄□ □$O((\dot{x}(t))^2 dt d\mathcal{B}_t) = O((d\mathcal{B}_t)^3/dt) = O(d\mathcal{B}_t)$□ □ □ □ □.

□ □ □ □, □ □$A^{(2)}(x(t),t)$□$x(t)$□依存□ □ □ □ □ □$\partial_{x(t)}\sqrt{A^{(2)}(x(t),t)} = 0$□ □Ito□ □Stratonovich□ □Langevin方□ □ □ □ □ □ □ □ □.

2.7.4 Brown□動 - overdamped Langevin方□式

□散移□方□ □ □ □ □ □ □ □ □ □ □ □ □ □ □

$$A^{(1)}(x;t) = -\mu\partial_x U_X(x), \tag{2.122}$$

$$A^{(2)}(x;t) = 2\mu\beta^{-1}. \tag{2.123}$$

□ □ □ □ □, Langevin方□ □ □

$$\dot{x}(t) = -\mu\partial_x U_X(x) + \sqrt{2\mu\beta^{-1}} \cdot \xi(t), \tag{2.124}$$

$$\langle \xi(t) \rangle = 0, \tag{2.125}$$

$$\langle \xi(t)\xi(t') \rangle = \delta(t - t'), \tag{2.126}$$

□ □ □ □ □ □. □ □Langevin方□ □ □ □ □ □ □ □子□Brown□動□ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □. 例□ □ □ □ □$\xi(t)$□ □ □ □ □ □ □, □ □Langevin方□ □ □

$$\mu^{-1}\dot{x}(t) = -\partial_x U_X(x), \tag{2.127}$$

□□□, □□□□□□□$\mu^{-1}\dot{x}(t)$□□□□□□□力$-\partial_x U_X(x)$□□□□□□□□□□□□□□□□□□□□□.□□□□□動度□□数μ^{-1}□□□□□係数□□□. □□□□□□□□□□□□□□□力□□□□□□□□□□□, □度□平方□□□例□□□□□□□□□力$\sqrt{2\mu\beta^{-1}}\cdot\xi(t)$□加□□□□□□□□□□□□□□□□□□□. □□Langevin方□□□□□overdamped Langevin方□□□□□□□□□.

2.7.5 Brown□動 - underdamped Langevin方□式

□動方□□□□□□□加□□□□□□□Langevin方□□□□□□□□□□□□. □□□, □子□□度$v(t)$□対□□m□□□□□□

$$m\mu\dot{v}(t) = -v(t) + \sqrt{2\mu\beta^{-1}}\cdot\xi(t), \tag{2.128}$$

$$\langle\xi(t)\rangle = 0, \tag{2.129}$$

$$\langle\xi(t)\xi(t')\rangle = \delta(t-t'), \tag{2.130}$$

□□□□Langevin方□□□□□□□□□□□□□□. □□□□□□□□□□□□□

$$m\dot{v}(t) = -\mu^{-1}v(t), \tag{2.131}$$

□□□□□□加□□□□□□□□□□□動方□□□□□□□□. □□□□□□□□□□□□□力$\sqrt{2\mu\beta^{-1}}\cdot\xi(t)$□加□□□□□□□□□□□□□□□□□. □□Langevin方□□□□□underdamped Langevin方□□□□□□□□□.

対□□□Fokker-Planck方□□□□刻t□□□度v□□□□□□分布$P_V(v;t)$□対□□,

$$\partial_t P_V(v;t) = \partial_v\left[\frac{v}{m\mu}P_V(v;t)\right] + \partial_v^2\left[\frac{1}{m^2\mu\beta}P_V(v;t)\right] \tag{2.132}$$

$$= -\partial_v[j_V(v;t)], \tag{2.133}$$

$$j_V(v;t) = -\frac{v}{m\mu}P_V(v;t) - \frac{1}{m^2\mu\beta}\partial_v P_V(v;t), \tag{2.134}$$

□□□□□□. □□Fokker-Planck方□□□□□□平衡□□□□□□□□□. $j_V(v;t) = 0$□□□□□□□定常分布$P_V^{\mathrm{ss}}(v)$□

$$-\beta m v = \partial_v \ln P_V^{\mathrm{ss}}(v), \tag{2.135}$$

$$\ln P_V^{\mathrm{ss}}(v) = -\beta\frac{mv^2}{2} + \mathrm{const.}, \tag{2.136}$$

□□□□□□□,

$$P_V^{\mathrm{ss}}(v) = \frac{\exp\left(-\beta\frac{mv^2}{2}\right)}{\int dv\exp\left(-\beta\frac{mv^2}{2}\right)}, \tag{2.137}$$

□□動□□□□□$mv^2/2$□対□□□□□□□分布□□□□□□示□□. □□□□□□Brown□動□□□□□□□□□□□.

2.7.6 Kramers方□式と平□の条件

□□□□, underdamped Langevin方□□□□□□□□□力$-\mu\partial_x U_X(x)$□加□□□□□□□□□□. □□□□□□□□□□□度$v(t)$□位□$x(t)$□□□□□□□□□□□□□

□□□□.

$$
\begin{aligned}
m\mu\dot{v}(t) &= -v(t) - \mu\partial_x U_X(x) + \sqrt{2\mu\beta^{-1}}\cdot\xi(t), && (2.138)\\
\dot{x}(t) &= v(t) && (2.139)\\
\langle\xi(t)\rangle &= 0, && (2.140)\\
\langle\xi(t)\xi(t')\rangle &= \delta(t-t'), && (2.141)
\end{aligned}
$$

対□□□□刻t□□位□x□□度v□□□□□□分布$P_{X,V}(x,v;t)$□□□□□□□□□□□□□□□□□□□. □□□度□□□□□□□□□□□(2.138)□分□寄□□

$$
\partial_v\left[\left[\frac{v}{m\mu}+\frac{\partial_x U_X(x)}{m}\right]P_{X,V}(x,v;t)\right]+\partial_v^2\left[\frac{1}{m^2\mu\beta}P_V(v;t)\right], \tag{2.142}
$$

□□□, 位□□□□□□□□□□□□(2.139)□□分□寄□□

$$
-\partial_x\left[vP_{X,V}(x,v;t)\right], \tag{2.143}
$$

□□□□□□□□□□□□, 分布$P_{X,V}(x,v;t)$□□□□□□□□□

$$
\begin{aligned}
\partial_t P_{X,V}(x,v;t) = \partial_v&\left[\left[\frac{v}{m\mu}+\frac{\partial_x U_X(x)}{m}\right]P_{X,V}(x,v;t)\right]\\
&+\partial_v^2\left[\frac{1}{m^2\mu\beta}P_V(v;t)\right]-\partial_x\left[vP_{X,V}(x,v;t)\right].
\end{aligned} \tag{2.144}
$$

□□□□□□. □□方□□□Kramers方□□□□□□□□□.

□□Kramers方□□□$x(t)$□$v(t)$□2□□□Fokker-Planck方□□□□□□□□, 実□Kramers方□□□平衡□□□条□□□□□□□□□□□□□□□□Fokker-Planck方□□□平衡□条□(2.68)□□□□□□. □□,

$$
\begin{aligned}
\partial_t P_{X,V}(x,v;t) &= -\partial_v\left[j_V(x,v;t)\right]-\partial_x[j_X(x,v;t)],\\
j_V(x,v;t) &= -\left[\frac{v}{m\mu}+\frac{\partial_x U_X(x)}{m}\right]P_{X,V}(x,v;t)-\frac{1}{m^2\mu\beta}\partial_v P_{X,V}(x,v;t),\\
j_X(x,v;t) &= vP_{X,V}(x,v;t),
\end{aligned} \tag{2.145}
$$

□□□□□□, 条□(2.68)□□□$j_X(x,v;t)=0$□□$j_V(x,v;t)=0$□□□□□□□□□□定常分布$P^{\mathrm{ss}}_{X,V}(x,v)$□□□□□存□□□□□□□□□□□□□□. □□□□条□$j_X(x,v;t)=0$□$P^{\mathrm{ss}}_{X,V}(x,v)$□$v=0$□□□□□□□□□□数□□□□□□□□□□□, □方□$j_V(x,v;t)=0$□条□$j_X(x,v;t)=0$□□□□□□分□□□□□$P^{\mathrm{ss}}_{X,V}(x,v)$□□□□$v\neq 0$□□□□□□□□□□□□□□, □□□□□□条□□□□□□□□.

□方□定常分布□条□

$$
0=-\partial_v\left[j_V(x,v;t)\right]-\partial_x[j_X(x,v;t)], \tag{2.146}
$$

□□□□□□□定常分布$P^{\mathrm{ss}}_{X,V}(x,v)$□

$$
P^{\mathrm{ss}}_{X,V}(x,v)=\frac{\exp\left(-\beta\left[\frac{mv^2}{2}+U_X(x)\right]\right)}{\int dv\int dx\exp\left(-\beta\left[\frac{mv^2}{2}+U_X(x)\right]\right)}, \tag{2.147}
$$

□□□□□□□(2.147)□□(2.146)□□□□□□□□□□□□□□□□□□□□□□□. □□定常分布$P^{\mathrm{ss}}_{X,V}(x,v)$□□□□□□分布□□□□□, 条□(2.146)□平衡分布□□□□□□□□□□□□□□. □□□Kramers方□□□□□□□平衡□□□条□□□(2.68)□□

□(2.146)□条□□□□□□□□□□□.□□Kramers方□□□□□□□数□□□位□□□度□□□□存□□□□□□□, x□v□□□□□□□□□□□□□□□□□□□, 平衡□□□□□□□位□□□□□寄□$\partial_x[j_X(x,v;t)]$□□度□□□□寄□$\partial_v\,[j_V(x,v;t)]$□□□□□□□□□□□□□□.

□□□□□位□□□度□□□□存□□□□□□平衡□□□条□□□□□, □□□□□□□方□□□□□□□□□□□□.□□□□□□条□□平衡□□□表□□□□□, □□□□□□条□□定□□位□x, (x')□□度v, (v')□□□□□□□□□□□□□□□□□□□□□.□□□□□□□□□□□□条□□定□□□□□□□□□□□□. 位□x, □度v□□位□x', □度v'□□□□□□□□□移□□□$W(x',v'|x,v)$□対□□

$$W(x',v'|x,v)P^{\rm ss}_{X,V}(x,v) = W(x,-v|x',-v')P^{\rm ss}_{X,V}(x',-v'), \tag{2.148}$$

□□□条□□, □□□□□□□□□□□条□□□□. □□□平衡□□□分布□v'□□□□□□数$P^{\rm ss}_{X,V}(x',-v') = P^{\rm ss}_{X,V}(x',v')$□□□□□□,

$$W(x',v'|x,v)P^{\rm ss}_{X,V}(x,v) = W(x,-v|x',-v')P^{\rm ss}_{X,V}(x',v'), \tag{2.149}$$

□□□□□□.

□□□□□□□□条□□□x, x'□□□x□□x'□□□□□□

$$J^+(x'|x) = W(x',v'|x,v)P^{\rm ss}_{X,V}(x,v), \tag{2.150}$$

□x'□□x□□□□□□□

$$J^-(x'|x) = W(x,-v|x',-v')P^{\rm ss}_{X,V}(x',-v'), \tag{2.151}$$

□□□□□□□条□$J^+(x'|x) = J^-(x'|x)$□□□□□. □□□□□□□□□□度v, v'□□□□□□, □□□□□□□□□□□□□$-v$, $-v'$□□□□□□□□□□□□□定□□□□. □□□□□, □□□□□□□□□対□□□□□数□□□□□□□□, □□□□□□条□□修□□□□□□□□□□□□□□ [2]. □□□□□□□□□□対□□□□数□□□□□□□□□□□□□□□□□□□, □□□□□□□□□□□□□□□, □□□力学□□察□□□□□□□□□□対□□□□□数□-1□□□□□□□作□□□□□□□面□□□□□.

□3□

ゆらぎの熱力学

□□□□, □□□□方□□□Fokker-Planck方□□□□力学□□□□□□, 非平衡□□□力学□□□□□□□□方□□(□□□□□力学/stochastic thermodynamics)□□□□□□□.

3.1 流れと力

□□□□□□□□□□□□□□平衡□非平衡□□□□係□, □力学□□□□□□□□□□□□□. □□□□□□□□□力学□□□□□□□, □□□Onsager□Prigogine□□□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□□□□□□□□□1976年□Schnakenberg□□□□□□文 [1]□□□□. □日□□, □□□□□力学(stochastic thermodynamics)□□□□□分□□□□日□□□□□□□.

□□, □散□□$x \in \{1, \ldots, N\}$, $x' \in \{1, \ldots, N\}$□対□□master方□□□対□□□力学□□□□行□□. □M□□□□存□□□□□□□□□定□□□数□$\nu \in \{1, \ldots, M\}$□□□□. □□□□□□度□□□□□□□x□□□□□□□□□□□□□□□□, □□□□方□□□

$$\frac{\partial}{\partial t} p_X(x;t) = \sum_{\nu=1}^{M} \sum_{x'=1}^{N} [J^{+(\nu)}(x|x';t) - J^{-(\nu)}(x'|x;t)]. \tag{3.1}$$

$$J^{+(\nu)}(x|x';t) = W^{(\nu)}(x|x';t) p_X(x';t), \tag{3.2}$$

$$J^{-(\nu)}(x|x';t) = W^{(\nu)}(x'|x;t) p_X(x;t), \tag{3.3}$$

□□□□□□□. □□□$J^{+(\nu)}(x|x';t)$□□ν□□□□□□x'□□x□□□□□□□, $J^{-}(x|x';t)$□□ν□□□□□□x□□x'□□□□□□□□, $W^{(\nu)}(x|x';t)$□□移□□□$W(x|x';t)$□□□□□□□□寄□□

$$\sum_{\nu=1}^{M} W^{(\nu)}(x|x';t) = W(x|x';t), \tag{3.4}$$

□□□□分□□□□□□□□. □□□□□□Kramers方□□□□□□□□□□□□□位□□□度□□方□□□□□□□□, □(2.150)□□(2.151)□□□□□□□□□定□□□□□□□□, □□□□力学□□□□□□□□□□□□□□.

□□, $W^{(\nu)}(x|x';t) > 0$□□□$W^{(\nu)}(x'|x;t) > 0$□□□□□□□□. □□□□ν□□□□x'□□x□□□移□□□□□□□, □□□ν□□□□□□□□x□□x'□□□移□□□□

□□□□力学□□□□□□□□□．□□非□□□□移□□□$W^{(\nu)}(x|x';t)$□□□□□□，□□□移□□□□□定□□□数ρ

$$\rho \in \{(x,x',\nu)|W^{(\nu)}(x|x';t) \neq 0\}, \tag{3.5}$$

□□□□□□□□．□□□

$$J^{+(\nu)}(x|x';t) = J_\rho^+(t), \tag{3.6}$$
$$J^{-(\nu)}(x|x';t) = J_\rho^-(t), \tag{3.7}$$

□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□．□□□$J_\rho^+(t) > 0$, $J_\rho^+(t) > 0$□□□．□□平衡□□□□□□□□□□□条□□□□□x', x, □□ν□対□□

$$J^{+(\nu)}(x|x';t) = J^{-(\nu)}(x|x';t), \tag{3.8}$$

□□□□□□□ρ□対□□

$$J_\rho^+(t) = J_\rho^-(t), \tag{3.9}$$

□□□□□□□□□□．□□□□□□□□□寄□□□□□□□□□□□

$$J_\rho(t) = J_\rho^+(t) - J_\rho^-(t), \tag{3.10}$$

□□□□．□□□平衡□□□□□□ρ□対□□$J_\rho(t) = 0$□□□□□□□□□．□□条□□□□□定常□□$P_X^{\mathrm{ss}}(x)$□平衡□□□定□□□□□□□□分布□□□□□□．□□□□□□□□□□□□条□□□□，$\Delta s^{\mathrm{bath}(\nu)}(x'|x;t)$□□□□□□□刻$t$□$x'$□□$x$□□移□□□□，□□□□□□□□□□$\nu$□□□□□□□□□□□□□

$$\ln \frac{W^{(\nu)}(x|x';t)}{W^{(\nu)}(x'|x;t)} = \Delta s^{\mathrm{bath}(\nu)}(x|x';t), \tag{3.11}$$

□□□□□□□□□□□．

□□□□□□(□力学□□)力□□□□□□□□□□□□□□．

$$F_\rho(t) = \ln \frac{J_\rho^+(t)}{J_\rho^-(t)}, \tag{3.12}$$

□□$\rho = (x,x',\nu)$□□□$F_\rho(t) = F^{(\nu)}(x|x';t)$□□表□□□□□□□．□□□□□□$J_\rho(t)$□□□□□□□．□□□□

$$J_\rho(t) > 0 \Leftrightarrow F_\rho(t) > 0 \quad (\Leftrightarrow J_\rho^+(t) > J_\rho^-(t)), \tag{3.13}$$
$$J_\rho(t) < 0 \Leftrightarrow F_\rho(t) < 0 \quad (\Leftrightarrow J_\rho^+(t) < J_\rho^-(t)), \tag{3.14}$$
$$J_\rho(t) = 0 \Leftrightarrow F_\rho(t) = 0 \quad (\Leftrightarrow J_\rho^+(t) = J_\rho^-(t)), \tag{3.15}$$

□□□□□□□□□□□□□．□□□□□□条□□□□力$F_\rho(t)$□□□□□□$F_\rho(t) = 0$□□□□□□□□□□□．□□□□刻t□□□x□□□□□□□□□□□□□□

$$s^{\mathrm{sys}}(x;t) = -\ln p(x;t), \tag{3.16}$$

□定□□，□刻t□□□□x'□□x□□□□□□□□□□□□□

$$\Delta s^{\mathrm{sys}}(x|x';t) = s^{\mathrm{sys}}(x;t) - s^{\mathrm{sys}}(x';t), \tag{3.17}$$

□□□□. □□□$\rho = (x, x', \nu)$□対□□□□□□□□□□□□□□□□

$$\Delta s_\rho^{\mathrm{sys}}(t) = s^{\mathrm{sys}}(x;t) - s^{\mathrm{sys}}(x';t), \tag{3.18}$$

$$\Delta s_\rho^{\mathrm{bath}}(t) = \Delta s^{\mathrm{bath}(\nu)}(x|x';t), \tag{3.19}$$

□□□□, 力$F_\rho(t)$□

$$F_\rho(t) = \Delta s_\rho^{\mathrm{sys}}(t) + \Delta s_\rho^{\mathrm{bath}}(t), \tag{3.20}$$

□□□□□□□□□□□□□. □□□力$F_\rho(t)$□□□□□□□□□□□□□□□□□□□□□.

3.2 熱力学□二法則

3.2.1 エントロピー□成□

□□$J_\rho(t)$□力$F_\rho(t)$□□□□□□□. □□□□, □□□力□□□

$$J_\rho(t) F_\rho(t) \geq 0, \tag{3.21}$$

□常□非□□□□, □□□□条□□$F^{(\nu)}(x|x';t) = J^{(\nu)}(x|x';t) = 0$, □□□□$J_\rho^+(t) = J_\rho^-(t)$□□□$\rho$□対□□□□□□□□□□□□.

□ρ□□□□□□$x > x'$□□□□□□制□□加□□□□

$$\mathcal{E} = \{(x, x', \nu) | x > x', W^{(\nu)}(x|x';t) \neq 0\}, \tag{3.22}$$

□対□□□

$$\sigma(t) = \sum_{\rho \in \mathcal{E}} J_\rho(t) F_\rho(t), \tag{3.23}$$

□□□□□. □□$\mathcal{E}$□$x > x'$□□□□制□□加□□□□, (x, x', ν)□寄□□(x', x, ν)□寄□□□□数□□□□□□□□□□□□□□□. □□$\sigma(t)$□□□□□□□□□□□□□□□□□, □□□□□□□□□□□.

$$\sigma(t) \geq 0, \tag{3.24}$$

□□$\sigma(t) = 0$□□□□□□□□□□□□□条□□□□□□□□. □□非□□(3.24)□□力学□□□則□□□□□. □□□□□□前□$J_\rho(t) F_\rho(t)$□□□□□□移ρ□対□□□分□□□□□□□□□□□□□□□□□□.

3.2.2 熱力学□二法則との対応□係

□□□□□□□□□□□□□□□$\sigma(t)$□, □力学□□□□□□□□□□力学□□□則□□□□□対□□□□□□□□□□□□□□. $\sigma(t)$□□□□□□□□□□□□□□□□

$$\sigma(t) = \sum_{x,x'|x>x'} [J^{+(\nu)}(x|x';t) - J^{-(\nu)}(x|x';t)] F^{(\nu)}(x|x';t) \tag{3.25}$$

$$= \sum_{x,x',\nu|x \neq x'} J^{+(\nu)}(x|x';t) F^{(\nu)}(x|x';t), \tag{3.26}$$

□□□$F^{(\nu)}(x|x';t) = -F^{(\nu)}(x'|x;t)$, $J^{+(\nu)}(x|x';t) = -J^{-(\nu)}(x'|x;t)$□□□□. □□□□□□方□□□□散□□表□

$$\begin{aligned} p_X(x;t+dt) &= \sum_{x'=1}^{N}\left(\delta_{xx'} + \sum_{\nu=1}^{M} W^{(\nu)}(x|x';t)dt\right)p_X(x';t) \\ &= \sum_{x'=1}^{N}\sum_{\nu=1}^{M}\Big(\delta_{\nu 1}\delta_{xx'} + W^{(\nu)}(x|x';t)dt\Big)p_X(x';t), \end{aligned} \tag{3.27}$$

□□□□□□□□□□□□□. □□□x□□x□□□□□移□$\nu = 1$□□□□□□□□□□□. □□□□□□方□□□□散□□

$$p_X(x;t+dt) = \sum_{x'=1}^{N}\sum_{\nu=1}^{M} p(x;t+dt,x';t,\nu), \tag{3.28}$$

□□□□□□□□分布$p(x;t+dt,x';t,\nu)$□□□□□□□□□□, $x \neq x'$□□□□□□□□分布□

$$p(x;t+dt,x';t,\nu) = J^{+(\nu)}(x|x';t)dt, \tag{3.29}$$

□□□□□□□$J^{+(\nu)}(x|x';t)$□□□□□□□□□□□□. □□□, □□□□□□□□□$\sigma(t)$□dt□□□□□□□,

$$\begin{aligned} \sigma(t)dt &= \sum_{x,x',\nu|x\neq x'} p(x;t+dt,x';t,\nu)F^{(\nu)}(x|x';t), \\ &= \sum_{x,x',\nu} p(x;t+dt,x';t,\nu)F^{(\nu)}(x|x';t), \\ &= \sum_{x,x',\nu} p(x;t+dt,x';t,\nu)[\Delta s^{\mathrm{bath}(\nu)}(x|x';t) + \Delta s^{\mathrm{sys}}(x|x';t)], \end{aligned} \tag{3.30}$$

□□□□□□□□□□. □□□□□□□□□□□□□□$F^{(\nu)}(x|x;t) = 0$□□□□実□□□□□□. □□□□□期□□$\langle\cdots\rangle = \sum_{x,x',\nu} p(x;t+dt,x';t,\nu)\cdots$□表□□□□□

$$\begin{aligned} \sigma(t)dt &= \langle F(t)\rangle \\ &= \langle \Delta s^{\mathrm{bath}}(t)\rangle + \langle \Delta s^{\mathrm{sys}}(t)\rangle, \end{aligned} \tag{3.31}$$

□□□□□□□□□□□□□□. □□□, $\sigma(t)dt$□□□□□□□□□□□□□□□□期□□□□□□□□□□□□□□□□□. □□□, □力学□□□則(3.24)□

$$\langle \Delta s^{\mathrm{bath}}(t)\rangle + \langle \Delta s^{\mathrm{sys}}(t)\rangle \geq 0, \tag{3.32}$$

□□□□□□□□□□□□□□□期□□□□□非□□□□□□□□□□□□. □□□□□□条□□□□□□□□条□□□□□□□□, □□□□平衡□□□□□□□□.

□□□□□□□□□分□$\Sigma(\tau) = \int_{t=0}^{t=\tau}\sigma(t)dt$□□刻0□□$\tau$□□□□□□□□□□□□□□□, □力学□□□則□□□□□□□□□□□□□□□□,

$$\begin{aligned} \Sigma(\tau) &= \int_{t=0}^{t=\tau}\langle F(t)\rangle \\ &= \int_{t=0}^{t=\tau}\langle \Delta s^{\mathrm{bath}}(t)\rangle + \int_{t=0}^{t=\tau}\langle \Delta s^{\mathrm{sys}}(t)\rangle \\ &\geq 0. \end{aligned} \tag{3.33}$$

□刻0□□τ□□□□□□□□□□□□□□行□□□□□□□□□□□□□□定□□□対□□係□□□□□，□$\int_{t=0}^{t=\tau}\langle\Delta s^{\mathrm{sys}}(t)\rangle$□□□□□□□□□□$\oint dS^{\mathrm{SYS}}$□□□，□$\int_{t=0}^{t=\tau}\langle\Delta s^{\mathrm{bath}}(t)\rangle$□□□□□□□□□□□$-\oint\sum_i[\delta Q_i/T_i]$□□□□□□□□□□□□対□□□□□．□□□，$S^{\mathrm{SYS}}$□□□□□□□□力学□□□□□□□□，$\delta Q_i$□□度$T_i$□□□□□□□□□，$\oint$□□□□□□□□□□□□□□□分□□□．

3.2.3 □のエントロピー変化とShannonエントロピーの変化

□□□□□□□□□□□□力学□□□□□□□□□□□□□□対□□□□□□□□□□□□□□□□□□□□期□□$\langle\Delta s_{\mathrm{sys}}\rangle$□□□□□□□□□□□□□□□□．□□□□□力学□□□□□，□□□$\langle\Delta s_{\mathrm{sys}}\rangle$□□□□□□□□□□□□□□□□□□□度□□□□□□Shannon□□□□□□$H(X;t)$□□□□□□□□□□□□□□□□示□．□□

$$
\begin{aligned}
\langle\Delta s_{\mathrm{sys}}(t)\rangle &= \sum_{x,x',\nu} p(x;t+dt,x';t,\nu)[\ln p_X(x';t) - \ln p_X(x;t)] \\
&= \sum_{x'=1}^{N} p_X(x';t)\ln p_X(x';t) - \sum_{x=1}^{N} p_X(x;t+dt)\ln p_X(x;t) \qquad (3.34)
\end{aligned}
$$

□□□□□□．□□□□

$$
\begin{aligned}
&\sum_{x=1}^{N} p_X(x;t+dt)\ln p_X(x;t+dt) \\
&= \sum_{x=1}^{N} p_X(x;t+dt)\ln p_X(x;t) + \sum_{x=1}^{N} p_X(x;t)dt\frac{\partial_t p_X(x;t)}{p_X(x;t)} + O(dt^2) \\
&= \sum_{x=1}^{N} p_X(x;t+dt)\ln p_X(x;t) + dt\partial_t\left[\sum_{x=1}^{N} p_X(x;t)\right] + O(dt^2) \\
&= \sum_{x=1}^{N} p_X(x;t+dt)\ln p_X(x;t) + O(dt^2), \qquad (3.35)
\end{aligned}
$$

□$O(dt)$□□□□□□□□□$\sum_x p_X(x;t)=1$□□□□□□□□□，$O(dt^2)$□□□□□□□□□□□，

$$
\begin{aligned}
\langle\Delta s_{\mathrm{sys}}\rangle &= \sum_{x=1}^{N} p_X(x;t)\ln p_X(x;t) - \sum_{x=1}^{N} p_X(x;t+dt)\ln p_X(x;t+dt) \\
&= H(X;t+dt) - H(X;t) \qquad (3.36) \\
&= \frac{dH(X;t)}{dt}dt \qquad (3.37)
\end{aligned}
$$

□□刻t□□□□□数X□□□□Shannon□□□□□□$H(X;t)$□□□□□□□□□□□□□□．□□□Shannon□□□□□□$H(X;t)$□

$$
H(X;t) = -\sum_{x=1}^{N} p_X(x;t)\ln p_X(x;t), \qquad (3.38)
$$

□□□□定□□□□．□□□□□□分□□□□

$$
\int_{t=0}^{t=\tau}\langle\Delta s_{\mathrm{sys}}\rangle = H(X;\tau) - H(X;0), \qquad (3.39)
$$

□□□□□□□□Shannon□□□□□□□□分□□□□.

Shannon□□□□□□□□分□表□□□□□□力学□□□則(3.24)□□□□□□

$$H(X;\tau) - H(X;0) \geq -\int_{t=0}^{t=\tau} \langle \Delta s^{\mathrm{bath}}(t) \rangle, \tag{3.40}$$

□□□□，□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□対□□，□□□□□□□□□□□□□□□□□□力学□□□□□□□□□.□□□，□□□□□力学□□□□□方□□□□□□□□□□□□□□□□□□□□□□□□，□□□□□□力学□□□□□□□体□□□□□□□□□□□□□□□□.

3.2.4 エントロピー□成□と熱力学□一法則

□□□□□□□□□□□□□□□□□□定□□□力学□□□則□整□□□□□□□□□□□□□.□□□□□□□□□□□□□定□□□力学□□□則□□整□□□□□□□□□□□.

$M = 1$□□□，□□度β□□□□□□□□□□□□□□□□.□□□依存□□□□□□□□$U_X(x;t)$□□□□□□□□□条□

$$\ln \frac{W^{(1)}(x|x';t)}{W^{(1)}(x'|x;t)} = -\beta(U_X(x;t) - U_X(x';t)), \tag{3.41}$$

□□□□□□□□察□□□.□□□□□□□□$U_X(x;t)$□期□□$\langle U_X(t) \rangle$□

$$\langle U_X(t) \rangle = \sum_{x=1}^{N} U_X(x;t) p_X(x;t), \tag{3.42}$$

□□□□□□.□□□$\langle U_X(t) \rangle$□□□分□□□□□□分□□□□□□□□□.

$$\frac{\langle U_X(t) \rangle}{dt} = \sum_{x=1}^{N} (\partial_t U_X(x;t)) p_X(x;t) + \sum_{x=1}^{N} U_X(x;t) \partial_t p_X(x;t). \tag{3.43}$$

□□□□□□□□□$U_X(x;t)$□□□依存□□□□□□□

$$\sum_{x=1}^{N} (\partial_t U_X(x;t)) p_X(x;t) = \frac{\delta \mathcal{W}}{\delta t}(t) \tag{3.44}$$

□□□，□□□□□□□□□□□□□□□.□□□□□□□□□力学□□□則

$$\frac{\langle U_X(t) \rangle}{dt} = \frac{\delta \mathcal{Q}}{\delta t}(t) + \frac{\delta \mathcal{W}}{\delta t}(t), \tag{3.45}$$

□□□□□□□$\delta\mathcal{Q}/\delta t(t)$□□□□□□□□.

$$\begin{aligned} \sum_{x=1}^{N} U_X(x;t) \partial_t p_X(x;t) &= \frac{\langle U_X(t) \rangle}{dt} - \frac{\delta \mathcal{W}}{\delta t}(t) \\ &= \frac{\delta \mathcal{Q}}{\delta t}(t). \end{aligned} \tag{3.46}$$

□□□□□□$\delta\mathcal{Q}/\delta t(t)$□□□□，□□□□□□□□□$\sigma(t)$□

$$\sigma(t) = \frac{dH(X;t)}{dt} - \beta \frac{\delta \mathcal{Q}}{\delta t}(t), \tag{3.47}$$

□□□□□□□□□□□□□□□□□□□□□.

$$
\begin{aligned}
&\frac{dH(X;t)}{dt} - \beta\frac{\delta\mathcal{Q}}{\delta t}(t) \\
&= -\sum_{x=1}^{N}\ln p_X(x;t)\partial_t p_X(x;t) - \sum_{x=1}^{N}\beta U_X(x;t)\partial_t p_X(x;t) \\
&= -\sum_{x=1}^{N}[\ln p_X(x;t) + \beta U_X(x;t)]\sum_{x'=1}^{N}J^{(1)}(x|x';t) \\
&= -\frac{1}{2}\sum_{x=1}^{N}\sum_{x'=1}^{N}[\ln p_X(x;t) + \beta U_X(x;t)]J^{(1)}(x|x';t) \\
&\quad -\frac{1}{2}\sum_{x=1}^{N}\sum_{x'=1}^{N}[\ln p_X(x';t) + \beta U_X(x';t)]J^{(1)}(x'|x;t) \\
&= \frac{1}{2}\sum_{x=1}^{N}\sum_{x'=1}^{N}\left[\ln\frac{p_X(x';t)}{p_X(x;t)} - \beta(U_X(x;t) - U_X(x';t))\right]J^{(1)}(x'|x;t) \\
&= \frac{1}{2}\sum_{x=1}^{N}\sum_{x'=1}^{N}\ln\frac{W^{(1)}(x|x';t)p_X(x';t)}{W^{(1)}(x'|x;t)p_X(x;t)}J^{(1)}(x'|x;t) \\
&= \sum_{x,x'|x>x'}F^{(1)}(x'|x;t)J^{(1)}(x'|x;t) \\
&= \sigma(t).
\end{aligned} \tag{3.48}
$$

□□□□□□□□□□, □□□□□□□□□条□(3.41), □□定□(3.46), □□□□方□□$\partial_t p_X(x;t) = \sum_{x'=1}^{N} J^{(1)}(x|x';t)$□□□□□対称□$J^{(1)}(x'|x;t) = -J^{(1)}(x|x';t)$□□□□□□. □□□

$$
\frac{\langle \Delta s_{\rm sys}\rangle}{dt} = \frac{dH(X;t)}{dt} \tag{3.49}
$$

□□□□□□□□□□□□, □□□□□□□□□□□□□□□□寄□□

$$
\frac{\langle \Delta s_{\rm bath}\rangle}{dt} = -\beta\frac{\delta\mathcal{Q}}{\delta t}(t), \tag{3.50}
$$

□□□□□□□□□□□□□□□□□□□□.

3.3 □平□定常状態での熱力学とKirchhoffの法則

非平衡□□□□□定常□□□□□□□□□□□□□□□□□□□□□□□力学□□□□□□□□□□□□□□□. □□□□□□□□□□□□□□□□□□, □移□□定□□ρ□□□□□□, □□□□定□□x□□□□□□□□□□表□□□□□, □□□□□□察□□□□□□□□□□□□□□. □□□□□□□□表□□□□□□□力学□□□Schnakenberg□□□□□□□□ [1]□□□□□□□. □□, 非平衡定常□□□□□□Schnakenberg□□□□□□□□□□□□□□□□行□.

□移□□□$W^{(\nu)}(x|x';t)$□□□□依存□□□□□□,$W^{(\nu)}(x|x';t) = W^{(\nu)}(x|x')$□□□□□□□□□□. 定常分布$p_X^{\rm ss}(x)$□□□□$\rho = (x, x', \nu)$□対□□定常分布□対□□□□□

$$
J_\rho^{\rm ss} = J_\rho^{+\rm ss} - J_\rho^{-\rm ss}, \tag{3.51}
$$

$$
J_\rho^{+\rm ss} = W^{(\nu)}(x|x')p_X^{\rm ss}(x'), \tag{3.52}
$$

$$
J_\rho^{-\rm ss} = W^{(\nu)}(x'|x)p_X^{\rm ss}(x), \tag{3.53}
$$

□□□. □□ρ□□□□□□, □□□□x''□□□□□□□

$$\mathcal{E}^{+}(x'') = \{(x, x', \nu)|x = x'', x > x', W^{(\nu)}(x|x') \neq 0\}, \tag{3.54}$$

□□□x''□□□□□□□□

$$\mathcal{E}^{-}(x'') = \{(x, x', \nu)|x' = x'', x > x', W^{(\nu)}(x|x') \neq 0\}, \tag{3.55}$$

□□□□, 定常□□□条□□□□□x□対□□

$$\sum_{\rho \in \mathcal{E}^{+}(x)} J_{\rho}^{\mathrm{ss}} - \sum_{\rho \in \mathcal{E}^{-}(x)} J_{\rho}^{\mathrm{ss}} = 0, \tag{3.56}$$

□□□□□□□□□. □□定常□□□条□□□□□□□Krichhoff□□□□則(□□則)□対□□□□□□□□□□. □□□□Kirchhoff□□□□則□□□□□□□□□□□□□□□□□□□□□□□実□□□□□□□□□.

Kirchhoff□□□□則□□□□, □□□□□□□□□□□□□□□□□□□□□□□□□□実□□, □□□□□□□□□□□□□□□□□□□□□□, □□□□□□□□□定常□□□□J_{ρ}^{ss}□対□□□□□□□□□□□□□□□□. □□□□□□, □□数学□□□□□□□□□□□, 例□□□□□□□□□□□□□□□□□□□□□□行□□□□□文□ [6]□□□□□□.

□□□□□□□□□□□$\rho_i = (x_i, x_i', \nu_i)$□□□$(i \in \{0, \ldots, n\})$□, □□$x_i' = x_{i+1}$, $x_0 = x_n'$□□□□□□□□□□□□□□. □□□□□□□□$\rho_0, \rho_1, \ldots \rho_n$□□□□, □□□□□$x_0 = x_n'$□□□□□□□□□□□□□□. □□□□□□□□□□□□□, □□□□□□□□□□□□□□, □□□□$i \neq j$□$\rho_i \neq \rho_j$□□, □□□□□□□(x_i, x_i', ν_i)□□□□□□□□□□□□□□, □□□□□□□(x_i', x_i, ν_i)□□□□□□□□□□□□□□□□.

□□□□□□□□□□□□□□□□□□□□□□□□□□行列$\mathcal{S}_{\rho}(\mathcal{C})$□□□□. □□□□□□$\mathcal{C}$□□移$\rho = (x, x', \nu)$□□□□□□□□$\mathcal{S}_{\rho}(\mathcal{C}) = 1$□, □□□□$\mathcal{C}$□□移$\rho = (x, x', \nu)$□□□□□□移$(x', x, \nu)$□□□□□□□□$\mathcal{S}_{\rho}(\mathcal{C}) = -1$□, □□□□□□□□□□□□□□□□□$\mathcal{S}_{\rho}(\mathcal{C}) = 0$□□□□行列□□□. □□□□□□□□□$\mathcal{C}$□□□□□□□□□底$\{\mathcal{C}_{\mu}|\mu = 1, \cdots, n_{\mathrm{C}}\}$□□□□□□□□□□□□. □□□□□□□$\mathcal{C}$□□□□□□□□□底$\{\mathcal{C}_{\mu}|\mu = 1, \cdots, n_{\mathrm{C}}\}$□□□□□□, □□□□□□□□□□□□□□$\mathcal{C}$□行列$\mathcal{S}_{\rho}(\mathcal{C})$対□□, 常□係数$a_{\mu}$□表□□□□□□□□底$\mathcal{S}_{\rho}(\mathcal{C}_{\mu})$□□□□□□, □□□□

$$\mathcal{S}_{\rho}(\mathcal{C}) = \sum_{\mu=1}^{n_{\mathrm{C}}} a_{\mu} \mathcal{S}_{\rho}(\mathcal{C}_{\mu}), \tag{3.57}$$

□□□□□.

□□□□□行列$\mathcal{S}_{\rho}(\mathcal{C}_{\mu})$□□□□□□, □□□□□□□$\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_{\mu})$□

$$J_{\rho}^{\mathrm{ss}} = \sum_{\mu=1}^{n_{\mathrm{C}}} \mathcal{S}_{\rho}(\mathcal{C}_{\mu}) \mathcal{J}^{\mathrm{ss}}(\mathcal{C}_{\mu}), \tag{3.58}$$

□□□□ρ□□□□□□□□□□□□□□□□□□. □□□□□□□□□□□□□底$\{\mathcal{C}_{\mu}|\mu = 1, \cdots, n_{\mathrm{C}}\}$□□□□$\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_{\mu})$□□□□□□□□□□□□定□, □□□定□□□□□□□□□□□□□□底□□□方□制□□□□□□□□□. □□□□□□□□□□□底□□□方□□□

□fundamental set of cycle□□□□□□□ [1]. □□□□□□□□□□定□(3.58)□, 定常□□□条□□□□□□□□□□□□□□□□□□□□□□□□□□.

$$
\begin{aligned}
&\sum_{\rho\in\mathcal{E}^{+}(x)} J_\rho^{\rm ss} - \sum_{\rho\in\mathcal{E}^{-}(x)} J_\rho^{\rm ss} \\
&= \sum_{\rho\in\mathcal{E}^{+}(x)} \sum_{\mu=1}^{n_{\rm C}} \mathcal{S}_\rho(\mathcal{C}_\mu)\mathcal{J}^{\rm ss}(\mathcal{C}_\mu) - \sum_{\rho\in\mathcal{E}^{-}(x)} \sum_{\mu=1}^{n_{\rm C}} \mathcal{S}_\rho(\mathcal{C}_\mu)\mathcal{J}^{\rm ss}(\mathcal{C}_\mu) \\
&= \sum_{\mu=1}^{n_{\rm C}} \left[\sum_{\rho\in\mathcal{E}^{+}(x)} \mathcal{S}_\rho(\mathcal{C}_\mu) - \sum_{\rho\in\mathcal{E}^{-}(x)} \mathcal{S}_\rho(\mathcal{C}_\mu) \right] \mathcal{J}^{\rm ss}(\mathcal{C}_\mu) \\
&= 0.
\end{aligned} \tag{3.59}
$$

□□□, □□□□□定□□□$\sum_{\rho\in\mathcal{E}^{+}(x)} \mathcal{S}_\rho(\mathcal{C}_\mu) = \sum_{\rho\in\mathcal{E}^{-}(x)} \mathcal{S}_\rho(\mathcal{C}_\mu)$□□□□□□□□□.

□□□□□定常□□□ρ□□□□力

$$
F_\rho^{\rm ss} = \ln \frac{J_\rho^{+\rm ss}}{J_\rho^{-\rm ss}}, \tag{3.60}
$$

□□□□□, □□□□□□□□分□□□□□□□□. □□□□□力$\mathcal{F}^{\rm ss}(\mathcal{C}_\mu)$□□□□□□□□定□□□□.

$$
\mathcal{F}^{\rm ss}(\mathcal{C}_\mu) = \sum_{\rho\in\mathcal{E}} \mathcal{S}_\rho(\mathcal{C}_\mu) F_\rho^{\rm ss}. \tag{3.61}
$$

□□□□□□□力□定□□□□□□□□□□□□□□□, Krichhoff□□□□則(□□則)□□□□□, □□□□□力$\mathcal{F}^{\rm ss}(\mathcal{C}_\mu)$□□□力□□□□□□□□□□. □□□□Kirchhoff□□□則□, □□□□□□□力□□□荷□□□□□□□□□□□□□□□□□□□□実□□□□□□□□□.

□□□□表□□□□□□定常□□□□□□□□□□□□□□□□$\sigma^{\rm ss} := \sum_{\rho\in\mathcal{E}} J_\rho^{\rm ss} F_\rho^{\rm ss}$□

$$
\begin{aligned}
\sigma^{\rm ss} &= \sum_{\rho\in\mathcal{E}} J_\rho^{\rm ss} F_\rho^{\rm ss} \\
&= \sum_{\rho\in\mathcal{E}} \sum_{\mu} \mathcal{S}_\rho(\mathcal{C}_\mu)\mathcal{J}^{\rm ss}(\mathcal{C}_\mu) F_\rho^{\rm ss} \\
&= \sum_{\mu} \mathcal{J}^{\rm ss}(\mathcal{C}_\mu)\mathcal{F}^{\rm ss}(\mathcal{C}_\mu),
\end{aligned} \tag{3.62}
$$

□□□□□. □□□□□□□□力□□□□□□□□□□□□□□□□□□表□□□□□□□□□□□. □□□□□□□□□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□□□□□□力□□□□□□, 定常□□□□□□□□□□□□□□□□□□力□□□□□□□□□□□□□□□□□□□□□.

平衡□□□□□□□□□□□□□□□□□□$\sigma^{\rm ss} = 0$□□□, 非平衡定常□□□□□□$\sigma^{\rm ss} \neq 0$□□□. □□平衡□□□□□□□□□□□□□□□条□,

$$
J_\rho^{\rm ss} = F_\rho^{\rm ss} = 0, \tag{3.63}
$$

□□□□□□□□,

$$
\mathcal{F}^{\rm ss}(\mathcal{C}_\mu) = \mathcal{J}^{\rm ss}(\mathcal{C}_\mu) = 0 \tag{3.64}
$$

□□□. □□□, $\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)$□□□□□□□□□□□定□□□利□□□. (3.58)□□□$\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)=0$□□□□□□□□□. □□□, 平衡□□□非平衡定常□□□□□□□, □□□□□□□□存□□有□□□□□□□□□□□□□□□□□□. □□□定常□□□平衡□□□□□□, □□□□□□□$\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)$□存□□□□.

3.4 □形不可□熱力学とOnsager□反□係

定常□□□平衡□□□□□□□□□□□□□□□□□□□. □□□□, □□□□□□□□

$$
\begin{aligned}
J_\rho^{+\mathrm{eq}} &:= W^{\mathrm{eq}(\nu)}(x|x')p_X^{\mathrm{eq}}(x') \\
&= W^{\mathrm{eq}(\nu)}(x'|x)p_X^{\mathrm{eq}}(x) := J_\rho^{-\mathrm{eq}}
\end{aligned}
\tag{3.65}
$$

□□□□平衡□□$p^{\mathrm{eq}}(x)$□□□平衡□□□□□□□移□□□$W^{\mathrm{eq}(\nu)}(x|x')$□□□□. □□□□□移□□□□例□□□$\nu$□□□□□□□□□

$$
W^{(\nu)}(x|x') = W^{\mathrm{eq}(\nu)}(x|x') + O(\epsilon)
\tag{3.66}
$$

□□□□□ϵ□□□□□□□□□□□, 平衡□□□□□新□□非平衡定常□□$p_X^{\mathrm{ss}}(x)$□実□□□□. □□□, □□□ρ□□□新□□非平衡定常□□□J_ρ^{ss}□

$$
J_\rho^{\mathrm{ss}} = J_\rho^{+\mathrm{ss}} - J_\rho^{-\mathrm{ss}} = \mathcal{O}(\epsilon),
\tag{3.67}
$$

□□□□□□□□□. □□

$$
J_\rho^{-\mathrm{eq}} = J_\rho^{-\mathrm{ss}} + \mathcal{O}(\epsilon),
\tag{3.68}
$$

□□□. □□□□

$$
\begin{aligned}
F_\rho^{\mathrm{ss}} &= \ln\left(1 + \frac{J_\rho^{\mathrm{ss}}}{J_\rho^{-\mathrm{ss}}}\right) \\
&= \frac{J_\rho^{\mathrm{ss}}}{J_\rho^{-\mathrm{ss}}} + \mathcal{O}(\epsilon^2) \\
&= \frac{J_\rho^{\mathrm{ss}}}{J_\rho^{-\mathrm{eq}}} + \mathcal{O}(\epsilon^2)
\end{aligned}
\tag{3.69}
$$

□□□. □□□

$$
\alpha_\rho = \frac{1}{J_\rho^{-\mathrm{eq}}} = \frac{1}{J_\rho^{+\mathrm{eq}}}
\tag{3.70}
$$

□□□□□□□□□□,

$$
F_\rho^{\mathrm{ss}} = \alpha_\rho J_\rho^{\mathrm{ss}} + \mathcal{O}(\epsilon^2)
\tag{3.71}
$$

□□□□□□力□□□□□□係□□□□□□□□□□□. □□□□□例係数α_ρ□□□□平衡□□□□□□□移□□□□平衡分布□□□□□□□□□□.

$\mathcal{O}(\epsilon^2)$□□□□□□□□□□係□□□□□□□□□力□□□□□□□□□□,

$$
\begin{aligned}
\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu) &= \sum_{\rho\in\mathcal{E}} \mathcal{S}_\rho(\mathcal{C}_\mu) F_\rho^{\mathrm{ss}} \\
&= \sum_{\rho\in\mathcal{E}} \mathcal{S}_\rho(\mathcal{C}_\mu)\alpha_\rho J_\rho^{\mathrm{ss}} \\
&= \sum_{\nu=1}^{n_{\mathrm{C}}} \left[\sum_{\rho\in\mathcal{E}} \mathcal{S}_\rho(\mathcal{C}_\mu)\alpha_\rho \mathcal{S}_\rho(\mathcal{C}_\nu)\right] \mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu).
\end{aligned}
\tag{3.72}
$$

□□□□.□□□

$$L_{\mu\nu} = \sum_{\rho\in\mathcal{E}} \mathcal{S}_\rho(\mathcal{C}_\mu)\alpha_\rho \mathcal{S}_\rho(\mathcal{C}_\nu), \tag{3.73}$$

□□□□□□,

$$\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu) = \sum_{\nu=1}^{n_\mathrm{C}} L_{\mu\nu}\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu). \tag{3.74}$$

□平衡□□□□□□□□□□力$\mathcal{F}(\mathcal{C}_\mu)$□□□□□□□□$\mathcal{J}(\mathcal{C}_\nu)$□□□□係□□□□□□□□□□□□□.□□□□行列$L_{\mu\nu}$□平衡□□□□α_ρ□□□□□□□□□□.□□□□□係□□□□□□平衡□□□□□定常□□□□定□□力学□□□□□枠□□□,□□非□□□力学(linear irreversible thermodynamics)□□□□□□□.

□□□□非□□□力学□□□□□$L_{\mu\nu}$□□則□□□,□行列$M_{\mu\nu} = L_{\mu\nu}^{-1}$□存□□□.□則□□存□□□□□□□□□□□□□□□□□□□□.

□□□□□μ□$F^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□,□□□$\mu$□$J^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□□□□□□□□□□□示□.□□□$\mu$□$F^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□,$\sigma^{\mathrm{ss}} = 0$□□平衡□□□□□.□□□□$J_\rho^{\mathrm{ss}} = 0$□□□.$J^{\mathrm{ss}}(\mathcal{C}_\mu)$□□□$J_\rho^{\mathrm{ss}} = 0$□□□□□定□□□□□□定□□□□□□,□□□$\mu$□$J^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□□□□□□□.

□□□$L_{\mu\nu}$□□則□□□□□□□,□□□□□□□□0□□□□□,□□□□□□□□□非□□□$J^{\mathrm{ss}}(\mathcal{C}_\mu)$□□□□□□□□□□□,□□□$\mu$□$F^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□□.□□□□□□$\mu$□$F^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□,□□□$\mu$□$J^{\mathrm{ss}}(\mathcal{C}_\mu) = 0$□□□□□□□□□□□□□実□□□□□.□□□ $L_{\mu\nu}$□□則.

□□□□□行列$M_{\mu\nu} = L_{\mu\nu}^{-1}$□□□□,□□□

$$\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu) = \sum_{\mu=1}^{n_\mathrm{C}} M_{\mu\nu}\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu), \tag{3.75}$$

□□□□□□□□□.□□□行列$M_{\mu\nu}$□, Onsager係数□□□□□□□.

□□□□, $L_{\mu\nu}$□定□□□行列□対称□

$$L_{\mu\nu} = L_{\nu\mu}, \tag{3.76}$$

□示□□.□□対称行列□□行列□対称□□□

$$M_{\mu\nu} = M_{\nu\mu}, \tag{3.77}$$

□□□□.□□□□Onsager□□□係□□□□□.□□□□□平衡□□□

$$\frac{\partial\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu)}{\partial\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu)} = \frac{\partial\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\nu)}{\partial\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)}, \tag{3.78}$$

$$\frac{\partial\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)}{\partial\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\nu)} = \frac{\partial\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu)}{\partial\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu)}, \tag{3.79}$$

□□□□□□□,□□□平衡□□□□□□□□□□□□□□□□力□□□□□□□□□係□□□□□□□□□□□.

□□□定常□□□□□□□□□□□□□□

$$
\begin{aligned}
\sigma^{\mathrm{ss}} &= \sum_{\mu=1}^{n_{\mathrm{C}}} \mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu)\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu) \\
&= \sum_{\mu=1}^{n_{\mathrm{C}}}\sum_{\nu=1}^{n_{\mathrm{C}}} L_{\mu\nu}\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu) \\
&= \sum_{\mu=1}^{n_{\mathrm{C}}}\sum_{\nu=1}^{n_{\mathrm{C}}} M_{\mu\nu}\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu)\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\nu),
\end{aligned}
\tag{3.80}
$$

□□□, □力学□□□則□

$$
\sum_{\mu,\nu} L_{\mu\nu}\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\mu)\mathcal{J}^{\mathrm{ss}}(\mathcal{C}_\nu) \geq 0, \tag{3.81}
$$

$$
\sum_{\mu,\nu} M_{\mu\nu}\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\mu)\mathcal{F}^{\mathrm{ss}}(\mathcal{C}_\nu) \geq 0, \tag{3.82}
$$

□行列$L_{\mu\nu}$, $M_{\mu\nu}$□□□□□□□定□行例□□□□□□□□□□.

□□□□定□□□数学□□別表□□□□□行列□□□行列□□□□非□□□□□□□□□□□□□□□□□□□. □□定□□□□力学□□□則□□来□□□□□□, $L_{\mu\nu}$, $M_{\mu\nu}$□□□□□□□行列□□□□非□□□力学□□□則□別表□□□□. 例□□$n_{\mathrm{C}}=2$□□□

$$
\begin{vmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{vmatrix} = L_{11}L_{22} - L_{12}L_{21} \geq 0, \tag{3.83}
$$

$$
L_{11} \geq 0, \tag{3.84}
$$

$$
L_{22} \geq 0, \tag{3.85}
$$

□□□□

$$
\begin{vmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{vmatrix} = M_{11}M_{22} - M_{12}M_{21} \geq 0, \tag{3.86}
$$

$$
M_{11} \geq 0, \tag{3.87}
$$

$$
M_{22} \geq 0, \tag{3.88}
$$

□□□□□□□力学□□□□, □力学□□□則□別表□□□□.

3.5　Fokker-Planck方□式における熱力学□二法則

□□□□□□散□master方□□□対□□, □力学□□□則□□□□□□. □, over-damped□Langevin方□□

$$
\dot{x}(t) = -\mu\partial_x U_X(x;t) + \sqrt{2\mu\beta^{-1}}\cdot\xi(t), \tag{3.89}
$$

$$
\langle\xi(t)\rangle = 0, \tag{3.90}
$$

$$
\langle\xi(t)\xi(t')\rangle = \delta(t-t'), \tag{3.91}
$$

□□□□□□□□Fokker-Planck方□□

$$
\partial_t P_X(x;t) = -\partial_x(\nu_X(x;t)P_X(x;t)), \tag{3.92}
$$

$$
\nu_X(x;t) = -\mu\partial_x[U_X(x;t) + \beta^{-1}\partial_x \ln P_X(x;t)], \tag{3.93}
$$

□対□□, □力学□□□則□□□□□□□□□□□□□□□□□□□□□□□□.

□散□□□□□□□力学□□□則□□□□□方□□□□□方□□，□□□□□□□□□□□□□□□□□定□□□□□□□□□□□．□□，□□□□□□□□□□□□□期□□$\langle U(t)\rangle$

$$\langle U_X(t)\rangle = \int dx U_X(x;t) P_X(x;t), \tag{3.94}$$

□□□□，□□□□□□□□期□□□□□□□分□□□□□寄□$\delta\mathcal{W}/\delta t(t)$□□□寄□$\delta\mathcal{Q}/\delta t(t)$□分□□□□□□□．

$$\frac{d}{dt}\langle U_X(t)\rangle = \frac{\delta\mathcal{W}}{\delta t} + \frac{\delta\mathcal{Q}}{\delta t}, \tag{3.95}$$

$$\frac{\delta\mathcal{W}}{\delta t}(t) = \int dx (\partial_t U_X(x;t)) P_X(x;t), \tag{3.96}$$

$$\frac{\delta\mathcal{Q}}{\delta t}(t) = \int dx U_X(x;t) \partial_t P_X(x;t). \tag{3.97}$$

□□□□□□□□□□$U_X(x;t)$□□□依存□□□□□□□□□□□□寄□$\delta\mathcal{W}/\delta t(t)$□□□□□□□□□□□□□．□□□(3.95)□□力学□□□則□□□□□□□□□□，□□定□(3.97)□□□□□□□．

□□□Shannon□□□□□□□□□□□□□□□□分□□□□□□□$\mathcal{H}(X;t)$□

$$\mathcal{H}(X;t) = -\int dx P_X(x;t) \ln P_X(x;t), \tag{3.98}$$

□□□□□□□□，□□□□□□□□□□□□□□□□□．□□$\sigma(t)$□定□□□□□□□□□□□□．

$$\sigma(t) = \frac{d\mathcal{H}(X;t)}{dt} - \beta\frac{\delta\mathcal{Q}}{\delta t}. \tag{3.99}$$

□□□□□□□□□□□□□□□□□□□□□□□□．

$$\begin{aligned}
\sigma(t) &= -\int dx \ln P_X(x;t)\partial_t P_X(x;t) - \int dx \partial_t P_X(x;t) - \beta\frac{\delta\mathcal{Q}}{\delta t} \\
&= -\beta\int dx [U_X(x;t) + \beta^{-1}\ln P_X(x;t)]\partial_t P_X(x;t) \\
&= \beta\int dx [U_X(x;t) + \beta^{-1}\ln P_X(x;t)]\partial_x(\nu_X(x;t)P_X(x;t)) \\
&= \beta\int dx [-\partial_x[U_X(x;t) + \beta^{-1}\ln P_X(x;t)]](\nu_X(x;t)P_X(x;t)) \\
&= \frac{\beta}{\mu}\int dx (\nu_X(x;t))^2 P_X(x;t).
\end{aligned} \tag{3.100}$$

□□□□□□□□□□□条□$\int dx\partial_t P_X(x;t) = \partial_t(1) = 0$□□□，$P_X(x;t)$□□□□□□□□□□□□定□□□□□分□分□行□□□．□□□，□□□□□□□□□□□非□□□

$$\sigma(t) = \frac{\beta}{\mu}\int dx (\nu_X(x;t))^2 P_X(x;t) \geq 0, \tag{3.101}$$

□□□□□□□□□，□力学□□□則□□□□□□□．□□$P_X(x;t)$□□□□分布□□□□□□□x□非□□□□□□□□□□□□□□□分布□対□□□，□□□x□対□□$\nu_X(x;t) = 0$□□□□□□□□□□□条□□□□□□□，□□□□平衡□□□□□□□□□□□□□□□□□0□□□□□□□□□．

□4□

情報□とゆらぎの熱力学

Shannon□□□□□□□□□□□□□□□□□□□□□, □□□□□力学□□□□□□□□□□□□□□□□. □□□□□□□□[7]□□□□□□□□□□□□□□□, □□□□□□□□□□□力学□□□□□□□□□□□□□□□□□.

4.1 Shannonエントロピーと微分エントロピー

□□□□前□□□□Shannon□□□□□□□□分□□□□□□□□改□□□□□□□□.

4.1.1 Shannonエントロピー

□□□数□□$\boldsymbol{X}=\{X_1,\cdots,X_n\}$□□□□□散□□$\boldsymbol{x}\in\{1,\dots,N\}^n$□対□□□□分布□$p_{\boldsymbol{X}}(\boldsymbol{x})$□□□. □□□数□□$\boldsymbol{X}=\{X_1,\cdots,X_n\}$□□□□□Shannon□□□□□□□

$$H(\boldsymbol{X})=-\sum_{x}p_{\boldsymbol{X}}(\boldsymbol{x})\ln p_{\boldsymbol{X}}(\boldsymbol{x}), \tag{4.1}$$

□定□□□□. □□□$p_{\boldsymbol{X}}(\boldsymbol{x})=0$□□□□□□□□□□□□□□□□□□□□□寄□□$p_{\boldsymbol{X}}(\boldsymbol{x})\ln p_{\boldsymbol{X}}(\boldsymbol{x})=0$□□□. □□□□$0\le p_{\boldsymbol{X}}(\boldsymbol{x})\le 1$□□非□

$$H(\boldsymbol{X})\ge 0, \tag{4.2}$$

□□□. □□□□条□□□□$\boldsymbol{x}$□対□□$p_{\boldsymbol{X}}(\boldsymbol{x})=1$□□□□□□. □□□□$1\ln 1=0$□$0\ln 0=0$□寄□□□□□□□□□□□□$0$□□□□. □□Shannon□□□□□□□期□□□表□□□□□□□□□□□. □□□□

$$H(\boldsymbol{X})=\langle -\ln p_{\boldsymbol{X}}\rangle_{p_{\boldsymbol{X}}}, \tag{4.3}$$

□□□□□□□□□□□□. □□□□□□□□□字□□□分布□期□□□□□□□□□□□□□. 例□□, □数$f(\boldsymbol{x})$□□□□$p_{\boldsymbol{X}}(\boldsymbol{x})$□□□期□□□$\langle f\rangle_{p_{\boldsymbol{X}}}=\sum_{\boldsymbol{x}}f(\boldsymbol{x})p_{\boldsymbol{X}}(\boldsymbol{x})$□□□□□□.

□□□□□□数□□$\boldsymbol{X}_1=\{X_1,\cdots,X_m\}$□□□□□散□□□$\boldsymbol{x}_1\in\{1,\dots,N\}^m$, □□□数□□$\boldsymbol{X}_2=\{X_{m+1},\cdots,X_n\}$□□□□□散□□□$\boldsymbol{x}_2\in\{1,\dots,N\}^{n-m}$□□□. □□□□条□□□□□$p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1)$□□□□, □□□数□□$\boldsymbol{X}_1$□条□□□□□□□数□□$\boldsymbol{X}_2$□□□□□条□□□Shannon□□□□□□□

$$H(\boldsymbol{X}_2|\boldsymbol{X}_1)=-\sum_{\boldsymbol{x}_1,\boldsymbol{x}_2}p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2)\ln p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1), \tag{4.4}$$

□□□□定□□□. □□□, ln□前□□□□□分布$p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2)$□□□□□□□□□□□□. □□□□非□□□□. 期□□□□□□□□□□□

$$H(\boldsymbol{X}_2|\boldsymbol{X}_1) = \langle -\ln p_{\boldsymbol{X}_2|\boldsymbol{X}_1} \rangle_{p_{\boldsymbol{X}_1,\boldsymbol{X}_2}}, \tag{4.5}$$

□□□□□□.

□□分布□Chain rule $p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2) = p_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1)p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)$□□, 条□□□Shannon□□□□□□□

$$H(\boldsymbol{X}_2|\boldsymbol{X}_1) = H(\boldsymbol{X}_2,\boldsymbol{X}_1) - H(\boldsymbol{X}_1), \tag{4.6}$$

□□□□Shannon□□□□□□□□□□□□. □□□□□□□□数□□$\boldsymbol{X} = \{X_1,\cdots,X_n\}$□対□□

$$H(\boldsymbol{X}) = H(X_1) + \sum_{k=1}^{n-1} H(X_{k+1}|X_k,\ldots,X_1), \tag{4.7}$$

□□□□分□□□□□□□. □□Shannon□□□□□□□分□□□方□, 条□□□□□□□□□□□chain rule□□□.

4.1.2 微分エントロピー

□□□□□□$\boldsymbol{x} \in \mathsf{R}^n$□□□□□□□$P_{\boldsymbol{X}}(\boldsymbol{x})$□分布□□□□□, 期□□□□□□表□□Shannon□□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□. □□□数□□$\boldsymbol{X}$□□□□□分□□□□□□□

$$\mathcal{H}(\boldsymbol{X}) = -\int d\boldsymbol{x} P_{\boldsymbol{X}}(\boldsymbol{x}) \ln P_{\boldsymbol{X}}(\boldsymbol{x}) = \langle -\ln P_{\boldsymbol{X}} \rangle_{P_{\boldsymbol{X}}}, \tag{4.8}$$

□定□□□□□□□分□□□□□□□□□. □□□, □数$f(\boldsymbol{x})$□□□□$P_{\boldsymbol{X}}(\boldsymbol{x})$□□□期□□□$\langle f \rangle_{P_{\boldsymbol{X}}} = \int d\boldsymbol{x} f(\boldsymbol{x}) P_{\boldsymbol{X}}(\boldsymbol{x})$□□□□□□. □□□□□数□□$\boldsymbol{X}_1 = \{X_1,\cdots,X_m\}$□□□□□□□□□$\boldsymbol{x}_1 \in \mathsf{R}^m$, □□□数□□$\boldsymbol{X}_2 = \{X_{m+1},\cdots,X_n\}$□□□□□散□□□$\mathsf{R}^{n-m}$□□□. □□□□□□条□□□□□$P_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1)$□対□□□条□□□□分□□□□□□□

$$\begin{aligned} \mathcal{H}(\boldsymbol{X}_2|\boldsymbol{X}_1) &= -\int d\boldsymbol{x} P_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2) \ln P_{\boldsymbol{X}_2|\boldsymbol{X}_1}(\boldsymbol{x}_2|\boldsymbol{x}_1) \\ &= \langle -\ln P_{\boldsymbol{X}_2|\boldsymbol{X}_1} \rangle_{P_{\boldsymbol{X}_1,\boldsymbol{X}_2}}, \end{aligned} \tag{4.9}$$

□□□□

□□□□Shannon□□□□□□□□□□□□幾□□□□□□□□□□□. 例□□, Shannon□□□□□□□□□分布□$P_{\boldsymbol{X}}(\boldsymbol{x})$□1□□□□□□□, □分□□□□□□□□□□□非□□□□□. □方□Chain rule□□□□□□□□□□□□,

$$\mathcal{H}(\boldsymbol{X}) = \mathcal{H}(X_1) + \sum_{k=1}^{n-1} \mathcal{H}(X_{k+1}|X_k,\ldots,X_1), \tag{4.10}$$

□示□□.

4.1.3 Shannonエントロピーと微分エントロピーの具体例

□体例□□□□□□．□□, 2□ ($x \in \{1, 2\}$)□□□分布$p_X(x)$□□

$$p_X(1) = q, \tag{4.11}$$

$$p_X(2) = 1 - q, \tag{4.12}$$

□□□□□□□□□□□□ ($q > 0$)．□□□, Shannon□□□□□□□

$$H(X) = -q \ln q - (1-q)\ln(1-q), \tag{4.13}$$

□□□．□□Shannon□□□□□□□$q = 0, 1$□最□□0□, $q = 1/2$□□□最□□$\ln 2$□□□□□□□□□．

□□平□μ, 分散σ^2□□□□分布

$$P_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \tag{4.14}$$

□□□□□分□□□□□□□

$$\begin{aligned} \mathcal{H}(X) &= \frac{1}{2}\ln[2\pi\sigma^2] + \frac{\langle (x-\mu)^2 \rangle_{P_X}}{2\sigma^2} \\ &= \frac{1}{2}\ln[2\pi\sigma^2] + \frac{1}{2}, \end{aligned} \tag{4.15}$$

□□□□□□．□□□□□□分布□□分□□□□□□□分散σ^2□□□□数□□□, 平□μ□依存□□□．分散$\sigma^2 \to 0$□□□ (□□□□$P_X(x)$□□□□□数□□□□□) □□$\mathcal{H}(X) \to -\infty$□, $\sigma^2 \to \infty$□□□ (□□□□$P_X(x)$□□□分布□□□□□) □□$\mathcal{H}(X) \to \infty$□□□□□□□□□□, □分□□□□□□□□□□□非□□□□□□□□□□□□□□□．

4.2 Kullback-Leiblerダイバージェンス

4.2.1 Kullback-Leiblerダイバージェンスの定義

Shannon□□□□□□□□分□□□□□□□分布$p_{\boldsymbol{X}}(\boldsymbol{x})$ ($P_{\boldsymbol{X}}(\boldsymbol{x})$)□□□□□□□□□□□□．□□□□□□□分布□□□□□度□□□, Kullback-Leibler□□□□□□□□□□□□□□□□□□□□．

Kullback-Leibler□□□□□□□□□定□□□□□□．□□□散□□$\boldsymbol{x} \in \{1, \ldots, N\}^n$□□□□□□□分布$p_{\boldsymbol{X}}(\boldsymbol{x})$□$q_{\boldsymbol{X}}(\boldsymbol{x})$□対□□,

$$\begin{aligned} D_{\mathrm{KL}}(p_{\boldsymbol{X}} \| q_{\boldsymbol{X}}) &= \sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) \ln \frac{p_{\boldsymbol{X}}(\boldsymbol{x})}{q_{\boldsymbol{X}}(\boldsymbol{x})} \\ &= \langle \ln p_{\boldsymbol{X}} - \ln q_{\boldsymbol{X}} \rangle_{p_{\boldsymbol{X}}}, \end{aligned} \tag{4.16}$$

□□□□定□□□□．定□□□

$$D_{\mathrm{KL}}(p_{\boldsymbol{X}} \| q_{\boldsymbol{X}}) \neq D_{\mathrm{KL}}(q_{\boldsymbol{X}} \| p_{\boldsymbol{X}}), \tag{4.17}$$

□□□□□, □□Kullback-Leibler□□□□□□□□□数学□□□□□□□□□□□□□□□□□．□□□□□□分布□□□□□□□分布$P_{\boldsymbol{X}}(\boldsymbol{x})$□$Q_{\boldsymbol{X}}(\boldsymbol{x})$□対□□

$$\begin{aligned} D_{\mathrm{KL}}(P_{\boldsymbol{X}} \| Q_{\boldsymbol{X}}) &= \int d\boldsymbol{x} P_{\boldsymbol{X}}(\boldsymbol{x}) \ln \frac{P_{\boldsymbol{X}}(\boldsymbol{x})}{Q_{\boldsymbol{X}}(\boldsymbol{x})} \\ &= \langle \ln P_{\boldsymbol{X}} - \ln Q_{\boldsymbol{X}} \rangle_{P_{\boldsymbol{X}}}, \end{aligned} \tag{4.18}$$

□□□□定□□□□.

4.2.2 Kullback-Leiblerダイバージェンスの□□性

□□Kullback-Leibler□□□□□□□□□, □□$\boldsymbol{x}$□□散□□□□□□□□□□□□□□□□□, □□□□□非□□□□□.

$$D_{\mathrm{KL}}(p_{\boldsymbol{X}}||q_{\boldsymbol{X}}) \geq 0, \tag{4.19}$$

$$D_{\mathrm{KL}}(P_{\boldsymbol{X}}||Q_{\boldsymbol{X}}) \geq 0. \tag{4.20}$$

□□□□散□□□□□$p_{\boldsymbol{X}} = q_{\boldsymbol{X}}$□□□□□$D_{\mathrm{KL}}(p_{\boldsymbol{X}}||p_{\boldsymbol{X}}) = 0$□□□, □□□□□□□□□□□□ $P_{\boldsymbol{X}} = Q_{\boldsymbol{X}}$□□□□□$D_{\mathrm{KL}}(P_{\boldsymbol{X}}||Q_{\boldsymbol{X}}) = 0$□□□.

□□□□□示□□□□, □□□□□Jensen□□□□□□□□□□□. □□$\boldsymbol{x}$□□□□□数$g(\boldsymbol{x})$□□数$f(g)$□□□□. Jensen□□□□□□□数f□□□□□□数□□□□□□□

$$\langle f(g)\rangle_{p_{\boldsymbol{X}}} \leq f(\langle g\rangle_{p_{\boldsymbol{X}}}), \tag{4.21}$$

□□□□□□□□□. □□$\boldsymbol{x}$□□□□□□□□□□□Jensen□□□□

$$\langle f(g)\rangle_{P_{\boldsymbol{X}}} \leq f(\langle g\rangle_{P_{\boldsymbol{X}}}), \tag{4.22}$$

□□□□□.

Jensen□□□□□□□□□□□示□. □□f□□□□□□数□□□□□, $\langle g\rangle_{p_{\boldsymbol{X}}}$□□□□□, $f(g)$□□□常□□□□□□□□□□□存□□□. □□□□

$$f(g(\boldsymbol{x})) \leq a(g(\boldsymbol{x}) - \langle g\rangle_{p_X}) + f(\langle g\rangle_{P_{\boldsymbol{X}}}), \tag{4.23}$$

□□□□$g(\boldsymbol{x})$□□□□□□a□存□□□. □□□□□(4.23)□□□□対□□期□□$\langle\cdots\rangle_{p_{\boldsymbol{X}}}$□□□□□□□□□□□□□□□, □□□□

$$\begin{aligned}\langle f(g)\rangle_{p_{\boldsymbol{X}}} &\leq \langle a(g - \langle g\rangle_{p_{\boldsymbol{X}}}) + f(\langle g\rangle_{p_{\boldsymbol{X}}})\rangle_{p_{\boldsymbol{X}}} \\ &= f(\langle g\rangle_{p_{\boldsymbol{X}}}),\end{aligned} \tag{4.24}$$

□Jensen□□□□□□□□□□□□示□□. □□□□□□□条□□$f(g) = ag$□□□□□□, □□□□□□□数f□対□□非□□□□□□□条□□□□□$\boldsymbol{x}$□対□□$g(\boldsymbol{x}) = \langle g\rangle_{p_{\boldsymbol{X}}} = \mathrm{const.}$□□□.□

□□Jensen□□□□□□□□, Kullback-Leibler□□□□□□□□□非□□□示□. □□□□□数□□□$f(g) = \ln(g)$□□□□. □□□対□□, $g(\boldsymbol{x}) = q_{\boldsymbol{X}}(\boldsymbol{x})/p_{\boldsymbol{X}}(\boldsymbol{x})$□□□□□□□□□□□□□非□□□示□□.

$$\begin{aligned}-D_{\mathrm{KL}}(p_{\boldsymbol{X}}||q_{\boldsymbol{X}}) &= \left\langle \ln\left(\frac{q_{\boldsymbol{X}}}{p_{\boldsymbol{X}}}\right)\right\rangle_{p_{\boldsymbol{X}}} \\ &\leq \ln\left(\left\langle \frac{q_{\boldsymbol{X}}}{p_{\boldsymbol{X}}}\right\rangle_{p_{\boldsymbol{X}}}\right) \\ &= \ln(1) \\ &= 0.\end{aligned} \tag{4.25}$$

□□□□条□□$q_{\boldsymbol{X}}(\boldsymbol{x})/p_{\boldsymbol{X}}(\boldsymbol{x}) = \langle q_{\boldsymbol{X}}/p_{\boldsymbol{X}}\rangle_{p_{\boldsymbol{X}}} = 1$□□□. □□□$q_{\boldsymbol{X}} = p_{\boldsymbol{X}}$□□□□□□□□□□□. □□Kullback-Leibler□□□□□□□□□非□□□示□□□, □□□□□散□□□□□□□□□利□□□□□□□□, □□□□□□$D_{\mathrm{KL}}(P_{\boldsymbol{X}}||Q_{\boldsymbol{X}})$□非□□□□□□□条□□示□□.

4.3 Fisher情報□列

4.3.1 情報幾何

分布$p_{\boldsymbol{X}}$ ($P_{\boldsymbol{X}}$)□$q_{\boldsymbol{X}}$ ($Q_{\boldsymbol{X}}$)□□分□□□□ $q_{\boldsymbol{X}} = p_{\boldsymbol{X}} + dp_{\boldsymbol{X}}$ ($Q_{\boldsymbol{X}} = P_{\boldsymbol{X}} + dP_{\boldsymbol{X}}$) □□□□□. □□□$dp_{\boldsymbol{X}}$ ($dP_{\boldsymbol{X}}$)□□□□分布□□□□□□□. □□□□□□□散□□□分布□□Kullback-Leibler□□□□□□□□□□□□□□□□□□□□□□□□□□□□□.

$$
\begin{aligned}
&D_{\mathrm{KL}}(p_{\boldsymbol{X}}||p_{\boldsymbol{X}} + dp_{\boldsymbol{X}}) \\
&= D_{\mathrm{KL}}(q_{\boldsymbol{X}} - dp_{\boldsymbol{X}}||q_{\boldsymbol{X}}) \\
&= -\sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) \ln \frac{p_{\boldsymbol{X}}(\boldsymbol{x}) + dp_{\boldsymbol{X}}(\boldsymbol{x})}{p_{\boldsymbol{X}}(\boldsymbol{x})} \\
&= -\sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) \left(\ln 1 + \frac{dp_{\boldsymbol{X}}(\boldsymbol{x})}{p_{\boldsymbol{X}}(\boldsymbol{x})} - \frac{1}{2}\frac{(dp_{\boldsymbol{X}}(\boldsymbol{x}))^2}{(p_{\boldsymbol{X}}(\boldsymbol{x}))^2} \right) + \mathcal{O}(dp_{\boldsymbol{X}}^3) \\
&= \frac{1}{2}\sum_{\boldsymbol{x}} \frac{(dp_{\boldsymbol{X}}(\boldsymbol{x}))^2}{p_{\boldsymbol{X}}(\boldsymbol{x})} + \mathcal{O}(dp_{\boldsymbol{X}}^3) \\
&= \frac{1}{2}\sum_{\boldsymbol{x}} \frac{(dp_{\boldsymbol{X}}(\boldsymbol{x}))^2}{q_{\boldsymbol{X}}(\boldsymbol{x})} + \mathcal{O}(dp_{\boldsymbol{X}}^3).
\end{aligned}
\tag{4.26}
$$

□□□□□□□□□□□□, □□分布□□□□条□

$$
1 = \sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_{\boldsymbol{x}} (p_{\boldsymbol{X}}(\boldsymbol{x}) + dp_{\boldsymbol{X}}(\boldsymbol{x})), \tag{4.27}
$$

□□

$$
\sum_{\boldsymbol{x}} dp_{\boldsymbol{X}}(\boldsymbol{x}) = 0, \tag{4.28}
$$

□□□□□□□□□□. □□□□, □□□□□Kullback-Leibler□□□□□□□□□対称□□□□□分布□□□□対□□□□□□□,

$$
D_{\mathrm{KL}}(p_{\boldsymbol{X}}||p_{\boldsymbol{X}} + dp_{\boldsymbol{X}}) = D_{\mathrm{KL}}(p_{\boldsymbol{X}} + dp_{\boldsymbol{X}}||p_{\boldsymbol{X}}) + \mathcal{O}(dp_{\boldsymbol{X}}^3), \tag{4.29}
$$

$$
D_{\mathrm{KL}}(P_{\boldsymbol{X}}||P_{\boldsymbol{X}} + dP_{\boldsymbol{X}}) = D_{\mathrm{KL}}(P_{\boldsymbol{X}} + dP_{\boldsymbol{X}}||P_{\boldsymbol{X}}) + \mathcal{O}(dP_{\boldsymbol{X}}^3). \tag{4.30}
$$

□□□□□□□□分布□□□□対□□対称□□, Kullback-Leibler□□□□□□□□□非□□□□□□□, Kullback-Leibler□□□□□□□□□□□分幾何学□□□□□□□□□□. □□□□□□分幾何学□□□幾何学 [8]□□□□□□□.

□□□分布□□□□□□□□□□□□□ds^2□Kullback-Leibler□□□□□□□□□□□□□□□□□□□□□, □散□□□分布□□□□□

$$
\begin{aligned}
ds^2 &= \sum_{\boldsymbol{x}} \frac{(dp_{\boldsymbol{X}}(\boldsymbol{x}))^2}{p_{\boldsymbol{X}}(\boldsymbol{x})} \\
&= \langle (d \ln p_{\boldsymbol{X}})^2 \rangle_{p_{\boldsymbol{X}}} \\
&= 2D_{\mathrm{KL}}(p_{\boldsymbol{X}}||p_{\boldsymbol{X}} + dp_{\boldsymbol{X}}) + \mathcal{O}(dP_{\boldsymbol{X}}^3) \\
&= 2D_{\mathrm{KL}}(p_{\boldsymbol{X}} + dp_{\boldsymbol{X}}||p_{\boldsymbol{X}}) + \mathcal{O}(dP_{\boldsymbol{X}}^3),
\end{aligned}
\tag{4.31}
$$

□□□□□分布□□□□□

$$\begin{aligned}
ds^2 &= \int d\boldsymbol{x} \frac{(dP_{\boldsymbol{X}}(\boldsymbol{x}))^2}{P_{\boldsymbol{X}}(\boldsymbol{x})} \\
&= \langle (d\ln P_{\boldsymbol{X}})^2 \rangle_{P_{\boldsymbol{X}}} \\
&= 2D_{\mathrm{KL}}(P_{\boldsymbol{X}} || P_{\boldsymbol{X}} + dP_{\boldsymbol{X}}) + \mathcal{O}(dP_{\boldsymbol{X}}^3) \\
&= 2D_{\mathrm{KL}}(P_{\boldsymbol{X}} + dP_{\boldsymbol{X}} || P_{\boldsymbol{X}}) + \mathcal{O}(dP_{\boldsymbol{X}}^3),
\end{aligned} \tag{4.32}$$

□定□□□□.

4.3.2 Fisher情報□列

□□□□□□□□□□□$\boldsymbol{\theta} = \{\theta_1, \ldots, \theta_{n_\Theta}\}$□□□□分布□□定□□□□□, 分布□□□□□□□

$$d\ln p_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_i [\partial_{\theta_i} \ln p_{\boldsymbol{X}}(\boldsymbol{x})] d\theta_i + O(d\boldsymbol{\theta}^2), \tag{4.33}$$

$$d\ln P_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_i [\partial_{\theta_i} \ln P_{\boldsymbol{X}}(\boldsymbol{x})] d\theta_i + O(d\boldsymbol{\theta}^2), \tag{4.34}$$

□□□□□□□□□, $O(d\boldsymbol{\theta}^3)$□□□□□□, □□□□□□□□□□□□□□□表□□□□□.

$$ds^2 = \sum_{i,j} g_{ij} d\theta_i d\theta_j. \tag{4.35}$$

□□□g_{ij}□□散□□□□□□□

$$g_{ij} = \langle [\partial_{\theta_i} \ln p_{\boldsymbol{X}}][\partial_{\theta_j} \ln p_{\boldsymbol{X}}] \rangle_{p_{\boldsymbol{X}}}, \tag{4.36}$$

□□□□□□□□□

$$g_{ij} = \langle [\partial_{\theta_i} \ln P_{\boldsymbol{X}}][\partial_{\theta_j} \ln P_{\boldsymbol{X}}] \rangle_{P_{\boldsymbol{X}}}, \tag{4.37}$$

□□□□□□. □□g_{ij}□Fisher□□行列□□□. ds^2□非□□□□, Fisher□□行列□□□定□行列□□□, □□幾何学□□□□□□□□□割□果□□□□□.

4.3.3 Cramér-Raoの不□式

□, □□□□□□$\boldsymbol{\theta} = \{\theta_1\}$□□□□□□度$\theta_1 = \theta$□□□□□□□□□□□. □□□□,

$$ds^2 = g_{11} d\theta^2, \tag{4.38}$$

□□□□Fisher□□行列g_{11}□, □□□θ□□□□Fisher□□□□□□,

$$g_{11} = \left(\frac{ds}{d\theta}\right)^2, \tag{4.39}$$

□□□□□□□□. θ□□□□Fisher□□□□$\boldsymbol{x}$□□散□□□□□

$$\left(\frac{ds}{d\theta}\right)^2 = \langle [\partial_\theta \ln p_{\boldsymbol{X}}]^2 \rangle_{p_{\boldsymbol{X}}}, \tag{4.40}$$

$\boldsymbol{x}$□□□□□□□□

$$\left(\frac{ds}{d\theta}\right)^2 = \langle[\partial_\theta \ln P_{\boldsymbol{X}}]^2\rangle_{P_{\boldsymbol{X}}}, \tag{4.41}$$

□□□□□□.

□□Fisher□□□□□体□□□□□□□□□□Cramér-Rao□□□□□□□□□□□□□有□□□□.□□□□□□$\boldsymbol{x}$□□数$R(\boldsymbol{x})$□分散

$$\mathrm{Var}_{p_{\boldsymbol{X}}}[R] = \langle[R - \langle R\rangle_{p_{\boldsymbol{X}}}]^2\rangle_{p_{\boldsymbol{X}}}, \tag{4.42}$$

□□□□□□□□□□□□□□.$\boldsymbol{x}$□□散□□□□□,□□□□数$f(\boldsymbol{x})$, $g(\boldsymbol{x})$□対□□Cauchy-Schwartz□□□□

$$\langle f^2\rangle_{p_{\boldsymbol{X}}}\langle g^2\rangle_{p_{\boldsymbol{X}}} \geq (\langle fg\rangle_{p_{\boldsymbol{X}}})^2, \tag{4.43}$$

□$f(\boldsymbol{x}) = \partial_\theta \ln p_{\boldsymbol{X}}(\boldsymbol{x})$, $g(\boldsymbol{x}) = R(\boldsymbol{x}) - \langle R\rangle_{p_{\boldsymbol{X}}}$□□□□□□□□,

$$\begin{aligned}
\left(\frac{ds}{d\theta}\right)^2 \mathrm{Var}_{p_{\boldsymbol{X}}}[R] &\geq (\langle[\partial_\theta \ln p_{\boldsymbol{X}}(\boldsymbol{x})][R - \langle R\rangle_{p_{\boldsymbol{X}}}]\rangle_{p_{\boldsymbol{X}}})^2 \\
&= \left(\sum_{\boldsymbol{x}} \frac{\partial p_{\boldsymbol{X}}(\boldsymbol{x})}{\partial\theta}[R(\boldsymbol{x}) - \langle R\rangle_{p_{\boldsymbol{X}}}]\right)^2 \\
&= \left(\frac{d}{d\theta}\langle R\rangle_{p_{\boldsymbol{X}}}\right)^2,
\end{aligned} \tag{4.44}$$

□□□□□.□□□$d/d\theta[\sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x})] = d/d\theta[1] = 0$□□□□.□□□□条□□Cauchy-Schwartz□□□□□□□□□条□□□,何□□□□例係数$\alpha(\theta)$□□□□

$$\partial_\theta \ln p_{\boldsymbol{X}}(\boldsymbol{x}) = \alpha(\theta)[R(\boldsymbol{x}) - \langle R\rangle_{p_{\boldsymbol{X}}}] \tag{4.45}$$

□□□□□□□□□□□□.□□□$\boldsymbol{x}$□□□□□□□□

$$\left(\frac{ds}{d\theta}\right)^2 \mathrm{Var}_{P_{\boldsymbol{X}}}[R] \geq \left(\frac{d}{d\theta}\langle R\rangle_{P_{\boldsymbol{X}}}\right)^2, \tag{4.46}$$

□□□□□.□□□□□□Cramér-Rao□□□□□□□□□□□.

□□□Cramér-Rao□□□□□期□□$\langle\Theta\rangle_{P_{\boldsymbol{X}}} = \theta$□□□□□□$R(\boldsymbol{x}) = \Theta(\boldsymbol{x})$□対□□□□□察□□□.□□□□□$\Theta(\boldsymbol{x})$□$\theta$□□□□定□□□□□□□□□.□□□□,Cramér-Rao□□□□(4.47)□

$$\mathrm{Var}_{P_{\boldsymbol{X}}}[\Theta] \geq \frac{1}{\left(\frac{ds}{d\theta}\right)^2}, \tag{4.47}$$

□□□□□□.□□□θ□□□□Fisher□□□□□数□,θ□□□□定□$\Theta(\boldsymbol{x})$□分散□□□□□□□□□□□□□□.□□□,□□□□□θ□□□□定□□期□□□□□定□□□□□□定□□度□Fisher□□□□□数□□定□□,□□□□Fisher□□□□□定□□□□□□□□□Cramér-Rao□□□□□□□□□□□□□□□□□□□□□.

□□,Cramér-Rao□□□□(4.47)□□□□$\mathrm{Var}_{P_{\boldsymbol{X}}}[R]$□割□□,□□□対□□□□平方□□□□□□□

$$\frac{ds}{d\theta} \geq \frac{|\frac{d}{d\theta}\langle R\rangle_{P_{\boldsymbol{X}}}|}{\sqrt{\mathrm{Var}_{P_{\boldsymbol{X}}}[R]}} := v_R, \tag{4.48}$$

□□□□□□□□□□□□□□. □□□□□□□□θ□□□□□□□期□□□□□□□□$|d\langle R\rangle_{P_{\boldsymbol{X}}}/d\theta|$□□□□□$\sqrt{\mathrm{Var}_{P_{\boldsymbol{X}}}[R]}$□□□□□□□□□□□□□□. □□□□□□□□期□□$\langle R\rangle_{P_{\boldsymbol{X}}}$□□□□□□□□□□□□□□□初□□, □定□果□□有□□期□□□□□□□□□□□□□□□,□□□□□□□期□□$\langle R\rangle_{P_{\boldsymbol{X}}}$□□□□□□□□□□□□□□□□□□. □□□□□□□期□□$\langle R\rangle_{P_{\boldsymbol{X}}}$□□□□□□□$v_R$□□□□. □(4.48)□□□$v_R$□$R$□□□□□□□□□□□□□□□Fisher□□□□□□平方□$ds/d\theta$□□□□□□□□□□□□□□□□□□□□, $ds/d\theta$□R□□□□□□有□□□□□□□□□□□□□□. □□□□□□□幾何学□□□□ds^2□□□□□□□□□□□□□□□□□□□□□□□□□□□. □□□Cramér-Rao□□□□□, □□幾何学□□礎□□□□□□□□□□□.

4.4 情報□□における不□式

Kullback-Leibler□□□□□□□□□有□□□□例□□□, □□.

4.4.1 Shannonエントロピーの上□

□散□□$x\in\{1,\ldots,N\}$□□□□□□□数X□分布$p_X(x)$□□□□Shannon□□□□□$H(X)=\langle -\ln p_X\rangle_{p_X}$□□□□□□□□□□, Kullback-Leibler□□□□□□□□□非□□□□□□□□□□□□□. □□分布$p_X^{\mathrm{uni}}(x)=1/N$□分布$p_X(x)$□□Kullback-Leibler□□□□□□□□□□□□□□,

$$
\begin{aligned}
D_{\mathrm{KL}}(p_X||p_X^{\mathrm{uni}}) &= \langle \ln p_X - \ln p_X^{\mathrm{uni}}\rangle_{p_X} \\
&= -H(X) + \ln N,
\end{aligned}
\tag{4.49}
$$

□□, Kullback-Leibler□□□□□□□□□非□□$D_{\mathrm{KL}}(p_X||p_X^{\mathrm{uni}})\geq 0$□□

$$
\ln N \geq H(X),
\tag{4.50}
$$

□Shannon□□□□□□□□□□□□□□□□. □□□□□□□□分布$p_X(x)$□□□分布□□□□□.

4.4.2 条件付きShannonエントロピーに□する上□

□□□□散□□$\boldsymbol{x}\in\{1,\ldots,N\}^n$□□□□□□□. □□□数□□$\boldsymbol{X}_1=\{X_1,\cdots,X_m\}$□□□□□散□□□$\boldsymbol{x}_1\in\{1,\ldots,N\}^m$, □□□数□□$\boldsymbol{X}_2=\{X_{m+1},\cdots,X_n\}$□□□□□散□□□$\boldsymbol{x}_2\in\{1,\ldots,N\}^{n-m}$□□□. □□□□分布$p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2)$□, □□□□分布$p_{\boldsymbol{X}_1}(\boldsymbol{x}_1)=\sum_{\boldsymbol{x}_2}p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2)$, $p_{\boldsymbol{X}_2}(\boldsymbol{x}_2)=\sum_{\boldsymbol{x}_1}p_{\boldsymbol{X}_1,\boldsymbol{X}_2}(\boldsymbol{x}_1,\boldsymbol{x}_2)$□□□□□Kullback-Leibler□□□□□□□□□□□□□□□.

$$
\begin{aligned}
D_{\mathrm{KL}}(p_{\boldsymbol{X}_1,\boldsymbol{X}_2}||p_{\boldsymbol{X}_1}p_{\boldsymbol{X}_2}) &= \langle \ln p_{\boldsymbol{X}_1,\boldsymbol{X}_2} - \ln p_{\boldsymbol{X}_1} - \ln p_{\boldsymbol{X}_2}\rangle_{p_{\boldsymbol{X}_1,\boldsymbol{X}_2}} \\
&= H(\boldsymbol{X}_1) + H(\boldsymbol{X}_2) - H(\boldsymbol{X}_1,\boldsymbol{X}_2) \\
&= H(\boldsymbol{X}_1) - H(\boldsymbol{X}_1|\boldsymbol{X}_2) \\
&= H(\boldsymbol{X}_2) - H(\boldsymbol{X}_2|\boldsymbol{X}_1).
\end{aligned}
\tag{4.51}
$$

Kullback-Leibler□□□□□□□□□非□□$D_{\mathrm{KL}}(p_{\boldsymbol{X}_1,\boldsymbol{X}_2}||p_{\boldsymbol{X}_1}p_{\boldsymbol{X}_2})\geq 0$□□,

$$
H(\boldsymbol{X}_1) \geq H(\boldsymbol{X}_1|\boldsymbol{X}_2),
\tag{4.52}
$$

□□□□

$$H(\boldsymbol{X}_2) \geq H(\boldsymbol{X}_2|\boldsymbol{X}_1), \tag{4.53}$$

□□□□□. □□□条□□□□□□□Shannon□□□□□□□□□□□□□□□□□□. □□□□□, $p_{\boldsymbol{X}_1,\boldsymbol{X}_2} = p_{\boldsymbol{X}_1}p_{\boldsymbol{X}_2}$□□, □□□□□□数□□$\boldsymbol{X}_1$, $\boldsymbol{X}_2$□□□□□□□□.

□□□□□□数□□$\boldsymbol{X}_1' = \{X_1, \cdots, X_m\}$□□□□□散□□□$\boldsymbol{x}_1' \in \{1, \ldots, N\}^m$, □□□数□□$\boldsymbol{X}_2' = \{X_{m+1}, \cdots, X_l\}$□□□□□散□□□$\boldsymbol{x}_2' \in \{1, \ldots, N\}^{l-m}$, □□□数□□$\boldsymbol{X}_3' = \{X_{l+1}, \cdots, X_n\}$□□□□□散□□□$\boldsymbol{x}_3' \in \{1, \ldots, N\}^{n-l}$□□□, □□□□分布$p_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}(\boldsymbol{x}_1', \boldsymbol{x}_2', \boldsymbol{x}_3')$□, 分布$p_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}(\boldsymbol{x}_1'|\boldsymbol{x}_3')p_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}(\boldsymbol{x}_2'|\boldsymbol{x}_3')p_{\boldsymbol{X}_3'}(\boldsymbol{x}_3')$□□□□Kullback-Leibler□□□□□□□□□□□□□□□.

$$\begin{aligned}
&D_{\mathrm{KL}}(p_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}||p_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_3'}) \\
&= \langle \ln p_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'} - \ln p_{\boldsymbol{X}_1'|\boldsymbol{X}_3'} - \ln p_{\boldsymbol{X}_2'|\boldsymbol{X}_3'} - \ln p_{\boldsymbol{X}_3'} \rangle_{p_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}} \\
&= H(\boldsymbol{X}_3') + H(\boldsymbol{X}_1'|\boldsymbol{X}_3') + H(\boldsymbol{X}_2'|\boldsymbol{X}_3') - H(\boldsymbol{X}_1', \boldsymbol{X}_2', \boldsymbol{X}_3') \\
&= H(\boldsymbol{X}_1', \boldsymbol{X}_3') + H(\boldsymbol{X}_2', \boldsymbol{X}_3') - H(\boldsymbol{X}_3') - H(\boldsymbol{X}_1', \boldsymbol{X}_2', \boldsymbol{X}_3') \\
&= H(\boldsymbol{X}_1'|\boldsymbol{X}_3') - H(\boldsymbol{X}_1'|\boldsymbol{X}_2', \boldsymbol{X}_3') \\
&= H(\boldsymbol{X}_2'|\boldsymbol{X}_3') - H(\boldsymbol{X}_2'|\boldsymbol{X}_1', \boldsymbol{X}_3').
\end{aligned} \tag{4.54}$$

Kullback-Leibler□□□□□□□□□非□□$D_{\mathrm{KL}}(p_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}||p_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_3'}) \geq 0$□□,

$$H(\boldsymbol{X}_1'|\boldsymbol{X}_3') \geq H(\boldsymbol{X}_1'|\boldsymbol{X}_2', \boldsymbol{X}_3'), \tag{4.55}$$

□□□□

$$H(\boldsymbol{X}_2'|\boldsymbol{X}_3') \geq H(\boldsymbol{X}_2'|\boldsymbol{X}_1', \boldsymbol{X}_3'), \tag{4.56}$$

□□□□□. □□□条□□□□□□□条□□□□Shannon□□□□□□□□□. □□□□□, $p_{\boldsymbol{X}_1',\boldsymbol{X}_2'|\boldsymbol{X}_3'} = p_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}$□□, □□□□□□数□□$\boldsymbol{X}_1'$, $\boldsymbol{X}_2'$□□□□数□□$\boldsymbol{X}_3'$□□□□□□□□□□□□□□□□□.

□□□□$\boldsymbol{x} \in \mathsf{R}^n$□対□□分布$P_{\boldsymbol{X}}(\boldsymbol{x})$□□□□, □□□□□□□□□□□□□□□□□□□□□□□. Kullback-Leibler□□□□□□□□$D_{\mathrm{KL}}(P_{\boldsymbol{X}_1,\boldsymbol{X}_2}||P_{\boldsymbol{X}_1}P_{\boldsymbol{X}_2})$□非□□□□, □分□□□□□□□対□□

$$\mathcal{H}(\boldsymbol{X}_1) \geq \mathcal{H}(\boldsymbol{X}_1|\boldsymbol{X}_2), \tag{4.57}$$

□, Kullback-Leibler□□□□□□□□$D_{\mathrm{KL}}(P_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}||P_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}P_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}P_{\boldsymbol{X}_3'})$□非□□□□, 条□□□□分□□□□□□□対□□

$$\mathcal{H}(\boldsymbol{X}_1'|\boldsymbol{X}_3') \geq \mathcal{H}(\boldsymbol{X}_1'|\boldsymbol{X}_2', \boldsymbol{X}_3'), \tag{4.58}$$

□□□□□. □□□□条□□□□□□$\boldsymbol{X}_1$, $\boldsymbol{X}_2$□□□□□, $\boldsymbol{X}_3'$□□□□□$\boldsymbol{X}_1'$, $\boldsymbol{X}_2'$□条□□□□□□□□□.

4.4.3 □互情報□

条□□□□□□Shannon□□□□□□□□□□□分□□□□□□□□□分□, □□□□□□数□□有□□□□□□□□□□□, □□□□□□□□前□□□□□□. □□□数□

□$\boldsymbol{X}_1$□$\boldsymbol{X}_2$□□□□□□□□$I(\boldsymbol{X}_1;\boldsymbol{X}_2)$□□散□□□□□□□

$$I(\boldsymbol{X}_1;\boldsymbol{X}_2)=D_{\mathrm{KL}}(p_{\boldsymbol{X}_1,\boldsymbol{X}_2}||p_{\boldsymbol{X}_1}p_{\boldsymbol{X}_2}), \tag{4.59}$$

□, □□□□□□□□□

$$I(\boldsymbol{X}_1;\boldsymbol{X}_2)=D_{\mathrm{KL}}(P_{\boldsymbol{X}_1,\boldsymbol{X}_2}||P_{\boldsymbol{X}_1}P_{\boldsymbol{X}_2}), \tag{4.60}$$

□定□□□□. □□□条□□□□□□条□□□Shannon□□□□□□□□□□□分□□□□□□□□□□分□条□□□□□□□□□□□□□前□□□□□□. □□□数□□$\boldsymbol{X}_3'$□□□□□□□□□数□□$\boldsymbol{X}_1'$, $\boldsymbol{X}_2'$□□□□条□□□□□□□□$I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')$□□散□□□□□□□

$$I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')=D_{\mathrm{KL}}(p_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}||p_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}p_{\boldsymbol{X}_3'}), \tag{4.61}$$

□, □□□□□□□□□

$$I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')=D_{\mathrm{KL}}(P_{\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3'}||P_{\boldsymbol{X}_1'|\boldsymbol{X}_3'}P_{\boldsymbol{X}_2'|\boldsymbol{X}_3'}P_{\boldsymbol{X}_3'}), \tag{4.62}$$

□定□□□□. □□□□$\boldsymbol{X}_1$, $\boldsymbol{X}_2$□□□□□, $\boldsymbol{X}_3'$□□□□□$\boldsymbol{X}_1'$, $\boldsymbol{X}_2'$□条□□□□□□□0□□□非□□□

$$I(\boldsymbol{X}_1;\boldsymbol{X}_2)\geq 0, \tag{4.63}$$

$$I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')\geq 0, \tag{4.64}$$

□□□□□, □□□数□□□□□□□□□□□□□□□□□□□□□.

□□, □散□□□□□□□

$$I(\boldsymbol{X}_1;\boldsymbol{X}_2)=H(\boldsymbol{X}_1)+H(\boldsymbol{X}_2)-H(\boldsymbol{X}_1,\boldsymbol{X}_2), \tag{4.65}$$

□, □□□□□□□□□

$$I(\boldsymbol{X}_1;\boldsymbol{X}_2)=\mathcal{H}(\boldsymbol{X}_1)+\mathcal{H}(\boldsymbol{X}_2)-\mathcal{H}(\boldsymbol{X}_1,\boldsymbol{X}_2), \tag{4.66}$$

□□□□□□□, □□□□□$I(\boldsymbol{X}_1;\boldsymbol{X}_2)$□Shannon□□□□□□□□□□□分□□□□□□□□□□□□□□数$\boldsymbol{X}_1$, $\boldsymbol{X}_2$□□□□□分□□□□□□□□□□□. □□□□□□□对称□

$$\begin{aligned} I(\boldsymbol{X}_1;\boldsymbol{X}_2)&=I(\boldsymbol{X}_2;\boldsymbol{X}_1),\\ I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')&=I(\boldsymbol{X}_2';\boldsymbol{X}_1'|\boldsymbol{X}_3'), \end{aligned} \tag{4.67}$$

□□□□□□□□.

□□条□□□□□□□□□□□□□□□□□□□□□□□□Chain rule□□□□□.

$$I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')=I(\boldsymbol{X}_1';\{\boldsymbol{X}_2',\boldsymbol{X}_3'\})-I(\boldsymbol{X}_1';\boldsymbol{X}_3') \tag{4.68}$$

$$=I(\{\boldsymbol{X}_1',\boldsymbol{X}_3'\};\boldsymbol{X}_2')-I(\boldsymbol{X}_3';\boldsymbol{X}_2'). \tag{4.69}$$

□□□□□□□(4.68)□, 例□□□散□□□□□□, Shannon□□□□□□□Chain rule□□□□

$$\begin{aligned} &I(\boldsymbol{X}_1';\boldsymbol{X}_2'|\boldsymbol{X}_3')\\ &=H(\boldsymbol{X}_1',\boldsymbol{X}_3')+H(\boldsymbol{X}_2',\boldsymbol{X}_3')-H(\boldsymbol{X}_3')-H(\boldsymbol{X}_1',\boldsymbol{X}_2',\boldsymbol{X}_3')+H(\boldsymbol{X}_1')-H(\boldsymbol{X}_1')\\ &=[H(\boldsymbol{X}_2',\boldsymbol{X}_3')-H(\boldsymbol{X}_2',\boldsymbol{X}_3'|\boldsymbol{X}_1')]-[H(\boldsymbol{X}_1')-H(\boldsymbol{X}_1'|\boldsymbol{X}_3')]\\ &=I(\boldsymbol{X}_1';\{\boldsymbol{X}_2',\boldsymbol{X}_3'\})-I(\boldsymbol{X}_1';\boldsymbol{X}_3'), \end{aligned} \tag{4.70}$$

□□□□□□□. □□对称□□□(4.67)□□, □□□□□(4.69)□□□□□□□□□□□□□□□. □□□□□□□□□□□, Shannon□□□□□□□□分□□□□□□□□□□□□□□□□□□□□□□□.

4.4.4 データ処□不□式

□□□数□□$\boldsymbol{X}'_1$,$\boldsymbol{X}'_2$,$\boldsymbol{X}'_3$□$\boldsymbol{X}'_1 \to \boldsymbol{X}'_2 \to \boldsymbol{X}'_3$□□□Markov□□□□□□□□□□□□. □□□□$\boldsymbol{X}'_1$□$\boldsymbol{X}'_3$□$\boldsymbol{X}'_2$□□□条□□□□□□□□□□□□□□□. □□□□□□□□□□□□□□

$$I(\boldsymbol{X}'_1;\boldsymbol{X}'_2) \geq I(\boldsymbol{X}'_1;\boldsymbol{X}'_3), \tag{4.71}$$

□□□□□.

□□□□□□□□□□□, Markov□□□□□条□□□□□□

$$I(\boldsymbol{X}'_1;\boldsymbol{X}'_3|\boldsymbol{X}'_2) = 0, \tag{4.72}$$

□□, □□□□□条□□□□□□□□□非□□□Chain rule□□□□□□□□□示□□□.

$$\begin{aligned}0 &\leq I(\boldsymbol{X}'_1;\boldsymbol{X}'_2|\boldsymbol{X}'_3)\\ &= I(\boldsymbol{X}'_1;\{\boldsymbol{X}'_2,\boldsymbol{X}'_3\}) - I(\boldsymbol{X}'_1;\boldsymbol{X}'_3)\\ &= I(\boldsymbol{X}'_1;\boldsymbol{X}'_2) + I(\boldsymbol{X}'_1;\boldsymbol{X}'_3|\boldsymbol{X}'_2) - I(\boldsymbol{X}'_1;\boldsymbol{X}'_3)\\ &= I(\boldsymbol{X}'_1;\boldsymbol{X}'_2) - I(\boldsymbol{X}'_1;\boldsymbol{X}'_3).\end{aligned} \tag{4.73}$$

□□□□□□□□□□□例□□□□□□□□□□定□□□□察□□□. $\boldsymbol{X}'_1$□□□□□対□, $\boldsymbol{X}'_2$□対□□対□□何□□□□定□□□, $\boldsymbol{X}'_3$□□定□□□□何□□□□□□□□行□□□□□□□□□果□□□. □□□, □□□□□□□□□□$\boldsymbol{x}'_3$□□□$\boldsymbol{x}'_2$□□□□数$\boldsymbol{x}'_3 = f(\boldsymbol{x}'_2)$□□□□□□□□□□□□□□□□□. □□□□$\boldsymbol{X}'_1 \to \boldsymbol{X}'_2 \to \boldsymbol{X}'_3$□□□Markov□□□□□□□, □□□□□□□□□□□□□. □□□□□□□□□□□□□□□□□□□□, □□□□対□□□定□□□□□□□□□□$I(\boldsymbol{X}'_1;\boldsymbol{X}'_3)$□□□□□□果□□□□□対□□□□□□□$I(\boldsymbol{X}'_1;\boldsymbol{X}'_2)$□□□常□□□□□□□□□□□□□□□□□□□. □□□□□□, □□□□□$I(\boldsymbol{X}'_1;\boldsymbol{X}'_2)$□□□□"□□"□定□□□$\boldsymbol{X}'_2$□□□□□□□, □□□□□□□□□□□□□□□, □□□□□□果$\boldsymbol{X}'_3$□□□□□□対□$\boldsymbol{X}'_1$□□□$I(\boldsymbol{X}'_1;\boldsymbol{X}'_3)$□□□□□□□□□.□□□□, □□□□□□□□□□□□□□□□□□□□表□□□□□□□□□□□□□□.

□□, □□□□□f□□□□□□□□, □□

$$I(\boldsymbol{X}'_1;\boldsymbol{X}'_2) = I(\boldsymbol{X}'_1;\boldsymbol{X}'_3), \tag{4.74}$$

□□□□□□□□□□. □□□□□□条□□$I(\boldsymbol{X}'_1;\boldsymbol{X}'_2|\boldsymbol{X}'_3) = 0$, □□□□$\boldsymbol{X}'_3$□条□□□□□$\boldsymbol{X}'_1$, $\boldsymbol{X}'_2$□□条□□□□□□□□□□□□. □□□□□

$$p_{\boldsymbol{X}'_2|\boldsymbol{X}'_1,\boldsymbol{X}'_3} = p_{\boldsymbol{X}'_2|\boldsymbol{X}'_3}, \tag{4.75}$$

□□□□□□, □□□□対□$\boldsymbol{X}'_1$□□□□□□□果$\boldsymbol{X}'_3$□□□定□□□$\boldsymbol{X}'_2$□□□□□□□□, □□□□□□果$\boldsymbol{X}'_3$□□□□□□□□□定□□□$\boldsymbol{X}'_2$□□□□□□□□□条□□□□□□□□□□□□□□□□□□□□. □□□□□□□□□□□□□□$f(\boldsymbol{x}'_2)$□□□□数$\boldsymbol{X}'_3$□,□□□□□対□$\boldsymbol{X}'_1$□□□□□分□□□□□□□□□□□□□□□.

4.5 エントロピー□成とKullback-Leiblerダイバージェンス

4.5.1 □散状態でのエントロピー□成□

Kullback-Leibler□□□□□□□□非□□□, □□□□□力学□□□□□□□□□□□□□□非□□, □□□□□力学□□□則□□□□□□□□□□□□□□□□.

□□□散□□□master方□□□□□□□□□□□□. □刻t□□□x'□□□, □ν□□□□□刻$t+dt$□□□x□□□□□□□□□□□□分布$p(x;t+dt,x';t,\nu)$□□(3.27), (3.28)□□□□

$$p(x;t+dt,x';t,\nu) = \left(\delta_{\nu 1}\delta_{xx'} + W^{(\nu)}(x|x';t)dt\right) p_X(x';t) \tag{4.76}$$

□□□□□□□□□□□□□□□□. □□□□分布□

$$p_{X,X',N}(x,x',\nu) = p(x;t+dt,x';t,\nu) \tag{4.77}$$

□□□□□□□□□. □□□□□, 新□□分布□□□

$$p^{\dagger}{}_{X,X',N}(x,x',\nu) = p(x';t+dt,x;t,\nu) \tag{4.78}$$

□□□□□. □□□□, □□□分布$p_{X,X',N}$□$p^{\dagger}{}_{X,X',N}$□□□Kullback-Leibler□□□□□□□□□□□□□□,

$$\begin{aligned}
&D_{\mathrm{KL}}(p_{X,X',N}||p^{\dagger}{}_{X,X',N}) \\
&= \sum_{x,x',\nu} p_{X,X',N}(x,x',\nu) \ln \frac{p_{X,X',N}(x,x',\nu)}{p^{\dagger}{}_{X,X',N}(x,x',\nu)} \\
&= \sum_{x,x',\nu|x\neq x'} W^{(\nu)}(x|x';t)p_X(x';t)dt \ln \frac{W^{(\nu)}(x|x';t)p_X(x';t)}{W^{(\nu)}(x'|x;t)p_X(x;t)} \\
&= \sum_{x,x',\nu|x>x'} dt[W^{(\nu)}(x|x';t)p_X(x';t) - W^{(\nu)}(x'|x;t)p_X(x;t)] \ln \frac{W^{(\nu)}(x|x';t)p_X(x';t)}{W^{(\nu)}(x'|x;t)p_X(x;t)} \\
&= dt \sum_{\rho\in\mathcal{E}} (J_\rho^+ - J_\rho^-) \ln \frac{J_\rho^+}{J_\rho^-} \\
&= \sigma(t)dt
\end{aligned} \tag{4.79}$$

□□□. □□□$x=x'$□$\ln(p_{X,X',N}(x,x',\nu)/p^{\dagger}{}_{X,X',N}(x,x',\nu)) = \ln 1 = 0$□□□□□□□□□□□. □刻$t$□□$t'$□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□

$$\Sigma(t';t) = \int_t^{t'} ds\sigma(s) \tag{4.80}$$

□□□□□□□, Kullback-Leibler□□□□□□□□$D_{\mathrm{KL}}(p_{X,X',N}||p^{\dagger}{}_{X,X',N})$□□□□□□□□□

$$D_{\mathrm{KL}}(p_{X,X',N}||p^{\dagger}{}_{X,X',N}) = \Sigma(t+dt;t), \tag{4.81}$$

□□□□□□□□□□□□□□□□.

□□Kullback-Leibler□□□□□□□□□非□□$D_{\mathrm{KL}}(p_{X,X',N}||p^{\dagger}{}_{X,X',N}) \geq 0$□□

$$D_{\mathrm{KL}}(p_{X,X',N}||p^{\dagger}{}_{X,X',N}) = \sigma(t)dt \geq 0, \tag{4.82}$$

□□力学□□□則$\sigma(t) \geq 0$□示□，□□□□条□□$p_{X,X',N} = p^{\dagger}{}_{X,X',N}$□□□□□□□□□．□□□□条□$p_{X,X',N} = p^{\dagger}{}_{X,X',N}$□，□□刻$t$□□□$x'$□□□，□$\nu$□□□□□刻$t+dt$□□□$x$□□□□□□□，□□刻$t$□□□$x$□□□，□$\nu$□□□□□刻$t+dt$□□□$x'$□□□□□□□□□□□□□□□□□□□□．□□□，□□□□□□□□□□□表□□□□□□□□□□□□□．□□，□□□□□□□□□□□□□□条□□□□□□□□条□□□□□□□，平衡□□□□□□□□□□□□□□□□□□□□□□□□．

4.5.2 □□状態でのエントロピー□成□

□□□□□□□overdamped Langevin方□□

$$\dot{x}(t) = -\mu\partial_x U_X(x;t) + \sqrt{2\mu\beta^{-1}} \cdot \xi(t) \tag{4.83}$$
$$\langle \xi(t) \rangle = 0 \tag{4.84}$$
$$\langle \xi(t)\xi(t') \rangle = \delta(t-t') \tag{4.85}$$

□□□□□□□□□□□Fokker-Planck方□□□□□□□□□□□．

$$\partial_t P_X(x;t) = -\partial_x(\nu_X(x;t)P_X(x;t)) \tag{4.86}$$
$$\nu_X(x;t) = -\mu\partial_x[U_X(x;t) + \beta^{-1}\ln P_X(x;t)]. \tag{4.87}$$

Onsager-Machlup□数□□□□移□□□表□□□，□刻t□□□x'□□□□刻$t+dt$□□□x□□□□□□□分布□

$$P(x;t+dt,x';t) = \frac{1}{\sqrt{4\pi\beta^{-1}dt}} \exp\left[-\frac{\left[\frac{x-x'}{dt} + \mu\partial_x U(x';t)\right]^2}{4\mu\beta^{-1}} dt \right] P(x';t), \tag{4.88}$$

□□□□□□．□散□□□master方□□□□□□□□□□□□分布□

$$P_{X,X'}(x,x') = P(x;t+dt,x';t), \tag{4.89}$$

□□□，□刻t□□□x□□刻$t+dt$□□□x'□□□□□□□分布□

$$P^{\dagger}{}_{X,X'}(x,x') = P(x';t+dt,x;t) \tag{4.90}$$

□□□□，

$$D_{\mathrm{KL}}(P_{X,X'}||P^{\dagger}{}_{X,X'}) = \sigma(t)dt, \tag{4.91}$$

□□□□□□□□□□□□□□．

□□対数□□$\ln P_{X,X'}(x,x') - \ln P^{\dagger}{}_{X,X'}(x,x')$□

$$\begin{aligned} &\ln P_{X,X'}(x,x') - \ln P^{\dagger}{}_{X,X'}(x,x') \\ &= \beta(x-x')\frac{-\partial_x U(x;t) - \partial_{x'}U(x';t)}{2} + \ln P_X(x';t) - \ln P_X(x;t) \\ &= dx \circ [\partial_x[-\beta U(x;t)] - \partial_x \ln P_X(x;t)] \\ &= \frac{\beta}{\mu} dx \circ \nu_X(x;t), \end{aligned} \tag{4.92}$$

□□□□□□□□□.□□□, Ito□□□□□□□Taylor□□□□□□, Stratonovich□分□□□表□□使□□, $O(dt)$□□□□□□□□□□.

□□□□□□□数$A(x;t)$□dx□Stratonovich□□□□$dx \circ A(x;t)$□期□□□□□□□□□□

$$\langle dx \circ A(t) \rangle_{P_{X,X'}} = \int dx' \nu_X(x';t) A(x';t) P_X(x';t) dt, \tag{4.93}$$

□□□.□□□□□□□□□□□□□□□□□□□□□□.□□□, $O(dt)$□□□□□□□□□.

$$\begin{aligned}
&\langle dx \circ A(t) \rangle_{P_{X,X'}} \\
&= \int dx \int dx' P_{X,X'}(x;x') \left[(x-x') \frac{A(x;t)+A(x';t)}{2} \right] \\
&= \int dx \int dx' P_{X,X'}(x;x') \left[(x-x') A(x';t) + \frac{(x-x')^2}{2} \partial_{x'} A(x';t) \right] \\
&= \int dx' P_X(x';t) \left[(-\mu \partial_{x'} U(x';t) dt) A(x',t) + \mu \beta^{-1} dt \partial_{x'} A(x',t) \right] \\
&= \int dx' \left[(-\mu \partial_{x'} U(x';t) dt) A(x',t) P_X(x';t) - \mu \beta^{-1} dt A(x',t) \partial_{x'} P_X(x';t) \right] \\
&= \int dx' \nu_X(x';t) A(x';t) P_X(x';t) dt.
\end{aligned} \tag{4.94}$$

□□□□□□□□□$A(x';t) = 1/dt$□□□□□□.$\langle dx/dt \rangle_{P_{X,X'}} = \langle \nu_X(t) \rangle_{P_X(t)}$□□□□□□□□□□□, □度□$\nu_X(x';t)$□行□□□□□$x$□平□□□□□□□□□平□□度□□□□□□□□□.

□□□, □(4.92)□□(4.93)□□□□□, □□□分布$P_{X,X'}$, ${P^\dagger}_{X,X'}$□□□Kullback-Leibler□□□□□□□□□

$$\begin{aligned}
D_{\mathrm{KL}}(P_{X,X'} || {P^\dagger}_{X,X'}) &= \langle \ln P_{X,X'} - \ln {P^\dagger}_{X,X'} \rangle_{P_{X,X'}} \\
&= \langle \frac{\beta}{\mu} dx \circ \nu_X(t)) \rangle_{P_{X,X'}} \\
&= \frac{\beta}{\mu} \int dx' [\nu_X(x';t)]^2 P_X(x';t) dt \\
&= \sigma(t) dt,
\end{aligned} \tag{4.95}$$

□□□□□□□□□□□□.

4.5.3 エントロピー□成とKullback-Leiblerダイバージェンス

□散□□, □□□□□□□□□Kullback-Leibler□□□□□□□□□□□表□

$$\begin{aligned}
D_{\mathrm{KL}}(p_{X,X',N} || {p^\dagger}_{X,X',N}) &= \sigma(t) dt, \\
D_{\mathrm{KL}}(P_{X,X'} || {P^\dagger}_{X,X'}) &= \sigma(t) dt,
\end{aligned} \tag{4.96}$$

□, Markov□□□□有□□□□□□□□□□□□□□□□□□.

□dt□□□□□□□□□□, □刻0□□$(N-1)dt$□□□□□□.□Markov□□□□□□□□□□, □移□□

$$p(x_{n+1}; ndt, \nu_n | x_n; (n-1)dt) = \frac{p(x_{n+1}; ndt, x_n; (n-1)dt, \nu_n)}{p_X(x_n; (n-1)dt)}, \tag{4.97}$$

□□□□

$$P(x_{n+1}; ndt|x_n; (n-1)dt) = \frac{P(x_{n+1}; ndt, x_n; (n-1)dt)}{P_X(x_n; (n-1)dt)}, \tag{4.98}$$

□□□□，□□$\boldsymbol{x} = \{x_1, \cdots, x_N\}$□□□□□□動□□□□$\nu = \{\nu_1, \cdots, \nu_{N-1}\}$□□□□□$p_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x}, \boldsymbol{\nu})$□□□$\boldsymbol{x} = \{x_1, \cdots, x_N\}$□□□$P_{\boldsymbol{X}}(\boldsymbol{x})$□

$$p_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x}, \boldsymbol{\nu}) = \prod_{n=1}^{N-1} p(x_{n+1}; ndt, \nu_n|x_n; (n-1)dt)p_X(x_1; 0), \tag{4.99}$$

$$P_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{n=1}^{N-1} P(x_{n+1}; ndt|x_n; (n-1)dt)P_X(x_1; 0), \tag{4.100}$$

□□□□定□□□□．□□□□□□□□□□□

$$p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x}, \boldsymbol{\nu}) = \prod_{n=1}^{N-1} p(x_n; ndt, \nu_n|x_{n+1}; (n-1)dt)p_X(x_N; (N-1)dt), \tag{4.101}$$

$$P^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{n=1}^{N-1} P(x_n; ndt|x_{n+1}; (n-1)dt)P_X(x_N; (N-1)dt), \tag{4.102}$$

□□□□，$(N-1)dt = \tau$□□定□□$dt \to 0$□□□□□□□□Kullback-Leibler□□□□□□□□□

$$D_{\mathrm{KL}}(p_{\boldsymbol{X},\boldsymbol{N}}||p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}) = \int_0^{\tau} \sigma(t)dt = \Sigma(\tau; 0), \tag{4.103}$$

$$D_{\mathrm{KL}}(P_{\boldsymbol{X}}||P^{\dagger}{}_{\boldsymbol{X}}) = \int_0^{\tau} \sigma(t)dt = \Sigma(\tau; 0), \tag{4.104}$$

□□□□□□□□□□□□□□□示□□□□□□□．

□□□示□□□□□，□□□□□□□□□□□□□□□□□□□□□．

$$\begin{aligned}
p_{X_{n+1},N_n|X_n}(x_{n+1}, \nu_n|x_n) &= p(x_{n+1}; ndt, \nu_n|x_n; (n-1)dt), && (4.105)\\
p^{\dagger}{}_{X_n,N_n|X_{n+1}}(x_n, \nu_n|x_{n+1}) &= p(x_n; ndt, \nu_n|x_{n+1}; (n-1)dt), && (4.106)\\
p_{X_n}(x_n) &= p_X(x_n; (n-1)dt), && (4.107)\\
P_{X_{n+1}|X_n}(x_{n+1}|x_n) &= P(x_{n+1}; ndt|x_n; (n-1)dt), && (4.108)\\
P^{\dagger}{}_{X_n|X_{n+1}}(x_n|x_{n+1}) &= P(x_n; ndt|x_{n+1}; (n-1)dt), && (4.109)\\
P_{X_n}(x_n) &= P_X(x_n; (n-1)dt). && (4.110)
\end{aligned}$$

□□□□□□□□□□□□□□□

$$p_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{n=1}^{N-1} p_{X_{n+1},N_n|X_n}(x_{n+1}, \nu_n|x_n)p_{X_1}(x_1), \tag{4.111}$$

$$p^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{n=1}^{N-1} p^{\dagger}{}_{X_n,N_n|X_{n+1}}(x_n, \nu_n|x_{n+1})p_{X_N}(x_N), \tag{4.112}$$

$$P_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{n=1}^{N-1} P_{X_{n+1}|X_n}(x_{n+1}|x_n)P_{X_1}(x_1), \tag{4.113}$$

$$P^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{n=1}^{N-1} P^{\dagger}{}_{X_n|X_{n+1}}(x_n|x_{n+1})P_{X_N}(x_N), \tag{4.114}$$

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$$D_{\mathrm{KL}}(p_{X_{n+1},N_n|X_n}p_{X_n}||p^{\dagger}{}_{X_n,N_n|X_{n+1}}p_{X_{n+1}}) = \sigma((n-1)dt)dt, \tag{4.115}$$

$$D_{\mathrm{KL}}(P_{X_{n+1}|X_n}P_{X_n}||P^{\dagger}{}_{X_n|X_{n+1}}P_{X_{n+1}}) = \sigma((n-1)dt)dt, \tag{4.116}$$

□□□□□□□□□□□□.□□□

$$\begin{aligned}
&D_{\mathrm{KL}}(p_{\boldsymbol{X},\boldsymbol{N}}||p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}) \\
&= \left\langle \ln\left[\prod_{n=1}^{N-1} p_{X_{n+1},N_n|X_n}p_{X_1}\right] - \ln\left[\prod_{n=1}^{N-1} p^{\dagger}{}_{X_n,N_n|X_{n+1}}p_{X_N}\right]\right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}} \\
&= \sum_{n=1}^{N-1}\left\langle \ln\left[p_{X_{n+1},N_n|X_n}p_{X_n}\right] - \ln\left[p^{\dagger}{}_{X_n,N_n|X_{n+1}}p_{X_{n+1}}\right]\right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}} \\
&= \sum_{n=1}^{N-1} D_{\mathrm{KL}}(p_{X_{n+1},N_n|X_n}p_{X_n}||p^{\dagger}{}_{X_n,N_n|X_{n+1}}p_{X_{n+1}}) \\
&= \sum_{n=1}^{N-1}\sigma((n-1)dt)dt,
\end{aligned} \tag{4.117}$$

□□□□

$$\begin{aligned}
&D_{\mathrm{KL}}(P_{\boldsymbol{X}}||P^{\dagger}{}_{\boldsymbol{X}}) \\
&= \left\langle \ln\left[\prod_{n=1}^{N-1} P_{X_{n+1}|X_n}P_{X_1}\right] - \ln\left[\prod_{n=1}^{N-1} P^{\dagger}{}_{X_n|X_{n+1}}P_{X_N}\right]\right\rangle_{P_{\boldsymbol{X}}} \\
&= \sum_{n=1}^{N-1}\left\langle \ln\left[P_{X_{n+1}|X_n}P_{X_n}\right] - \ln\left[P^{\dagger}{}_{X_n|X_{n+1}}P_{X_{n+1}}\right]\right\rangle_{P_{\boldsymbol{X}}} \\
&= \sum_{n=1}^{N-1} D_{\mathrm{KL}}(P_{X_{n+1}|X_n}P_{X_n}||P^{\dagger}{}_{X_n|X_{n+1}}P_{X_{n+1}}) \\
&= \sum_{n=1}^{N-1}\sigma((n-1)dt)dt,
\end{aligned} \tag{4.118}$$

□□□, $(N-1)dt = \tau$□□定□□$dt \to 0$□□□□□□□□□□

$$\sum_{n=1}^{N-1}\sigma((n-1)dt)dt \to \Sigma(\tau;0), \tag{4.119}$$

□□□□□□□□□□□□□.

4.6 揺らぎの定□

4.6.1 □□ゆらぎの定□

□,□□□□□□□□

$$\begin{aligned}
\Sigma(\tau;0) &= \langle \ln p_{\boldsymbol{X},\boldsymbol{N}} - \ln p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}}, \\
\Sigma(\tau;0) &= \langle \ln P_{\boldsymbol{X}} - \ln P^{\dagger}{}_{\boldsymbol{X}}\rangle_{P_{\boldsymbol{X}}},
\end{aligned} \tag{4.120}$$

□□□□□□□□□□□□. □□期□□□□□前□□□□□□□□□□□□□□□□□□□

$$
\begin{aligned}
\hat{\Sigma}(\boldsymbol{x},\boldsymbol{\nu};\tau;0) &= \ln p_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu}) - \ln p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu}),\\
\hat{\Sigma}(\boldsymbol{x};\tau;0) &= \ln P_{\boldsymbol{X}}(\boldsymbol{x}) - \ln P^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x}),
\end{aligned}
\tag{4.121}
$$

□□□□□□. □□□□期□□□□□□□□□□□□□□□□□□□□.

$$
\begin{aligned}
\Sigma(\tau;0) &= \langle\hat{\Sigma}(\tau;0)\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}}\\
\Sigma(\tau;0) &= \langle\hat{\Sigma}(\tau;0)\rangle_{P_{\boldsymbol{X}}}.
\end{aligned}
\tag{4.122}
$$

□□□□□□□□□□□□□□□□定□□□□□□□

$$
\begin{aligned}
\frac{p_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu})}{p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu})} &= \exp[\hat{\Sigma}(\boldsymbol{x},\boldsymbol{\nu};\tau;0)],\\
\frac{P_{\boldsymbol{X}}(\boldsymbol{x})}{P^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x})} &= \exp[\hat{\Sigma}(\boldsymbol{x};\tau;0)],
\end{aligned}
\tag{4.123}
$$

□□□□□□□□数□□□□□□□□□□□□□□□□□□□□□□係□□. □□□□□□□□□□定□□□□□□□□.

□□□$p_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu})$ (□□□□$P_{\boldsymbol{X}}(\boldsymbol{x})$)□$p_{X_1}(x_1)$ (□□□□$P_{X_1}(x_1)$)□分布□□□□□□□□□方□□□□□□□□□□□□□□□□□□□□対□□, $p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu})$ (□□□□$P^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x})$)□$p_{X_N}(x_N)$ (□□□□$P_{X_N}(x_N)$)□分布□□□□□□□□□□方□□□□□□□□□□□□□□□□□□□□□□□□□□□. □□□□□□□□方□□□□□□□□□□□□□□方□□定□□□□□□□.

4.6.2 □分ゆらぎの定□

□□, □□□□□□□□定□□□□帰□□□□, □□□□□□□□□□□□示□□□□□□□.

$$
\begin{aligned}
\left\langle \exp[-\hat{\Sigma}(\tau;0)]\right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}} &= 1,\\
\left\langle \exp[-\hat{\Sigma}(\tau;0)]\right\rangle_{P_{\boldsymbol{X}}} &= 1,
\end{aligned}
\tag{4.124}
$$

□□□, 分布□□□□$\sum_{\boldsymbol{x},\boldsymbol{\nu}} p^{\dagger}{}_{\boldsymbol{X},\boldsymbol{N}}(\boldsymbol{x},\boldsymbol{\nu}) = 1$□$\int d\boldsymbol{x}P^{\dagger}{}_{\boldsymbol{X}}(\boldsymbol{x}) = 1$□□□□. □□□□□分□□□□定□□□□□□□□.

□数$f(g) = -\exp(-g)$□□□□□□数(□□□□$-f(g) = \exp(-g)$□□□□□□数)□□□□□□□, $f(g) = -\exp(-g)$□対□□Jensen□□□□(4.21), (4.22)□□分□□□□定□□□□□□

$$
\exp\left[-\left\langle\hat{\Sigma}(\tau;0)\right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}}\right] \le \left\langle \exp[-\hat{\Sigma}(\tau;0)]\right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}}, \tag{4.125}
$$

$$
\exp\left[-\left\langle\hat{\Sigma}(\tau;0)\right\rangle_{P_{\boldsymbol{X}}}\right] \le \left\langle \exp[-\hat{\Sigma}(\tau;0)]\right\rangle_{P_{\boldsymbol{X}}}, \tag{4.126}
$$

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$$
\exp\left[-\Sigma(\tau;0)\right] \le \exp[0], \tag{4.127}
$$

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$$\Sigma(\tau;0) \geq 0, \tag{4.128}$$

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4.6.3 Jarzynski□式

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$$\hat{\Sigma}(\boldsymbol{x},\boldsymbol{\nu};\tau;0) = \Delta S^{\mathrm{sys}}(\boldsymbol{x};\tau;0) + \Delta S^{\mathrm{bath}}(\boldsymbol{x};\tau;0), \tag{4.129}$$

$$\Delta S^{\mathrm{sys}}(\boldsymbol{x};\tau;0) = \ln p_X(x_1;0) - \ln p_X(x_N;\tau), \tag{4.130}$$

$$\Delta S^{\mathrm{bath}}(\boldsymbol{x};\tau;0) = \sum_{n=1}^{N-1} \ln \frac{p(x_{n+1};ndt,\nu_n|x_n;(n-1)dt)}{p(x_n;ndt,\nu_n|x_{n+1};(n-1)dt)}, \tag{4.131}$$

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$$\frac{p(x_{n+1};ndt,\nu_n|x_n;(n-1)dt)}{p(x_n;ndt,\nu_n|x_{n+1};(n-1)dt)} = \exp\left[-\beta\frac{\delta Q}{\delta t}((n-1)dt)dt\right], \tag{4.132}$$

□□□□．□□□$\delta Q/\delta t$□□位□□□□□□□□□□□□□□□．□□□，$dt \to 0$□□□□□□□□□□□□□□□□□□

$$\Delta S^{\mathrm{bath}}(\boldsymbol{x};\tau;0) = -\beta\int_0^\tau dt\frac{\delta Q}{\delta t} := -\beta\delta Q(\boldsymbol{x}), \tag{4.133}$$

□□□0□□τ□□□□□□□□□$\delta Q(\boldsymbol{x})$□□□□□□□□□□□□．

□□，□刻0□τ□平衡分布□□□，$U(x;t)$□□□□□□□□□□□，$F(t)$□Helmholtz□□□□□□□□□□□□，

$$p_X(x_1;0) = \exp[-\beta(U(x_1;0) - F(0))], \tag{4.134}$$

$$p_X(x_N;\tau) = \exp[-\beta(U(x_N;\tau) - F(\tau))], \tag{4.135}$$

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$$\Delta S^{\mathrm{sys}}(\boldsymbol{x};\tau;0) = \beta\Delta U(\boldsymbol{x}) - \beta\Delta F, \tag{4.136}$$

$$\Delta U(\boldsymbol{x}) = U(x_N;\tau) - U(x_1;0), \tag{4.137}$$

$$\Delta F = F(\tau) - F(0), \tag{4.138}$$

□□□□□□．□，□力学□□□則□□，□□□□□□$\delta W(\boldsymbol{x})$□

$$\delta W(\boldsymbol{x}) = \Delta U(\boldsymbol{x}) - \delta Q(\boldsymbol{x}), \tag{4.139}$$

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$$\hat{\Sigma}(\boldsymbol{x},\boldsymbol{\nu};\tau;0) = \beta(\delta W(\boldsymbol{x}) - \Delta F), \tag{4.140}$$

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□□□□分□□□□□定□□

$$\left\langle \exp[-\beta(\delta W - \Delta F)] \right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}} = 1, \tag{4.141}$$

□□□□□□□□□□□. □□ΔF□□□□□□$\boldsymbol{x}$□依存□□□□□□□□□

$$\left\langle \exp[-\beta\Delta F] \right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}} = \exp[-\beta\Delta F], \tag{4.142}$$

□□□□□□□□□□,

$$\exp[-\beta\Delta F] = \left\langle \exp[-\beta\delta W] \right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}}, \tag{4.143}$$

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□常□□力学□□□則□□□□□□□,

$$\left\langle \delta W(\boldsymbol{x}) \right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}} \geq \Delta F, \tag{4.144}$$

□□□. □□□力学□□□則□□□□平衡□□□□□□□□□□□□□□ΔF□□□□□□□δW□□□□□□□平□□□□□□□□□□□□□, □□□□□□□□□□刻0□□τ□□常□平衡□□□□□□□□□□□□□□. □方□□□Jarzynski□□□

$$\Delta F = -\beta^{-1} \ln \left\langle \exp[-\beta\delta W] \right\rangle_{p_{\boldsymbol{X},\boldsymbol{N}}}, \tag{4.145}$$

□□□□□□, □刻0□τ□□平衡□□□□□□□□□□□□□□□, □□□□移□非平衡□□移□□□□□□□, □□□□□□$\delta W(\boldsymbol{x})$□□□□□数$\exp[-\beta\delta W(\boldsymbol{x})]$□□□□□□□平□□□□□□□□□□□□□□□□□□□□, 非平衡□□□則□□□□□□□□□□□□. □□□実□□□□$\exp[-\beta\delta W(\boldsymbol{x})]$□□□□□□□□□□□平□□, $\delta W(\boldsymbol{x}) \ll 0$□□□□□□□□□□□□□□寄□□□□□□□□□□,□□□□□□□□□□□□□□□□□□□□, □□Jarzynski□□□□□□□□□□□□□□□□□□□□□□□□□□□.

4.7 □□□り合い条件におけるエントロピー□成□とKullback-Leiblerダイバージェンス

4.7.1 □散状態の場合のエントロピー□成□

Kullback-Leibler□□□□□□□□□□□□□□□□□□□□□□, 別□□係□□□□□□□□□□□. □, □移□□□□□□□依存□□□□□□$W^{(\nu)}(x'|x)$□□□. □□□□□□□□□条□□□□□□□

$$W^{(\nu)}(x'|x) p_X^{\mathrm{ss}}(x') = W^{(\nu)}(x|x') p_X^{\mathrm{ss}}(x'), \tag{4.146}$$

□□□□□□□$\rho = (x, x', \nu)$□□□□平衡分布$p_X^{\mathrm{ss}}(x')$□存□□□. □□□, □□□□□□□□□$\sigma(t)$□

$$\sigma(t) = -\frac{d}{dt} D_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}}), \tag{4.147}$$

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$$
\begin{aligned}
&-\frac{d}{dt}D_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}}) \\
&= -\sum_x \frac{dp_X(x;t)}{dt}\ln\frac{p_X(x;t)}{p_X^{\mathrm{ss}}(x)} + \sum_x \frac{dp_X(x)}{dt} \\
&= -\sum_x\sum_{x'}\sum_\nu [W^{(\nu)}(x|x')p_X(x';t) - W^{(\nu)}(x'|x)p_X(x;t)]\ln\frac{p_X(x;t)}{p_X^{\mathrm{ss}}(x)} \\
&= \sum_{x,x',\nu|x>x'} [W^{(\nu)}(x|x')p_X(x';t) - W^{(\nu)}(x'|x)p_X(x;t)]\left[\ln\frac{p_X(x';t)}{p_X^{\mathrm{ss}}(x')} - \ln\frac{p_X(x;t)}{p_X^{\mathrm{ss}}(x)}\right] \\
&= \sum_{x,x',\nu|x>x'} [W^{(\nu)}(x|x')p_X(x';t) - W^{(\nu)}(x'|x)p_X(x;t)]\ln\frac{W^{(\nu)}(x|x')p_X(x';t)}{W^{(\nu)}(x'|x)p_X(x;t)} \\
&= \sigma(t).
\end{aligned}
\tag{4.148}
$$

□□□□□, □□□□□□□□□□平衡分布□□□□分布□□□Kullback-Leibler□□□□□□□□□□□□分□□□□□□□□□□□. □□□□□□□□□□□□□□□□□定常□□$p_X^{\mathrm{ss}}(x')$□対□□$\sigma^{\mathrm{ex}}(t) = -d/dtD_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}})$□□□□□□□□□□□□□□□□□, □□□$\sigma^{\mathrm{ex}}(t)$□□□□□□□□□□□□□□□□□□剰□□□□□□□□□□□□□□□□□□□□.

4.7.2 □□状態の場合のエントロピー□成□

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$$
\partial_t P_X(x;t) = -\partial_x(\nu_X(x;t)P_X(x;t)) \tag{4.149}
$$

$$
\nu_X(x;t) = -\mu\partial_x[U_X(x) + \beta^{-1}\ln P_X(x;t)]. \tag{4.150}
$$

□□□□□□□□. □□□平衡分布$P_X^{\mathrm{ss}}(x')$□

$$
-\mu\partial_x[U_X(x) + \beta^{-1}\ln P_X^{\mathrm{ss}}(x')] = 0 \tag{4.151}
$$

□□□□分布□□□

$$
P_X^{\mathrm{ss}}(x) = \frac{\exp[-\beta U_X(x)]}{\int dx' \exp[-\beta U_X(x')]}, \tag{4.152}
$$

□□□□□□. □□□$-d/dtD_{\mathrm{KL}}(P_X(t)||P_X^{\mathrm{ss}})$□

$$
\begin{aligned}
&-\frac{d}{dt}D_{\mathrm{KL}}(P_X(t)||P_X^{\mathrm{ss}}) \\
&= -\int dx\partial_t P_X(x;t)\ln\frac{P_X(x;t)}{P_X^{\mathrm{ss}}(x)} - \int dx\partial_t P_X(x;t) \\
&= \int dx\partial_x(\nu_X(x;t)P_X(x;t))\left[\ln P_X(x;t) + \beta U_X(x) + \ln\int dx'\exp[-\beta U_X(x')]\right] \\
&= -\int dx(\nu_X(x;t)P_X(x;t))\partial_x\left[\ln P_X(x;t) + \beta U_X(x)\right] \\
&= \frac{\beta}{\mu}\int dx[\nu_X(x;t)]^2 P_X(x;t) \\
&= \sigma(t),
\end{aligned}
\tag{4.153}
$$

□□□.□□□□□□□□□□□□$\sigma(t)$□□□□□□□条□□□□□□□□□□□□□□
□□□□

$$\sigma(t) = -\frac{d}{dt} D_{\mathrm{KL}}(P_X(t)||P_X^{\mathrm{ss}}), \tag{4.154}$$

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4.8 熱力学□二法則と平□状態の安定性

4.8.1 力学□とmaster方□式

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$$\frac{dp_X(x;t)}{dt} = \sum_{x'} W(x|x')p_X(x';t), \tag{4.155}$$

□□□□□□行列表□$\boldsymbol{p}(t) = (p_X(1;t), p_X(2;t), \cdots, p_X(N;t))^{\mathrm{T}}$, $\mathsf{W}_{ij} = W(i|j)$□□□□□,

$$\frac{d}{dt}\boldsymbol{p}(t) = \mathsf{W}\boldsymbol{p}(t) := \boldsymbol{f}(\boldsymbol{p}(t)). \tag{4.156}$$

□□□□□□.□□master方□□□初期条□$\boldsymbol{p}(0)$□□□□□□数$\boldsymbol{f}(\boldsymbol{p}(t))$□□□□□□□□刻$t > 0$□□$\boldsymbol{p}(t)$□□□□□□□.

□□□

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(\boldsymbol{y}). \tag{4.157}$$

□□□□□数$\boldsymbol{f}(\boldsymbol{y})$□□□□□□□□□力学□□□□□□□□.□□□□□master方□□□□□分布□対□□力学□□□□.

力学□□□□□

$$\boldsymbol{f}(\boldsymbol{y}^*) = \boldsymbol{0}, \tag{4.158}$$

□□□□□$\boldsymbol{y} = \boldsymbol{y}^*$□□, $d\boldsymbol{y}/dt|_{\boldsymbol{y}=\boldsymbol{y}^*} = 0$□□$\boldsymbol{y}$□□□□□□□□□□.□□□$\boldsymbol{y}^*$□□定□□□□.master方□□□□□□定常分布$\boldsymbol{p}^{\mathrm{ss}} = (p_X^{\mathrm{ss}}(1;t), p_X^{\mathrm{ss}}(2;t), \cdots, p_X^{\mathrm{ss}}(N;t))^{\mathrm{T}}$□

$$\boldsymbol{f}(\boldsymbol{p}^{\mathrm{ss}}) = \boldsymbol{0}, \tag{4.159}$$

□□□□□□□□,□定□□□□□□□.

4.8.2 固定点の安定性とLyapunov□数

□□□力学□□□□□□定□$\boldsymbol{y}^*$□□□□分□□□□$\boldsymbol{y} = \boldsymbol{y}^* + \delta\boldsymbol{y}$□表□□□□□□□□.□□□,□分$\delta\boldsymbol{y}$□□□□□□

$$\frac{d\delta\boldsymbol{y}}{dt} = \boldsymbol{f}(\boldsymbol{y}^* + \delta\boldsymbol{y}). \tag{4.160}$$

□□□□□□.□□□□分□□□分$\delta y_i = (\delta\boldsymbol{y})_i$□□対□$|\delta y_i|$□

$$\frac{d}{dt}|\delta y_i| \leq 0 \tag{4.161}$$

□□□□□□□$\delta y_i = 0$□□□□□□□□，□□$t \to \infty$□□□□$\boldsymbol{y} \to \boldsymbol{y}^*$□□定□□□束□□□□□□□□□．□□□□□□□□□□□□□定□$\boldsymbol{y}^*$□□□□□□□安定□□□．

□□$d|\delta y_i|/dt \leq 0$□常□□□□□□□□□□，$t \to \infty$□□□□$\boldsymbol{y} \to \boldsymbol{y}^*$□□定□□□束□□□□□存□□□．□□□□□□□□□□□□□Lyapunov□数$\mathcal{L}(\boldsymbol{y}||\boldsymbol{y}^*)$□存□□□□□□$t \to \infty$□□□□$\boldsymbol{y} \to \boldsymbol{y}^*$□□定□□□束□，□□□□□□安定□□□．

Lyapunov□数$\mathcal{L}(\boldsymbol{y}||\boldsymbol{y}^*)$□□□□□□□□A, B□□□□数□□□．

□□A:

$$\mathcal{L}(\boldsymbol{y}||\boldsymbol{y}^*) \geq 0 \tag{4.162}$$

□□□□□□□$\boldsymbol{y} = \boldsymbol{y}^*$□□□．

□□B:

$$\frac{d}{dt}\mathcal{L}(\boldsymbol{y}||\boldsymbol{y}^*) \leq 0 \tag{4.163}$$

□□□□□□□$\boldsymbol{y} = \boldsymbol{y}^*$□□□．

□□□□□□A□条□□(4.162)□□□□□□数$\mathcal{L}(\boldsymbol{y}||\boldsymbol{y}^*)$□Lyapunov□補□数□□□□□□□，□□B□条□□(4.163)□□□□□□□□□定□□□□□□安定□□□□(□安定□)□□□□□方□□Lyapunov□□□□□□．□□$|\delta y_i|$□□分□□□□□□□□条□□(4.163)□□□□□□□，□□□□□□□□□□□□□□□□安定□□□．□□□□分□□□$|\delta y_i|$□□□□□□□□□□$t \to \infty$□□□□□□定□□□束□□保□□□□□，□度□定□$\boldsymbol{y}^*$□行□□□□，□□□□動$\delta \boldsymbol{y}$□加□□□□定□□□□□□□□□□□□□□□□．□□条□□(4.163)□□□□□□$\boldsymbol{y} = \boldsymbol{y}^*$□□□□□□□□条□□□□□□□□Lyapunov安定□□□□□□□．□□□□度□定□$\boldsymbol{y}^*$□行□□□□□□□□□□動$\delta \boldsymbol{y}$□加□□□□，□定□□□□□□□□□□□□□□□□□□定□□□□□□□□□□□□□□□□□□□□□□□．

4.8.3 熱力学□二法則と平□分布の安定性

master方□□□□□□□□□□□□□□□□□□，例□□□散□□□□□

$$\sigma(t) = -\frac{d}{dt}D_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}}), \tag{4.164}$$

□□□□□□□□□□□□□□□□□□□□□□．□□力学□□□則□□□

$$\frac{d}{dt}D_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}}) \leq 0, \tag{4.165}$$

□示□□．Kullback-Leibler□□□□□□□□□

$$D_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}}) \geq 0, \tag{4.166}$$

□□□□□□□$p_X(t) = p_X^{\mathrm{ss}}$□□□□□□□□□，$p_X^{\mathrm{ss}}$□master方□□□力学□□□□□□□□□□定□□□□．□□□平衡分布p_X^{ss}□□□□定□□□□□，□□□力学□□□則□Kullback-Leibler□□□□□□□□Lyapunov□数

$$\mathcal{L}(\boldsymbol{p}||\boldsymbol{p}^{\mathrm{ss}}) = D_{\mathrm{KL}}(p_X(t)||p_X^{\mathrm{ss}}), \tag{4.167}$$

□□□□□□□□□□□□□□□．□□□，□□□□□□□□□□master方□□□□□□□□□□□□□，平衡分布□□□□定□□□□□平衡分布□□□□□□□安定□□□，

$t \to \infty$□□□□$\boldsymbol{p} \to \boldsymbol{p}^{\mathrm{ss}}$□□束□□□□□保□□□□. □□□□□□□□□□□条□□□□□□□□, □力学□□□則□平衡分布□□□□□保□□□□□□□□□□□.

□5□

力学□と安定性

5.1 □□□□とパラメータの力学□

5.1.1 キュムラントとモーメント

□, □□□□$x \in \mathsf{R}$□□□分布$P_X(x)$□□□□□□□□□□□□□, n□□□□□□□□ □□□□□□□□□□□□. n□□□□□□□□c_n□定□□,

$$\ln\langle e^{sx}\rangle_{P_X} = \sum_{n=1}^{\infty} \frac{c_n}{n!} s^n \tag{5.1}$$

□□□□Taylor□□□係数□定□□□□. □□n□□□□□□□□c_n□□体□□□□□□,

$$c_n = (\partial_s)^n \ln\langle e^{sx}\rangle_{P_X}\big|_{s=0} \tag{5.2}$$

□□□□□□□□□□□□□. 例□□, 1□□□□□□□□□□□定□□□□□,

$$\begin{aligned} c_1 &= \partial_s \ln\langle e^{sx}\rangle_{P_X}\big|_{s=0} \\ &= \left.\frac{\langle x e^{sx}\rangle_{P_X}}{\langle e^{sx}\rangle_{P_X}}\right|_{s=0} \\ &= \langle x\rangle_{P_X}, \end{aligned} \tag{5.3}$$

□平□□□□□, 2□□□□□□□□□

$$\begin{aligned} c_2 &= (\partial_s)^2 \ln\langle e^{sx}\rangle_{P_X}\big|_{s=0} \\ &= \left.\left[\frac{\langle x^2 e^{sx}\rangle_{P_X}}{\langle e^{sx}\rangle_{P_X}} - \frac{\langle x e^{sx}\rangle_{P_X}^2}{\langle e^{sx}\rangle_{P_X}^2}\right]\right|_{s=0} \\ &= \langle x^2\rangle_{P_X} - \langle x\rangle_{P_X}^2, \end{aligned} \tag{5.4}$$

□分散□□□□□□□□□□.

□□□□□□□□□□□□n□□□□□□□m_n□□□□□□□□□□□□. □□□

$$\langle e^{sx}\rangle_{P_X} = 1 + \sum_{n=1}^{\infty} \frac{m_n}{n!} s^n \tag{5.5}$$

□□□□Taylor□□□係数□定□□□□. □□□n□□□□□□□□m_n□□体□□□□□□ □

$$m_n = (\partial_s)^n \langle e^{sx}\rangle_{P_X}\big|_{s=0} \tag{5.6}$$

□□□□□□□□, n□□□□□□□□

$$
\begin{aligned}
m_n &= (\partial_s)^n \langle e^{sx} \rangle_{P_X} |_{s=0} \\
&= \langle x^n e^{sx} \rangle_{P_X} |_{s=0} \\
&= \langle x^n \rangle_{P_X},
\end{aligned}
\tag{5.7}
$$

□x□n□□期□□□□□□□□. □□

$$
c_n = (\partial_s)^n \ln \left[1 + \sum_{n=1}^{\infty} \frac{m_n}{n!} s^n \right] \Bigg|_{s=0}, \tag{5.8}
$$

□□, n□□□□□□□□□n□□□□□□□□□□□□□□□□表□□□□□□□. 例□□, 1□□2□□□□□□

$$
c_1 = m_1, \tag{5.9}
$$

$$
c_2 = m_2 - m_1^2, \tag{5.10}
$$

□□□□表□□□□. □□□□□, n□□□□□□□□□

$$
m_n = (\partial_s)^n \exp \left[\sum_{n=1}^{\infty} \frac{c_n}{n!} s^n \right] \Bigg|_{s=0} \tag{5.11}
$$

□□, n□□□□□□□□□□□□□□□□□□表□□□□□□□. 例□□, 1□□2□□□□□□

$$
m_1 = c_1, \tag{5.12}
$$

$$
m_2 = c_2 + c_1^2, \tag{5.13}
$$

□□□□表□□□□.

□□分布$P_X(x)$□□□□□□□□□□□

$$
\Phi_X(k) = \int dx P_X(x) \exp(ikx) \tag{5.14}
$$

□□□□数□□□. □□□□□数□□□□□□□□□□□□□□分布$P_X(x)$□□□□□□□□, □□□数□□□□□□□分布$P_X(x)$□□定□□□. □, □□□□□□□□□□□□□数□

$$
\Phi_X(-is) = 1 + \sum_{n=1}^{\infty} \frac{m_n}{n!} (s)^n \tag{5.15}
$$

□□□□□□□□, □□□□□□□□□□定□□□□□分布$P_X(x)$□□□定□□□□□□□□□□□. □□□□□□□□□□□□□□□□□□□□□□□□, □□□□□□□□□□□□定□□□□□分布$P_X(x)$□□□定□□. □□□, □□□□□□□$\boldsymbol{m} = \{m_n | n = 1, \cdots\}$□□□□□□□□□□□□□$\boldsymbol{c} = \{c_n | n = 1, \cdots\}$□□□分布□□定□□□□□□□□□□□□□□□□□□□□.

例□□, □□分布$P_X(x)$□平□μ, 分散σ^2□□□□分布

$$
P_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(x-\mu)^2}{2\sigma^2} \right], \tag{5.16}
$$

□□□□,

$$
\begin{aligned}
\ln\langle e^{sx}\rangle_{P_X} &= \ln\left[\int dx \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2} + sx\right]\right] \\
&= \ln\left[\int dx \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu-\sigma^2 s)^2}{2\sigma^2} + \mu s + \frac{\sigma^2}{2}s^2\right]\right] \\
&= \mu s + \frac{\sigma^2}{2}s^2, \qquad (5.17)
\end{aligned}
$$

□□,□□□□分布□□□□□□□$c_1 = \mu$, $c_2 = \sigma^2$, $n \geq 3$□$c_n = 0$□□□□□□□□□□□□□□.

5.1.2 Fokker-Planck方□式とキュムラントの力学□

□□□□□□□□□□□□□□□□□□□□力学□□□□表□□□方□□□□□□□□. □体例□□□, □□□依存□□□□□□□□□□

$$
U_X(x;t) = \frac{k_U(t)}{2}(x - \mu_U(t))^2, \qquad (5.18)
$$

□□動□□□Fokker-Planck方□□

$$
\begin{aligned}
\partial_t P_X(x;t) &= \partial_x[[\mu\partial_x U_X(x;t)]P_X(x;t)] + \mu\beta^{-1}(\partial_x)^2 P_X(x;t) \\
&= \partial_x[\mu k_U(t)(x-\mu_U(t))P_X(x;t)] + \mu\beta^{-1}(\partial_x)^2 P_X(x;t), \qquad (5.19)
\end{aligned}
$$

□表□□□□□□□□□□□□□□, □□□□□□□□□□力学□

$$
\frac{d\boldsymbol{c}}{dt} = \boldsymbol{f}(\boldsymbol{c}), \qquad (5.20)
$$

□□□表□□□□□□. □□□□□□$k_U(t) > 0$□□□□□, $\mu > 0$□□□□□□□□□□.

□□□□□□□□□□, Fokker-Planck方□□□□□□□表□

$$
\partial_t P_X(x;t) = -\partial_x[A^{(1)}(x;t)P_X(x;t)] + \frac{1}{2}(\partial_x)^2[A^{(2)}(x;t)P_X(x;t)], \qquad (5.21)
$$

□□□, □□□□(5.19)□□□□係数$A^{(1)}(x;t)$, $A^{(2)}(x;t)$□x依存□□□示□□□□□□□

$$
\begin{aligned}
A^{(1)}(x;t) &= A_0^{(1)}(t) + xA_1^{(1)}(t), \\
A^{(2)}(x;t) &= A_0^{(2)}(t), \qquad (5.22)
\end{aligned}
$$

□□□□□□□□□□□□□□□□□□□. □□□, □□□$A_0^{(1)}(t) = \mu k_U(t)\mu_U(t)$, $A_1^{(1)}(t) = -\mu k_U(t)$, $A_0^{(2)}(t) = 2\mu\beta^{-1}$□□□.

□□□□, n□□□□□□□□$c_n(t)$□□□□□□

$$
\begin{aligned}
\frac{d}{dt}c_n(t) &= (\partial_s)^n \frac{\int dx e^{sx}\partial_t P_X(x;t)}{\langle e^{sx}\rangle_{P_X(t)}}\Bigg|_{s=0} \\
&= (\partial_s)^n \frac{\int dx e^{sx}\left[-\partial_x[A^{(1)}(x;t)P_X(x;t)] + \frac{1}{2}(\partial_x)^2[A^{(2)}(x;t)P_X(x;t)]\right]}{\langle e^{sx}\rangle_{P_X(t)}}\Bigg|_{s=0} \\
&= (\partial_s)^n \frac{\int dx e^{sx} s\left[A_0^{(1)}(t) + xA_1^{(1)}(t)]P_X(x;t) + \frac{1}{2}s^2 A_0^{(2)}(t)P_X(x;t)\right]}{\langle e^{sx}\rangle_{P_X(t)}}\Bigg|_{s=0} \\
&= (\partial_s)^n \frac{\left[sA_0^{(1)}(t)\langle e^{sx}\rangle_{P_X(t)} + sA_1^{(1)}(t)\partial_s\langle e^{sx}\rangle_{P_X(t)} + \frac{1}{2}s^2 A_0^{(2)}(t)\langle e^{sx}\rangle_{P_X(t)}\right]}{\langle e^{sx}\rangle_{P_X(t)}}\Bigg|_{s=0} \\
&= (\partial_s)^n \left[sA_0^{(1)}(t) + \frac{1}{2}s^2 A_0^{(2)}(t)\right]\Bigg|_{s=0} + (\partial_s)^n \left[sA_1^{(1)}(t)\partial_s \ln\langle e^{sx}\rangle_{P_X(t)}\right]\Bigg|_{s=0} \\
&= A_0^{(1)}(t)\delta_{n1} + A_0^{(2)}(t)\delta_{n2} + nA_1^{(1)}(t)c_n,
\end{aligned}
\tag{5.23}
$$

□□□□□□□□. □□□, 平□□$c_1(t) = \langle x\rangle_{P_X(t)}$□□□□□□

$$
\frac{d}{dt}c_1(t) = -\mu k_U(t)(c_1(t) - \mu_U(t)), \tag{5.24}
$$

分散$c_2(t) = \langle (x - \langle x\rangle_{P_X(t)})^2\rangle_{P_X(t)}$□□□□□□

$$
\frac{d}{dt}c_2(t) = -2\mu(k_U(t)c_2(t) - \beta^{-1}), \tag{5.25}
$$

$n \geq 3$□□□□□□n□□□□□□□□□□□□□□□

$$
\frac{d}{dt}c_n(t) = -\mu n k_U(t)c_n(t), \tag{5.26}
$$

□□□□□□.

□□□□, $t = 0$□□□□分布□□□□□, $n \geq 3$□$c_n(0) = 0$□□□. □□□□, □(5.26)□□$t \geq 0$□$c_n(t) = 0$□□□□□□示□□. □□□□□, □□□□□□□□□□Fokker-Planck方□□□□□□□□□□□動□□□□□□, 初期□□□□□□分布□□□□□□□□刻□□□□分布□□□□□□□□□□□□□□□□.

□□, □□Fokker-Planck方□□□対□□□Langevin方□□□, □□□□□□□□□□力学□□□□□□□□□. Langevin方□□□

$$
\begin{aligned}
\dot{x}(t) &= -\mu k_U(t)(x(t) - \mu_U(t)) + \sqrt{2\mu\beta}\cdot\xi(t), && (5.27)\\
\langle \xi(t)\rangle &= 0, && (5.28)\\
\langle \xi(t)\xi(t')\rangle &= \delta(t - t'), && (5.29)
\end{aligned}
$$

□□□□□□. □方□1□□□□□□□□□□□□□□□□□□□□(5.24)□

$$
\frac{d}{dt}\langle x\rangle_{P_X(t)} = -\mu k_U(t)(\langle x\rangle_{P_X(t)} - \mu_U(t)), \tag{5.30}
$$

□□□. □□1□□□□□□□□□□□□□力学□□Langevin方□□□体□平□□作□□□, □□□□□□$\langle \xi(t)\rangle = 0$□□□□□□□□□□対□□□□□.

5.1.3 キュムラントの固定点と安定性

□□, □□□□□□□□□□□□依存□□□□□, □□□□

$$U_X(x) = \frac{k_U}{2}(x-\mu_U)^2, \tag{5.31}$$

□□□□□□□□□□, □□□□□□$k_U > 0$□□□. □□□□, □□□□□□□□□□力学□□

$$\frac{d}{dt}c_n(t) = \mu k_U \mu_U \delta_{n1} + 2\mu\beta^{-1}\delta_{n2} - n\mu k_U c_n := f_n(\boldsymbol{c}(t)), \tag{5.32}$$

□□□□□□. □□力学□□□定□□□□□□□□.

□□□n□$f_n(\boldsymbol{c}^*) = 0$□□□□□定□$\boldsymbol{c}^*$□

$$c_1^* = \mu_U, \tag{5.33}$$
$$c_2^* = (\beta k_U)^{-1}, \tag{5.34}$$

□□$n \geq 3$□

$$c_n^* = 0, \tag{5.35}$$

□□□□□□□. □□□□□□□□□□□□定□□□□□□□□分布□平□μ_U, 分散$(\beta k_U)^{-1}$□□□□分布□□□□□□□□□□□□□, □□□□□□□□□定常分布□□□□□□□□□□□□分布

$$P_X^{\mathrm{ss}}(x) = \frac{1}{\sqrt{2\pi(\beta k_U)^{-1}}} \exp\left(-\beta\frac{k_U}{2}(x-\mu_U)^2\right) \propto \exp\left(-\beta U_X(x)\right) \tag{5.36}$$

□□□□□□□□□□□.

□□□平衡分布□□□□定□□□□, □□平行分布□□□□□□□安定□□□□□□, □□□□力学□□□則□□□係□既□□□□□, □□□□□□□□□□□□□□定□$\boldsymbol{c}^*$□□□□□□□安定□□□□□□□□□□□□□□□□□□□. $\delta c_n(t) = c_n(t) - c_n^*$□□□□□□□□□

$$\frac{d}{dt}\delta c_1(t) = -\mu k_U \delta c_1(t), \tag{5.37}$$
$$\frac{d}{dt}\delta c_2(t) = -2\mu k_U \delta c_2(t), \tag{5.38}$$
$$\tag{5.39}$$

□□$n \geq 3$□

$$\frac{d}{dt}\delta c_n(t) = -n\mu k_U \delta c_n(t), \tag{5.40}$$

□□□. $k_U > 0$, $\mu > 0$□□□□□□□定□□□□□□, □□□n□

$$\frac{d}{dt}|\delta c_n(t)| \leq 0, \tag{5.41}$$

□示□, □□□□□□□□定□$\boldsymbol{c}^*$□□□□□□□安定□□□.

5.2　レート方□式

5.2.1　化学反応とマスター方□式

□□, □□□□方□□□□□定□□□力学□□□□□□別□例□□□, □□□□□□学□□□□□□□学□□□度□□□□□□□□□□□□方□□□□□□□□□□□.

□□, □□□□□□学□□

$$\sum_{i=1}^{N}\nu_{i\rho}\mathrm{X}_i \underset{k_\rho^-}{\overset{k_\rho^+}{\rightleftharpoons}} \sum_{i=1}^{N}\kappa_{i\rho}\mathrm{X}_i, \tag{5.42}$$

□□□□. □□□, X_i□i□□□分子□□□, $i=1,...,N$□□□□□□□□□. □□ ρ□□□□□□□□□□字□□□, $\rho=1,...,M$□□□. □□$\nu_{i\rho}$, $\kappa_{i\rho}$□ρ□□□□□□□□□□□□数□表□□□□□, 非□□整数□□□□□学□□係数□□□□□. k_ρ^+, k_ρ^-□□□ρ□□□□□□□□□□□□□.

□□□□□□□□□□□体例□□□, □$\mathrm{H_2O}$□□□□□□□□□$\mathrm{CO_2}$□□□□□□□□□□□□□□□□□□.

$$2\mathrm{H}_2+\mathrm{O}_2 \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} 2\mathrm{H}_2\mathrm{O} \tag{5.43}$$

$$\mathrm{C}+\mathrm{O}_2 \underset{k_2^-}{\overset{k_2^+}{\rightleftharpoons}} \mathrm{CO}_2. \tag{5.44}$$

□□□□□, $\mathrm{X}_1=\mathrm{H}_2$, $\mathrm{X}_2=\mathrm{O}_2$, $\mathrm{X}_3=\mathrm{H_2O}$, $\mathrm{X}_4=\mathrm{C}$, $\mathrm{X}_5=\mathrm{CO}_2$□□□□, $\nu_{11}=2$, $\nu_{21}=1$, $\nu_{31}=\nu_{41}=\nu_{51}=0$, $\kappa_{31}=2$, $\kappa_{11}=\kappa_{21}=\kappa_{41}=\kappa_{51}=0$, $\nu_{22}=1$, $\nu_{42}=1$, $\nu_{12}=\nu_{32}=\nu_{52}=0$, $\kappa_{52}=1$, $\kappa_{12}=\kappa_{22}=\kappa_{32}=\kappa_{42}=0$□□学□□□表□□□□□□□□□.

分子X_i□□数□n_i□□, □□□□□□数□□□□□散□□$\boldsymbol{x}=(n_1,\cdots,n_N)^{\mathrm{T}}$□□□□□□分布□$p_{\boldsymbol{X}}(\boldsymbol{x};t)$□□□. □, □□□□$\rho$□□□□□□□□子□□□□$\mathsf{S}_{i\rho}=\kappa_{i\rho}-\nu_{i\rho}$□□, □□□□表□□□□ $\mathbf{S}_\rho=(\mathsf{S}_{1\rho},\cdots,\mathsf{S}_{N\rho})^{\mathrm{T}}$□□□□□□□□□方□□□

$$\begin{aligned}
&\frac{\partial}{\partial t}p_{\boldsymbol{X}}(\boldsymbol{x};t)\\
&=\sum_\rho[W^{+(\rho)}(\boldsymbol{x}|\boldsymbol{x}-\mathbf{S}_\rho)p_{\boldsymbol{X}}(\boldsymbol{x}-\mathbf{S}_\rho;t)+W^{-(\rho)}(\boldsymbol{x}|\boldsymbol{x}+\mathbf{S}_\rho)p_{\boldsymbol{X}}(\boldsymbol{x}+\mathbf{S}_\rho;t)]\\
&\quad-\sum_\rho[W^{+(\rho)}(\boldsymbol{x}+\mathbf{S}_\rho|\boldsymbol{x})+W^{-(\rho)}(\boldsymbol{x}-\mathbf{S}_\rho|\boldsymbol{x})]p_{\boldsymbol{X}}(\boldsymbol{x};t),
\end{aligned} \tag{5.45}$$

□□□□□□□□. □□□$W^{+(\rho)}(\boldsymbol{x}+\mathbf{S}_\rho|\boldsymbol{x})$□□□$\rho$□□方□□, □□$\boldsymbol{x}$□□□□$\boldsymbol{x}+\mathbf{S}_\rho$□移□□□□移□□□□□□, $W^{-(\rho)}(\boldsymbol{x}-\mathbf{S}_\rho|\boldsymbol{x})$□□□$\rho$□□方□□, □□$\boldsymbol{x}$□□□□$\boldsymbol{x}-\mathbf{S}_\rho$□移□□□□移□□□□□□. □□□移□□□□□□希薄□□□□□□, □□□□□□□子

□□□□体□Ω□□□□□□□□□□□□□□□□□□.

$$W^{+(\rho)}(\boldsymbol{x}|\boldsymbol{x}-\mathsf{S}_\rho) = k_\rho^+\Omega\prod_{i=1}^N\left(\frac{n_i-\mathsf{S}_{i\rho}}{\Omega}\right)^{\nu_{i\rho}}, \tag{5.46}$$

$$W^{+(\rho)}(\boldsymbol{x}+\mathsf{S}_\rho|\boldsymbol{x}) = k_\rho^+\Omega\prod_{i=1}^N\left(\frac{n_i}{\Omega}\right)^{\nu_{i\rho}}, \tag{5.47}$$

$$W^{-(\rho)}(\boldsymbol{x}|\boldsymbol{x}+\mathsf{S}_\rho) = k_\rho^-\Omega\prod_{i=1}^N\left(\frac{n_i+\mathsf{S}_{i\rho}}{\Omega}\right)^{\kappa_{i\rho}}, \tag{5.48}$$

$$W^{-(\rho)}(\boldsymbol{x}-\mathsf{S}_\rho|\boldsymbol{x}) = k_\rho^-\Omega\prod_{i=1}^N\left(\frac{n_i}{\Omega}\right)^{\kappa_{i\rho}}. \tag{5.49}$$

5.2.2 システムサイズ展□

希薄□□□□□□□□□□□□□□□□□□□子□□□□体□Ω□□分□□□□□□□□□. □子数n_i□□□□□□□□子□□□□体□Ω□割□□□, □□□□□度□□□$\tilde{x}_i = n_i/\Omega$□, □□ρ□□□□度□□□$\mathsf{S}_{i\rho}/\Omega$□□分$\Omega$□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□. □□□□□□度$\tilde{x}_i = n_i/\Omega$□□□□□□□□□□□□□□□, □□□□方□□□Kramers-Moyal□□□□□□□□□□□□□□□□□□□.

□□$\tilde{\boldsymbol{x}} = (\tilde{x}_1, \cdots, \tilde{x}_N)^{\mathrm{T}}$□□□□新□□□移□□□□□□□□□□□□□□□,

$$W^{+(\rho)}(\boldsymbol{x}|\boldsymbol{x}-\mathsf{S}_\rho) = \tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}-\mathsf{S}_\rho/\Omega), \tag{5.50}$$

$$W^{+(\rho)}(\boldsymbol{x}+\mathsf{S}_\rho|\boldsymbol{x}) = \tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}), \tag{5.51}$$

$$W^{-(\rho)}(\boldsymbol{x}|\boldsymbol{x}+\mathsf{S}_\rho) = \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}}+\mathsf{S}_\rho/\Omega), \tag{5.52}$$

$$W^{-(\rho)}(\boldsymbol{x}-\mathsf{S}_\rho|\boldsymbol{x}) = \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}}), \tag{5.53}$$

□□□. □□□, $\tilde{\boldsymbol{x}}$□□□□□□分布□□□

$$p_{\boldsymbol{X}}(\boldsymbol{x};t) = \frac{1}{\Omega^N}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t) \tag{5.54}$$

□□□□□□. □□□□□分布$p_{\boldsymbol{X}}(\boldsymbol{x};t)$□□□□$\sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x};t) = 1$□□

$$\sum_{\boldsymbol{x}} P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\Omega^{-N} = 1, \tag{5.55}$$

□□□□. □□□Ω□□分□□□□□□□Ω^{-N}□$d\tilde{\boldsymbol{x}}$, $\sum_{\boldsymbol{x}}$ □$\int$□□□□□□□□□□, □(5.55)□□□□□$\tilde{\boldsymbol{x}}$□□□□□□分布$P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)$□□□□

$$\int d\tilde{\boldsymbol{x}} P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t) = 1, \tag{5.56}$$

□□□□□□□□□□□□□.

□□□□, □□□□方□□□□□□□□□□□□□□□□□□□.

$$\begin{aligned}
&\frac{\partial}{\partial t}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t) \\
&= \sum_\rho[\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}-\mathsf{S}_\rho/\Omega)P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}}-\mathsf{S}_\rho/\Omega;t) + \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}}+\mathsf{S}_\rho/\Omega)P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}}+\mathsf{S}_\rho/\Omega;t)] \\
&\quad -\sum_\rho[\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}) + \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})]P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t),
\end{aligned} \tag{5.57}$$

□□□S_ρ/Ω□□□□□□□□□Taylor□□

$$\begin{aligned}
&\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}-\mathsf{S}_\rho/\Omega)P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}}-\mathsf{S}_\rho/\Omega;t)-\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\\
&=\sum_{k=1}^{\infty}\sum_{m_1,\cdots,m_N|\sum_i m_i=k}\left[\prod_{i=1}^{N}\frac{1}{m_i!}\left(-\frac{\mathsf{S}_{i\rho}}{\Omega}\right)^{m_i}(\partial_{\tilde{x}_i})^{m_i}\right][\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)],
\end{aligned}\tag{5.58}$$

$$\begin{aligned}
&\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}}+\mathsf{S}_\rho/\Omega)P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}}+\mathsf{S}_\rho/\Omega;t)-\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\\
&=\sum_{k=1}^{\infty}\sum_{m_1,\cdots,m_N|\sum_i m_i=k}\left[\prod_{i=1}^{N}\frac{1}{m_i!}\left(\frac{\mathsf{S}_{i\rho}}{\Omega}\right)^{m_i}(\partial_{\tilde{x}_i})^{m_i}\right][\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)],
\end{aligned}\tag{5.59}$$

□行□□, □□□□方□□□□□□□

$$\begin{aligned}
&\frac{\partial}{\partial t}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\\
&=\sum_\rho\sum_{k=1}^{\infty}\sum_{m_1,\cdots,m_N|\sum_i m_i=k}\left[\prod_{i=1}^{N}\frac{1}{m_i!}\left(-\frac{\mathsf{S}_{i\rho}}{\Omega}\right)^{m_i}(\partial_{\tilde{x}_i})^{m_i}\right][\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)]\\
&+\sum_\rho\sum_{k=1}^{\infty}\sum_{m_1,\cdots,m_N|\sum_i m_i=k}\left[\prod_{i=1}^{N}\frac{1}{m_i!}\left(\frac{\mathsf{S}_{i\rho}}{\Omega}\right)^{m_i}(\partial_{\tilde{x}_i})^{m_i}\right][\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)],
\end{aligned}\tag{5.60}$$

□□□分方□□□□□□□□. □□□□□□□□□□□□子□□□□体□Ω□□□□□□□□□□□□□□□□□□□□□□□□方□□□□□□□□□□□□□□. □, Ω□□分□□□□□□, $1/\Omega$□最低□□□□□似□□□,

$$\begin{aligned}
\frac{\partial}{\partial t}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)&=\sum_\rho\sum_i\left[\left(-\frac{\mathsf{S}_{i\rho}}{\Omega}\right)(\partial_{\tilde{x}_i})\right][\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)]\\
&\quad+\sum_\rho\sum_i\left[\left(\frac{\mathsf{S}_{i\rho}}{\Omega}\right)(\partial_{\tilde{x}_i})\right][\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)]\\
&=-\sum_\rho\sum_i\partial_{\tilde{x}_i}\left[\mathsf{S}_{i\rho}\frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})-\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\right],
\end{aligned}\tag{5.61}$$

□□□□□. □□, $(1/\Omega)^2$□寄□□□□□□□,

$$\begin{aligned}
\frac{\partial}{\partial t}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)&=-\sum_\rho\sum_i\partial_{\tilde{x}_i}\left[\mathsf{S}_{i\rho}\frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})-\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\right]\\
&+\frac{1}{2}\sum_\rho\sum_{i,j}(\partial_{\tilde{x}_i})(\partial_{\tilde{x}_j})\left[\mathsf{S}_{i\rho}\mathsf{S}_{j\rho}\frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})+\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega^2}P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)\right],
\end{aligned}\tag{5.62}$$

□□□□□. □□□□chemical Fokker-Planck方□□□□□□, 対□□□Langevin方□□□chemical Langevin方□□□□□□□□□□□□.

5.2.3 レート方□式

Fokker-Planck方□□□□Langevin方□□□□対□□□作□□□□□□□□□□□□□□□□□, $\tilde{x}_i$□□□□□□□□□□□□□□□□□□□□□. chemical Fokker-Planck方□□(5.62)□対□□□chemical Langevin方□□□□□□□□□□□. □□□□分散□□□□□□□□希薄□□□□移□□□□対□□□

$$\mathsf{S}_{i\rho}\mathsf{S}_{j\rho}\frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}})+\tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega^2}=O(1/\Omega)\tag{5.63}$$

□□□□□□□chemical Langevin方□□□□□□□□□Gaussian□□□□□分散□□(5.63)□□例□□□□□□□□□□□，□(5.62)□対□□□chemical Langevin方□□□

$$\frac{d\tilde{x}_i}{dt} = \sum_\rho \mathsf{S}_{i\rho} \frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}) - \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega} + O(1/\Omega)\cdot\xi_i, \tag{5.64}$$

□□□□$O(1/\Omega)$□□□□□□□□□□$O(1/\Omega)\cdot\xi_i$□□□Langevin方□□□□□．□$\Omega\to\infty$□□□□□，□□□□□$O(1/\Omega)\cdot\xi_i$□0□□□□□□□□□□□□□□□□□，$\Omega\to\infty$□□□□□□□□寄□□

$$\frac{d\tilde{x}_i}{dt} = \sum_\rho \mathsf{S}_{i\rho} \frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}) - \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega}, \tag{5.65}$$

□□□□定□□□常□分方□□□□□□□．□□常□分方□□□□(5.61)□Liouville方□□□□□□□□□□□□，□□Liouville方□□□対□□□常□分方□□□□□□□□．□□□□□希薄□□□□移□□□□□□□□□，

$$\frac{d\tilde{x}_i}{dt} = \sum_\rho \mathsf{S}_{i\rho} \left[k_\rho^+ \prod_{i=1}^N (\tilde{x}_i)^{\nu_{i\rho}} - k_\rho^- \prod_{i=1}^N (\tilde{x}_i)^{\kappa_{i\rho}} \right], \tag{5.66}$$

□□□□□．□□□□□□□方□□□□□□□□□，□□希薄□□□□学□□□□度□□□□□□□□□□□□□□□．□□□□□方□□□，非□□□常□分方□□□□□．□□□□□□□□□方□□□□□□力学□□□□□□，□似□行□□□□□□□非□□□力学□□□□□□□□□□．

□□，$1/\Omega$□最低□□□似□□前□□□□□方□□(5.60)□対□□，1□□□□□□□□□期□□$\langle\tilde{x}_i\rangle_{P_{\tilde{\boldsymbol{X}}}}$□□□□□□□□□□□□□

$$\begin{aligned}
\frac{d\langle\tilde{x}_i\rangle_{P_{\tilde{\boldsymbol{X}}}}}{dt} &= \int d\tilde{\boldsymbol{x}}\tilde{x}_i \frac{\partial}{\partial t} P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t) \\
&= \sum_\rho \int d\tilde{\boldsymbol{x}}(\partial_{\tilde{x}_i}\tilde{x}_i) \left[\mathsf{S}_{i\rho} \frac{\tilde{w}^{+(\rho)}(\tilde{\boldsymbol{x}}) - \tilde{w}^{-(\rho)}(\tilde{\boldsymbol{x}})}{\Omega} P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t) \right] && (5.67) \\
&= \sum_\rho \mathsf{S}_{i\rho} \left[k_\rho^+ \langle \prod_{i=1}^N \tilde{x}_i^{\nu_{i\rho}} \rangle_{P_{\tilde{\boldsymbol{X}}}} - k_\rho^- \langle \prod_{i=1}^N \tilde{x}_i^{\kappa_{i\rho}} \rangle_{P_{\tilde{\boldsymbol{X}}}} \right], && (5.68)
\end{aligned}$$

□□□□□□．□□□，$P_{\tilde{\boldsymbol{X}}}(\tilde{\boldsymbol{x}};t)$□□□□□寄□□0□□□□□□□定□□□□□分□分□行□，□□□分□分□□□□2□□□□□□分□□□□□□□1/Ω□□□□□□寄□□□□□□□□□□□□□□．□□□□□□□□□□□□，□密□□□□□□1□□□□□□$\langle\tilde{x}_i\rangle_{P_{\tilde{\boldsymbol{X}}}}$□□□□□□□□□□□□□□□□□□$\langle\prod_{i=1}^N \tilde{x}_i^{\nu_{i\rho}}\rangle_{P_{\tilde{\boldsymbol{X}}}}$□$\langle\prod_{i=1}^N \tilde{x}_i^{\kappa_{i\rho}}\rangle_{P_{\tilde{\boldsymbol{X}}}}$□□□□常□分方□□□□□□□□□□□□□□□．□□常□分方□□□□1□□□□□□□□□□□□□□□□□□□□□□□，□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□．

最□□□□□方□□□，□□□1□□□□□□□□□□□□□□□□□□□□□□．□□□□□□□□□□□□対□□

$$\langle \prod_{i=1}^N \tilde{x}_i^{k_i} \rangle_{P_{\tilde{\boldsymbol{X}}}} \simeq \prod_{i=1}^N (\langle\tilde{x}_i\rangle_{P_{\tilde{\boldsymbol{X}}}})^{k_i} \tag{5.69}$$

□□□□似□行□□□□□□□□□, □(5.68)□□□□方□□(5.66)□□□□□□□□□. □□□□□□□方□□□□度□期□□$\langle \tilde{x}_i \rangle_{P_{\tilde{\boldsymbol{x}}}}$□□□□□□□□□□□□□□, □□□□□□□□□1□□□□□□□□□□□似□□表□□□□□□□□□□□□□.

5.3 化学熱力学と平□状態の安定性

5.3.1 平□状態とエントロピー□成□

□□□□□力学□□□□□□□□□□方□□□□□□□□□学□□□□□□□□□, □□□方□□□□□□□力学, □□□□□学□力学□□□□□□□.□□□, □□□方□□□

$$\frac{d\tilde{x}_i}{dt} = \sum_\rho \mathsf{S}_{i\rho} \left[J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}) \right], \tag{5.70}$$

$$J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) = k_\rho^+ \prod_{i=1}^N (\tilde{x}_i)^{\nu_{i\rho}}, \tag{5.71}$$

$$J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}) = k_\rho^- \prod_{i=1}^N (\tilde{x}_i)^{\kappa_{i\rho}}, \tag{5.72}$$

□□□□表□□□□□□□. □□□□□□力学□□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}}$□,

$$\sum_\rho \mathsf{S}_{i\rho} \left[J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}^{\mathrm{ss}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}^{\mathrm{ss}}) \right] = 0, \tag{5.73}$$

□, □□□i□□□□□□□□□. □□□非□□方□□□□□, □定□□□□□□□数存□□□.

□□, □定□□□□□□□□ρ□対□□

$$J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}^{\mathrm{ss}}) = J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}^{\mathrm{ss}}), \tag{5.74}$$

□□□□□$\tilde{\boldsymbol{x}}^{\mathrm{ss}} = \tilde{\boldsymbol{x}}^{\mathrm{eq}}$□□□□□□. □□□$\tilde{\boldsymbol{x}}^{\mathrm{eq}}$□平衡□□□□□度□□□□. □□□□□□□□方□□□□□□□□□条□□□□□□□□□□□□□□□□. □□, □体□□$J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}^{\mathrm{eq}})$□$J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}^{\mathrm{eq}})$□□□□□□, □(5.74)□

$$\prod_{i=1}^N (\tilde{x}_i^{\mathrm{eq}})^{\mathsf{S}_{i\rho}} = \frac{k_\rho^+}{k_\rho^-}, \tag{5.75}$$

□□□□□□□. □□□□, 平衡□□□□度□□□□□□定数k_ρ^+/k_ρ^-□□□□□□□□□□□□□□□□□, □□作□□□則□□□□□□□.

□□□□方□□□□□□□□□□□□□□, □□□方□□□□□□□平衡□□□0□□□□□力学□□□□$J_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}})$□□力学□□力$F_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}})$□

$$J_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) = J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}), \tag{5.76}$$

$$F_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) = \ln \frac{J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}})}{J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}})}, \tag{5.77}$$

□定□□□□. 定□□□$J_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}})$□$F_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}})$□□□□□□□, □$J_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}^{\mathrm{eq}}) = F_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}^{\mathrm{eq}}) = 0$□□□.

□□□□□□方□□□□□□□□学□□□□□□□□□□□□□□□$\sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}})$□

$$\sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) = \sum_\rho J_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) F_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}), \tag{5.78}$$

□定□□□. □□□□非□

$$\sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) \geq 0, \tag{5.79}$$

□□□□□□□力学□□□則□□□□□. □□, $\sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) = 0$□□□□□□□作□□□則□□□□平衡□□$\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^{\mathrm{eq}}$□□□□□□□□□.

5.3.2 Kullback-Leiblerダイバージェンスの一般化とエントロピー□成□

□□□学□力学□□□□□□□□□□□□□□□, 平衡□□$\tilde{\boldsymbol{x}}^{\mathrm{eq}}$□存□□□定□□□□□, □□□□Lyapunov□数□□□□□□表□□□□□□□□□□□□□□□.

□□□□□□□□Kullback-Leibler□□□□□□□□□□□$D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{y}})$□□□□□□.

$$D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{y}}) = \sum_i \left(\tilde{x}_i \ln \frac{\tilde{x}_i}{\tilde{y}_i} + \tilde{y}_i - \tilde{x}_i \right) \tag{5.80}$$

$$= \sum_i \tilde{x}_i f\left(\frac{\tilde{y}_i}{\tilde{x}_i}\right). \tag{5.81}$$

$$f(x) = x - \ln x - 1. \tag{5.82}$$

□□□$f(x)$□□□□□□数□□□, $f(1) = 0$□□□□□□□□□□□□数□□(5.81)□□□□□□□□□f-□□□□□□□□□□□□□□□□, □□□□□□□□$\partial_x f(x)|_{x=1} = 0$□ $(\partial_x)^2 f(x)\big|_{x=1} = 1$□□□□□□□□□□□数□□数$f(x)$□□□□□□□□□$f$-□□□□□□□□□□□□□□□. □□□□□$\tilde{x}_i$□$\tilde{y}_i$□□□分布□□□□$\sum_i \tilde{x}_i = \sum_i \tilde{y}_i = 1$□□□□□□□$D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{y}}) = D_{\mathrm{KL}}(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{y}})$□Kullback-Leibler□□□□□□□□□□□□□.

□□□□□□有□□□□, □□分布□□□□$\sum_i \tilde{x}_i = \sum_i \tilde{y}_i = 1$□□□□□□□□□□, □□□$\tilde{x}_i \geq 0$, $\tilde{y}_i \geq 0$□□□□ Kullback-Leibler□□□□□□□□□□□□□□非□□

$$D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{y}}) \geq 0, \tag{5.83}$$

□□□□□条□

$$D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{y}}) = 0 \Leftrightarrow \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{y}}, \tag{5.84}$$

□□□□□□□□□□□□□□. □□□示□□□$x \geq 0$□

$$f(x) \geq 0, \tag{5.85}$$

$$f(x) = 0, \Leftrightarrow x = 1, \tag{5.86}$$

□□□□□□□□□□□□□□□□□□.□実□, $f(1) = 0, \partial_x f(x) = 1 - 1/x$, $\partial_x f(x)|_{x=1} = 0$, $(\partial_x)^2 f(x) = 1/(x^2) > 0$□□□□□□□□□□□□□□□□□.

実□□□Kullback-Leibler□□□□□□□□□□□□□□□□□, □□□□□力学□□□□□□□

$$\sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) = -\frac{d}{dt} D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}}), \tag{5.87}$$

□示□□□□□□□. 実□, $d\tilde{x}_i^{\mathrm{eq}}/dt = 0$□, □□作□□□則□□□□(5.75)□□□□□□□□□,

$$
\begin{aligned}
-\frac{d}{dt}D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}}) &= -\sum_i \left(\frac{d\tilde{x}_i}{dt} \ln \frac{\tilde{x}_i}{\tilde{x}_i^{\mathrm{eq}}} + \frac{d\tilde{x}_i}{dt} - \frac{d\tilde{x}_i}{dt} \right) \\
&= -\sum_\rho \sum_i \mathsf{S}_{i\rho} \left[J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}) \right] \ln \frac{\tilde{x}_i}{\tilde{x}_i^{\mathrm{eq}}} \\
&= \sum_\rho \left[J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}) \right] \ln \left[\prod_i \left(\frac{\tilde{x}_i}{\tilde{x}_i^{\mathrm{eq}}} \right)^{-\mathsf{S}_{i\rho}} \right] \\
&= \sum_\rho \left[J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}) \right] \ln \left[\prod_i \frac{k_\rho^+}{k_\rho^-} \frac{(\tilde{x}_i)^{\nu_{i\rho}}}{(\tilde{x}_i)^{\kappa_{i\rho}}} \right] \\
&= \sum_\rho \left[J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}}) - J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}}) \right] \ln \frac{J_\rho^{\mathrm{chem}+}(\tilde{\boldsymbol{x}})}{J_\rho^{\mathrm{chem}-}(\tilde{\boldsymbol{x}})} \\
&= \sum_\rho J_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) F_\rho^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) \\
&= \sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}}),
\end{aligned} \tag{5.88}
$$

□□□□□□□□□□.

□□□平衡□□$\tilde{\boldsymbol{x}}^{\mathrm{eq}}$□□□□定□□□□□, □力学□□□則$\sigma^{\mathrm{chem}}(\tilde{\boldsymbol{x}}) \geq 0$□□

$$
\frac{d}{dt}D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}}) \leq 0, \tag{5.89}
$$

□□, □□□□□□条□□□

$$
\frac{d}{dt}D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}}) = 0 \Leftrightarrow \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^{\mathrm{eq}}, \tag{5.90}
$$

□□□□□. □□□□(5.83), (5.84)□□

$$
D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}}) \geq 0, \tag{5.91}
$$
$$
D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}}) = 0 \Leftrightarrow \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^{\mathrm{eq}}, \tag{5.92}
$$

□□□□□, $D_f(\tilde{\boldsymbol{x}}||\tilde{\boldsymbol{x}}^{\mathrm{eq}})$□Lyapunov□数□□□□□□. □□Lyapunov□数□存□□□, □定□□□□□平衡□□$\tilde{\boldsymbol{x}}^{\mathrm{eq}}$□□□□□□□安定□□□□□□□□□□□□.

5.4 □□形性と不安定な固定点

5.4.1 レート方□式における不安定な固定点の例

□□□方□□□□□数□定□□存□□□□. □□□□□□定□□□□, □□作□□□則□□□□□□□□□平衡□□□□□□定□□□□□□□□□□□□□□□. □□□定□□□□□□安定□□□□□□□□□. □□□体例□□□, □□□□□□□□□□□□□□□□□□□.

$$
\mathrm{X}_1 + \mathrm{X}_2 \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} 2\mathrm{X}_1. \tag{5.93}
$$

□□□□, □□□方□□□

$$\frac{d\tilde{x}_1}{dt} = k_1^+\tilde{x}_1\tilde{x}_2 - k_1^-(\tilde{x}_1)^2, \tag{5.94}$$

$$\frac{d\tilde{x}_2}{dt} = -k_1^+\tilde{x}_1\tilde{x}_2 + k_1^-(\tilde{x}_1)^2, \tag{5.95}$$

□□□□□□. □□□□,

$$\frac{d}{dt}(\tilde{x}_1 + \tilde{x}_2) = 0, \tag{5.96}$$

□□保存□□□□

$$\tilde{x}_1 + \tilde{x}_2 = \tilde{x}_{\mathrm{tot}}, \tag{5.97}$$

□□□□□□. □□□$\tilde{x}_{\mathrm{tot}} > 0$□□□□□□□定□□□□□. □□□□□定□□□□□

$$\tilde{\boldsymbol{x}}^{\mathrm{ss}} = \begin{pmatrix} \tilde{x}_1^{\mathrm{ss}} \\ \tilde{x}_2^{\mathrm{ss}} \end{pmatrix} = \begin{pmatrix} \frac{k_1^+}{k_1^+ + k_1^-}\tilde{x}_{\mathrm{tot}} \\ \frac{k_1^-}{k_1^+ + k_1^-}\tilde{x}_{\mathrm{tot}} \end{pmatrix}, \tag{5.98}$$

□

$$\tilde{\boldsymbol{x}}^{\mathrm{ss}*} = \begin{pmatrix} \tilde{x}_1^{\mathrm{ss}*} \\ \tilde{x}_2^{\mathrm{ss}*} \end{pmatrix} = \begin{pmatrix} 0 \\ \tilde{x}_{\mathrm{tot}} \end{pmatrix}, \tag{5.99}$$

□□□□□□□□□□. □□□最初□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}}$□□□□□,

$$\frac{\tilde{x}_1^{\mathrm{ss}}}{\tilde{x}_2^{\mathrm{ss}}} = \frac{k_1^+}{k_1^-}, \tag{5.100}$$

□□□作□□□則□□□□□□, 平衡□□□□□. □方□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}*}$□□□作□□□則□□□□□□.

□□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}*}$□安定□□□□□□□□□□□□□□. □□□□, $\delta\tilde{\boldsymbol{x}}^* = \tilde{\boldsymbol{x}} - \tilde{\boldsymbol{x}}^{\mathrm{ss}*}$□□□□□□□□□□□□,

$$\frac{d\delta\tilde{x}_1^*}{dt} = -\frac{d\delta\tilde{x}_2^*}{dt} = k_1^+\delta\tilde{x}_1^*(\tilde{x}_{\mathrm{tot}} - \delta\tilde{x}_1^*) - k_1^-(\delta\tilde{x}_1^*)^2, \tag{5.101}$$

□□, □□□□□□$\epsilon > 0$□$\delta\tilde{x}_1^* = \epsilon$□□□□□□□□, $d|\delta\tilde{x}_1^*|/dt = k_1^+\tilde{x}_{\mathrm{tot}}\epsilon + O(\epsilon^2) > 0$□□□, □定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}*}$□安定□□□□□□□□□.

□□□平衡□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}}$□安定□□□□□□□□□□□□□□. □□□□, $\delta\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}} - \tilde{\boldsymbol{x}}^{\mathrm{ss}}$□□□□□□□□□□□□,

$$\begin{aligned} \frac{d\delta\tilde{x}_1}{dt} = -\frac{d\delta\tilde{x}_2}{dt} &= k_1^+\tilde{x}_1(\tilde{x}_2^{\mathrm{ss}} - \delta\tilde{x}_1) - k_1^-(\delta\tilde{x}_1 + \tilde{x}_1^{\mathrm{ss}})\tilde{x}_1 \\ &= -(k_1^+ + k_1^-)(\delta\tilde{x}_1)\tilde{x}_1 \\ &= (k_1^+ + k_1^-)(\delta\tilde{x}_2)\tilde{x}_1 \end{aligned} \tag{5.102}$$

□□□□□, $\tilde{x}_1 \geq 0$□□$d|\delta\tilde{x}_1|/dt < 0$, $d|\delta\tilde{x}_2|/dt < 0$□示□□□□, 平衡□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}}$□□□□□安定□□□□□□示□□.

5.4.2　□形安定性□析

力学□

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(\boldsymbol{y}). \tag{5.103}$$

□□□□$\boldsymbol{f}(\boldsymbol{y}^*) = \boldsymbol{0}$□□□□定□$\boldsymbol{y}^*$□□安定□□□□□□□□□□□□□□，□□□□安定□□□□□□□□□□□□□．□□□，□□□$\delta\boldsymbol{y} = \boldsymbol{y} - \boldsymbol{y}^*$□□□，1□□□□Taylor□□

$$\frac{d\delta\boldsymbol{y}}{dt} = \mathsf{J}(\boldsymbol{y}^*)\delta\boldsymbol{y} + O(|\delta\boldsymbol{y}|^2), \tag{5.104}$$

$$\mathsf{J}_{ij}(\boldsymbol{y}^*) = \partial_{y_j} f_i(\boldsymbol{y})\big|_{\boldsymbol{y}=\boldsymbol{y}^*} \tag{5.105}$$

□□□□□□，□□□行列$\mathsf{J}(\boldsymbol{y}^*)$□□有□□実□□□□□□□□□$\delta\boldsymbol{y}$□□□□□□□□□定□$\boldsymbol{y}^*$□□□□□□□安定□□□，□□□□$t \to \infty$□$\delta\boldsymbol{y} \to \boldsymbol{0}$□□□□□□□．□□□□□行列$\mathsf{J}(\boldsymbol{y}^*)$□□有□□□□□□□□□□，$t \to \infty$□□定□$\boldsymbol{y}^*$□□□□□□□□，□定□$\boldsymbol{y}^*$□□安定□□□．□□□□□□定□□□□□□□□行列□□□□定□□安定□□□□□□□方□□□安定□□析□□□．

実□□□□□□□□□□□□□例□□□安定□□析□行□□□□□．□□□□□□□□□□方□□□保存則$\tilde{x}_{\mathrm{tot}} = \tilde{x}_1 + \tilde{x}_2$□□□□□□□□□常□分方□□

$$\frac{d\tilde{x}_1}{dt} = k_1^+ \tilde{x}_1(\tilde{x}_{\mathrm{tot}} - \tilde{x}_1) - k_1^-(\tilde{x}_1)^2 := f_1(\tilde{x}_1), \tag{5.106}$$

□□□□□□□□，

$$\mathsf{J}_{11}(\tilde{x}_1) = k_1^+ \tilde{x}_{\mathrm{tot}} - 2(k_1^+ + k_1^-)\tilde{x}_1, \tag{5.107}$$

□□，$\mathsf{J}(\tilde{x}_1)$□1×1行列□□□□□□□□有□□$\mathsf{J}_{11}(\tilde{x}_1)$□□□□□□□□□，□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}}$，$\tilde{\boldsymbol{x}}^{\mathrm{ss*}}$□□□□□□□□□

$$\mathsf{J}_{11}(\tilde{x}_1^{\mathrm{ss}}) = -k_1^+ \tilde{x}_{\mathrm{tot}} < 0, \tag{5.108}$$

$$\mathsf{J}_{11}(\tilde{x}_1^{\mathrm{ss*}}) = k_1^+ \tilde{x}_{\mathrm{tot}} > 0, \tag{5.109}$$

□□□．□□□□□□□平衡□□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss}}$□□□□□安定□□□□□対□□，□定□$\tilde{\boldsymbol{x}}^{\mathrm{ss*}}$□安定□□□□□□示□□．

5.5　□□型性と分岐

5.5.1　分岐と標準形

□□□□□学□□□□□□非□□□□□定□□安定□□□□□□□□行□□□□□．□□□□□□□□方□□□□□分布□対□□力学□□□□□□□□□□□，□度□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□方□□□□□□非□□□□力学□□□□□□□□□□□，□安定□□定□□□□□□□□□□□□．□□□□□方□□□□□□□平衡□□□□□安定□□定□□存□□□□□□，例□□□□□□□□□□□□□□□□□□□□学□□□□□□□□□□□□□□□□□□□□□□□，非□□□□力学□□□□□□□□□，平衡□□□□□安定□□定□□□□□□□．□□□□□□定□□□□□定□□□□□□□□□□

□□□分□□□□□□□□□□□□□□. □□分□□□□□□□□, □□□□□□□□□□Strogatz□教科□ [9]□□□□□□□□□.

□□□□□□□□□□□□□□□□□□□□□$\boldsymbol{\lambda}$□依存□□力学□

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}_{\boldsymbol{\lambda}}(\boldsymbol{y}). \tag{5.110}$$

□□□□

$$\boldsymbol{f}_{\boldsymbol{\lambda}}(\boldsymbol{y}^*) = 0 \tag{5.111}$$

□□□□□定□$\boldsymbol{y}^*$□, □□□□□□□□□□□□□$\boldsymbol{\lambda}$□依存□□□. □□□□□□□□□$\boldsymbol{\lambda}$□□□□□□□□, □定□□定□□□□□□□□□□□□□□分□□□□. □□□□□□□枠□□□分□□□□□□□□□□□.

□□□□□□安定□□□□□□□□□, □定□$\boldsymbol{y}^*$□□□□□□□□□□□□□□□□□□□□□. □□□□□□□□□安定□□□□□□□□□□□□□□□□□分□□□□□□. □定□□□□□□□□□□□□座□□□□□□□□□□□□□□□□□□□□□□□□□□, □□□寄□$O(|\boldsymbol{y}|^n)$□□□□□□□□, 力学□□□□□□□□□□□□□□□□□分□□□□□分□□□□□□□□□□. □□□□□分□□□□常□分方□□□□□□□□□□□□□□.

例□□, 実数□□□1□□□□□($y_1 = x \in \mathsf{R}$)□□, 実数□□□□□□□数□1□($\lambda_1 = \lambda \in \mathsf{R}$)□□□□, □□□□□□□□□□□□察□□□

$$\frac{dx}{dt} = \lambda - x^2 + O(x^3), \tag{5.112}$$
$$\frac{dx}{dt} = \lambda x - x^2 + O(x^3), \tag{5.113}$$
$$\frac{dx}{dt} = \lambda x - x^3 + O(x^4). \tag{5.114}$$

□□

$$\frac{dx}{dt} = \lambda + x^2 + O(x^3), \tag{5.115}$$
$$\frac{dx}{dt} = \lambda x + x^2 + O(x^3), \tag{5.116}$$
$$\frac{dx}{dt} = \lambda x + x^3 + O(x^4). \tag{5.117}$$

□□□□□□□□□□□□□□□□□□□□□□□□□□察□□□. □□, □□□□散□□□□□□例□□

$$\frac{dx}{dt} = \lambda x + x^3 - x^5 + O(x^6). \tag{5.118}$$

□□□□□□□□□□□□□□□□□□□□□□□.

□□2□□($y_1 = x \in \mathsf{R}, y_2 = y \in \mathsf{R}$)□□□□, □□数表□$z = x + iy$□□□□

$$\frac{dz}{dt} = (\lambda + i)z - z|z|^2 + O(|z|^4), \tag{5.119}$$

□□□□

$$\frac{dz}{dt} = (\lambda + i)z + z|z|^2 + O(|z|^4), \tag{5.120}$$

□□□□□□□□□□□□□□□.□□□□□□□□□□□□力学□□□示□□□□□,

$$\frac{dx}{dt} = \lambda x - y - x(x^2 + y^2) + O(|\boldsymbol{y}|^4), \tag{5.121}$$
$$\frac{dy}{dt} = \lambda y + x - y(x^2 + y^2) + O(|\boldsymbol{y}|^4), \tag{5.122}$$

□□□□

$$\frac{dx}{dt} = \lambda x - y + x(x^2 + y^2) + O(|\boldsymbol{y}|^4), \tag{5.123}$$
$$\frac{dy}{dt} = \lambda y + x + y(x^2 + y^2) + O(|\boldsymbol{y}|^4), \tag{5.124}$$

□□□.

□□□□□□□□□□□,□数□□□定□□□□□□□□□□λ□□□□□□□□□□□□□□□□□□□□□□□□□□□,□□余□□1□□□□分□□□□□□□□□□.□□□余□□□□□□□□□□□□□□□□□□□□.□□余□□1□□□□分□□□□□□□,□□□□□□□□□□□□□□□□□□□□□.

5.5.2　サドルノード分岐

□□□□□□分□□□□□□

$$\frac{dx}{dt} = \lambda - x^2 + O(x^3), \tag{5.125}$$

□□□□

$$\frac{dx}{dt} = \lambda + x^2 + O(x^3), \tag{5.126}$$

□□□□□□.

□□□$O(x^3)$□□□□□

$$\frac{dx}{dt} = \lambda - x^2 := f_\lambda(x), \tag{5.127}$$

□□□□□□□□□.□□□□□□□□□$f_\lambda(x^{(i)*}) = 0$□□□□□定□$x^{(i)*}$□□□□□□λ□条□□分□□□.$\lambda > 0$□□□□定□□2□存□□,$x^{(1)*} = \sqrt{\lambda}$□$x^{(2)*} = -\sqrt{\lambda}$□□□□□□.□□$\lambda = 0$□□□□定□□1□□□□$x^{(1)*} = 0$,□□$\lambda < 0$□□□$f_\lambda(x^{(i)*}) = 0$□実数□□□□□,□定□□存□□□□.□□安定□□,

$$\mathsf{J}_{11}(x) = \partial_x f_\lambda(x) = -2x, \tag{5.128}$$

□□,$\lambda > 0$□□$\mathsf{J}_{11}(x^{(1)*}) < 0$□□□定□$x^{(1)*}$□安定,$\mathsf{J}_{11}(x^{(2)*}) > 0$□□□定□$x^{(2)*}$□□安定□□□.□□ $\lambda = 0$□□□□,$\mathsf{J}_{11}(x^{(1)*}) = 0$□□□,□$x$□□□□□□定□□□□□□$x$□□□□□□定□□□□□□□□□□□□□□□□□定□$x^{(1)*}$□安定□□□安定□□□.

□□□□□λ□□□□□□□□□□□□□□□□□□□□□□□,□定□□存□□□□□□□□□□□安定□□定□□□□□□□□,□□□定□□□□□安定□□定□□□安定□□定□□分□□□.□□安定□□定□□□□□,□安定□□定□□□□□□□□□□,□□□□□分□□□□□□□□分□□□□.□□□定□□□□□□□□□□□□□□定□□□□□□□□□□青□□霹靂□□□□□□,□□□□□□分□□□□□□□□□分□□□□□□□□□□□.

□□□□□□□□□□□□□□

$$\frac{dx}{dt} = \lambda + x^2 := f_\lambda(x), \tag{5.129}$$

□□□□□, □□□□□□□□□分□□□□□□($O(x^3)$□□□□□□□). □□□, $f_\lambda(x^{(i)*}) = 0$□□□□□定□$x^{(i)*}$□□□□□, $\lambda < 0$□□□2□存□□, $x^{(1)*} = \sqrt{-\lambda}$□□安定□□定□□□□, $x^{(2)*} = -\sqrt{-\lambda}$□安定□□定□□□□. □□$\lambda = 0$□□□□定□□1□□□□$x^{(1)*} = 0$□□□, x□□□□□□定□□□□□□x□□□□□□定□□□□□□□□□安定□□□. □□$\lambda > 0$□□□□定□□□□□□.

□□分□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□. □□□,

$$\frac{dx}{dt} = -\partial_x U(x), \tag{5.130}$$

□□□□□□□□□□□$U(x)$□□□□□□□□□, □(5.127)□□□□□□□分□□□□□□

$$U(x) = \frac{1}{3}x^3 - \lambda x + \text{const.}, \tag{5.131}$$

□(5.129)□□□□□□□分□□□□□□

$$U(x) = -\frac{1}{3}x^3 - \lambda x + \text{const.}, \tag{5.132}$$

□表□□□□. □□□, □定□$x^{(i)*}$□$\partial_x U(x^{(i)*}) = 0$□□□□□□□□□□□□□□□□, 安定□□定□□$(\partial_x)^2 U(x^{(i)*}) > 0$□□□□□□□□□□□□□□□□□□□□□□, □安定□□定□□$(\partial_x)^2 U(x^{(i)*}) < 0$□□□□□□□□□□□□□□□□□□□□□□□□□□. 例□□□(5.131)□□□□□□□□□□□□□□□□□分□□□□, □□□□□λ□□□□□□□□□□□□□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□□□□, □□□□□□□□子□□□□□□□□□□□□□□.

□□, □□□□□□□□□□□□□□□□□□□□□□□(5.131)□□(5.132)□□□□□, $x \to -x$, $\lambda \to -\lambda$□□□□□□□□□□□□□□□□□□□. □□□, □□□□□□□□□□□□□□□□□□方□□□□□□□, □□分□□□□□□□示□□□□□□□.

5.5.3 トランスクリティカル分岐

□□□□□□□□□□分□□□□□□

$$\frac{dx}{dt} = \lambda x - x^2 + O(x^3), \tag{5.133}$$

□□□□

$$\frac{dx}{dt} = \lambda x + x^2 + O(x^3), \tag{5.134}$$

□□□□□□.

□□□$O(x^3)$□□□□□□(5.133)□□□□□□□□□□□分□□□□□

$$\frac{dx}{dt} = \lambda x - x^2 := f_\lambda(x), \tag{5.135}$$

□□□□□□□□□. □□□□□□□□□ $f_\lambda(x^{(i)*})=0$ □□□□□定□ $x^{(i)*}$ □ $\lambda\neq 0$ □□□□□存□□, $x^{(1)*}=0$ □ $x^{(2)*}=\lambda$ □□□. □□ $\lambda=0$ □□□□定□□ $x^{(1)*}=0$ □□□□□□. □□, 安定□□□□□□

$$\mathsf{J}_{11}(x)=\partial_x f_\lambda(x)=\lambda-2x, \tag{5.136}$$

□□,

$$\mathsf{J}_{11}(x^{(1)*})=\lambda, \tag{5.137}$$
$$\mathsf{J}_{11}(x^{(2)*})=-\lambda, \tag{5.138}$$

□□□. □□□, □□□□定□□安定□□ λ □□□□□□□□□□□□□□□. □□ $\lambda>0$ □□□□, □定□ $x^{(1)*}$ □□安定, □定□ $x^{(2)*}$ □安定□□□□□対□□, $\lambda<0$ □□□□, □定□ $x^{(1)*}$ □安定, □定□ $x^{(2)*}$ □□安定□□□. $\lambda=0$ □□□□定□ $x^{(1)*}$ □ x □□□□□定□□□□ x □□□□□定□□□□□□□□□□安定□□□. □□□□□ λ □□□□□定□□安定□□□□(□□□□)□□分□□□□□□, □□□□□□□□□□分□□□□□□□□. □□, □□□□□□□□□□,

$$U(x)=\frac{1}{3}x^3-\frac{1}{2}\lambda x^2+\text{const.}, \tag{5.139}$$

□□□, □□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□.

□□ $O(x^3)$ □□□□□□(5.134)□□□□□□□□□□□分□□□□□

$$\frac{dx}{dt}=\lambda x+x^2:=f_\lambda(x), \tag{5.140}$$

□□□□□□□□□□. □□□□□, $f_\lambda(x^{(i)*})=0$ □□□□□定□ $x^{(i)*}$ □ $\lambda\neq 0$ □□□□存□□, $x^{(1)*}=0$ □ $x^{(2)*}=-\lambda$ □□□. □□ $\lambda=0$ □□□□定□□ $x^{(1)*}=0$ □□□□□□. □□, 安定□□□□□□

$$\mathsf{J}_{11}(x)=\partial_x f_\lambda(x)=\lambda+2x, \tag{5.141}$$

□□,

$$\mathsf{J}_{11}(x^{(1)*})=\lambda, \tag{5.142}$$
$$\mathsf{J}_{11}(x^{(2)*})=-\lambda, \tag{5.143}$$

□□□. □□□, □□□ $\lambda>0$ □□□□, □定□ $x^{(1)*}$ □□安定, □定□ $x^{(2)*}$ □安定□□□□□対□□, $\lambda<0$ □□□□, □定□ $x^{(1)*}$ □安定, □定□ $x^{(2)*}$ □□安定□□□. □□ $\lambda=0$ □□□□定□ $x^{(1)*}$ □ x □□□□□定□□□□□□□, x □□□□□定□□□□□□□□安定□□□. □□, □□□□□□□□□□,

$$U(x)=-\frac{1}{3}x^3-\frac{1}{2}\lambda x^2+\text{const.}, \tag{5.144}$$

□□□.

□□□□□□□□□□□□, □□□□□□□□□□□(5.139)□□(5.144)□□□□□□, $x\to -x$, $\lambda\to\lambda$ □□□□□□□□□□□□□□□□□. □□□, □□□□□□□□□□□□方□□□□□□□, □□分□□□□□□□示□□□□□□□.

□□□□□□□□□□□□□□方□□□

$$\frac{d\tilde{x}_1}{dt} = k_1^+ \tilde{x}_{\mathrm{tot}} \tilde{x}_1 - (k_1^- + k_1^+)(\tilde{x}_1)^2, \tag{5.145}$$

□□, $x = (k_1^- + k_1^+)\tilde{x}_1$, $\lambda = k_1^+ \tilde{x}_{\mathrm{tot}}$ □□□□数□□□□□□, □(5.133)□□□□□□□□□□□分□□□□□□□□. □□□, λ□常□□□□□保□□□. □□□□□□□□□□分□□□□□□. □□□□□□□□□□□□□□□□□, 分□□□□□□□□□□□□実□□□□□□□□□□□.

5.5.4 ピッチフォーク分岐

□□□□□□□□□□分□□□□□

$$\frac{dx}{dt} = \lambda x - x^3 + O(x^4)., \tag{5.146}$$

□□□□

$$\frac{dx}{dt} = \lambda x + x^3 + O(x^4)., \tag{5.147}$$

□□□□□□□. □□□□□□□□□□□□□□□□□□□, □□□□

$$U(x) = \frac{1}{4}x^4 - \frac{1}{2}\lambda x^2 + \mathrm{const.}, \tag{5.148}$$

□

$$U(x) = -\frac{1}{4}x^4 - \frac{1}{2}\lambda x^2 + \mathrm{const.}, \tag{5.149}$$

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□□, 前□□□□□□□□□□□□□□□□□□□□□分□□□□□(5.146)□□□□□□□□□□. □□□□□

$$\frac{dx}{dt} = \lambda x - x^3 := f_\lambda(x), \tag{5.150}$$

□$f_\lambda(x^{(i)*}) = 0$□□□□□定□$x^{(i)*}$□, □□$x^{(1)*} = 0$□□□. □□, $\lambda > 0$□□□□□□2□存□□□, $x^{(2)*} = \sqrt{\lambda}$□$x^{(3)*} = -\sqrt{\lambda}$□□定□□□□. □□, 安定□□□□□□

$$\mathsf{J}_{11}(x) = \partial_x f_\lambda(x) = \lambda - 3x^2, \tag{5.151}$$

□□, □定□$x^{(1)*}$□□□□□$\mathsf{J}_{11}(x^{(1)*}) = \lambda$□□$\lambda < 0$□□□安定□□□□□対□□$\lambda > 0$□□□安定□□□. □□, $\lambda = 0$□□□□□□安定□□析□□□□□$\mathsf{J}_{11}(x^{(1)*}) = 0$□□□□□□□□, □□□□□□□$\lambda = 0$□□□$d|x|/dt < 0$□□□□□□$x^{(1)*} = 0$□□定□□安

定□□□□□□□．□□$\lambda > 0$□□□□定□$x^{(2)*}$□$\mathsf{J}_{11}(x^{(2)*}) = -2\lambda$□□安定，$\lambda > 0$□□□□定□$x^{(3)*}$□$\mathsf{J}_{11}(x^{(2)*}) = -2\lambda$□□安定□□□．□□□，□□□□□□□□□□□□□□□□□□□分□□$\lambda < 0$□□□□□□□安定□□定□□□□□□□，$\lambda > 0$□□□□□□□□□定□□□安定□□□，□□□安定□□定□□分□□□．□□□定□□分□□□□□□□□□□□□□□□□□□□似□□□□□，□□分□□□□□□□□□□分□□□□□□□□．□(5.148)□□□□□□□□□□□□□□，$\lambda < 0$□□□□□□□□□□□対□□，$\lambda > 0$□□□□□□□□□□，$x^{(2)*}$□$x^{(3)*}$□□□□□□□□□□□□□□□□□□□□□□□□□□□□□．

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$$\frac{dx}{dt} = \lambda x + x^3 - x^5 := f_\lambda(x), \tag{5.152}$$

□□□□□□察□行□□□□□□□．□□□□□□□定□□$x^{(1)*} = 0$□，$-1/4 < \lambda < 0$□□□□□定□ $x^{(2)*} = \sqrt{(1-\sqrt{1+4\lambda})/2}$, $x^{(3)*} = -\sqrt{(1-\sqrt{1+4\lambda})/2}$□，$-1/4 \le \lambda$□□□□□定□ $x^{(4)*} = \sqrt{(1+\sqrt{1+4\lambda})/2}$, $x^{(5)*} = -\sqrt{(1+\sqrt{1+4\lambda})/2}$□存□□□．

$$\mathsf{J}_{11}(x) = \partial_x f_\lambda(x) = \lambda + 3x^2 - 5x^4, \tag{5.153}$$

□□，$\mathsf{J}_{11}(x^{(1)*}) = \lambda$□□□定□$x^{(1)*} = 0$□$\lambda < 0$□安定□□□，$\lambda > 0$□□安定□□□．□□$\lambda = 0$□□，$x \simeq 0$□□□□□□□□□□□□□$x^3$□方□□□□□$-x^5$□□□□□□□□$d|x|/dt > 0$□□□□□□安定□□□．□□□定□$x^{(2)*}$□$x^{(3)*}$□$-1/4 < \lambda < 0$□

$$\begin{aligned}
\mathsf{J}_{11}(x^{(3)*}) &= \mathsf{J}_{11}(x^{(2)*}) \\
&= \lambda + 3\frac{1-\sqrt{1+4\lambda}}{2} - 5\frac{(1-\sqrt{1+4\lambda})^2}{4} \\
&= -(4\lambda+1) + \sqrt{1+4\lambda} \\
&> 0,
\end{aligned} \tag{5.154}$$

□□安定□□□．□□□定□$x^{(4)*}$□$x^{(5)*}$□$-1/4 < \lambda$□

$$\begin{aligned}
\mathsf{J}_{11}(x^{(4)*}) &= \mathsf{J}_{11}(x^{(5)*}) \\
&= \lambda + 3\frac{1+\sqrt{1+4\lambda}}{2} - 5\frac{(1+\sqrt{1+4\lambda})^2}{4} \\
&= -(4\lambda+1) - \sqrt{1+4\lambda} \\
&< 0,
\end{aligned} \tag{5.155}$$

□□安定□□□，□□$\lambda = -1/4$□$\mathsf{J}_{11}(x^{(4)*}) = \mathsf{J}_{11}(x^{(5)*}) = 0$□□□□□□．□□□$x^{(4)*}$□□定□□対□□□$x > x^{(4)*}$□$x^{(4)*}$□□□□$x < x^{(4)*}$□$x^{(4)*}$□□□□□□□□□，$x^{(4)*}$□□定□□□安定□□□．□□□$x^{(5)*}$□□定□□対□□□$x < x^{(5)*}$□$x^{(5)*}$□□□□$x > x^{(5)*}$□$x^{(5)*}$□□□□□□□□□，$x^{(5)*}$□□定□□□安定□□□．

□□□□，λ□□□□□□□□□□□□□□行□□□□□，□□□□□□$x^{(1)*}$□安定□□定□□□□□□□□，$\lambda = 0$□□□□□□定□□□安定□□□，安定□□定□□$\mathsf{J}_{11}(x^{(4)*})$□□□□$\mathsf{J}_{11}(x^{(5)*})$□□□□□．□方□，$\lambda$□□□□□□□□□□□□□□□行□□□□□$\mathsf{J}_{11}(x^{(4)*})$□□□□$\mathsf{J}_{11}(x^{(5)*})$□安定□□定□□$\lambda = -1/4$□□□□□□□□□□□，□□□$x^{(1)*}$□安定□□定□□□□□□．□□□□□安定□□定□□移動□□□

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$$U(x) = \frac{1}{6}x^6 - \frac{1}{4}x^4 - \frac{1}{2}\lambda x^2 + \mathrm{const.}, \tag{5.156}$$

□□□□□□□□□□□□□□□□□□□□□□□□□□□□. $\lambda < 0$□□□□□□□□□□□□□□□□□□□□対□□, $\mathsf{J}_{11}(x^{(4)*})$□□□□$\mathsf{J}_{11}(x^{(5)*})$□□□□□□□□□□□□□$\lambda > -1/4$□□□□□□. □□□□□□□□□□□□□□□□□□□□□□□□$\lambda = -1/4$□$\lambda = 0$□□□□□□□, 最初□□□□□□□□□□□□□□□□□□依存□□□□□□, □□□□□□□□□□□□□□□□□□□□.

□□□□□□□□□□分□□, □□□□□□□□□□□移□文□□□□□□□□□□□□. 例□□, □□移□文□□□λ□□□□□度□□□□□□□□□□□□ x□□□□□□□□□□表□秩序□□□□□□□□□□□□. □□□□移□文□□□□□□□安定□□定□□□□□分□□□□□□□□□□□□□□□□□□□□□□□分□□, 2□□□移□□□□□. □方□□□□□安定□□定□□□□□分□□□□□□□□□□□□□□□□□□□□分□□, □□移□文□□□1□□□移□□□□□. □□□□□□□□□□体□□□□□□□□,□□体□□□□□□□□□□□□□融□□□□度□□□□□□□□□□□□□□□□□□存□□□□□□1□□□移□□□□□□□□□□, □□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□□□□□□□□.

5.5.5 ホップ分岐

□□□□□分□□□□□

$$\frac{dz}{dt} = (\lambda + i)z - z|z|^2 + O(|z|^4), \tag{5.157}$$

□□□□

$$\frac{dz}{dt} = (\lambda + i)z + z|z|^2 + O(|z|^4), \tag{5.158}$$

□□□□□□□□□. □□□z□実数□2□□($y_1 = x \in \mathsf{R}, y_2 = y \in \mathsf{R}$)□対□□, □□数表□$z = x + iy$□□□□□□□□□□□□□□□□□□□. □□□, □□□使□□□数□□$z = |r|\exp(i\theta)$□□□□. □□□$|r| \in \mathsf{R}, \theta \in \mathsf{R}$□実数□□□, $|r| \geq 0$□□□. □□□$x = |r|\cos\theta$, $y = |r|\sin\theta$□□□□□. □□□数□□□□□□□, □□□分□□□□□□

$$\frac{d|r|}{dt} = \lambda|r| - |r|^3 + O(|r|^4), \tag{5.159}$$

$$\frac{d\theta}{dt} = 1, \tag{5.160}$$

□□□□

$$\frac{d|r|}{dt} = \lambda|r| + |r|^3 + O(|r|^4), \tag{5.161}$$

$$\frac{d\theta}{dt} = 1, \tag{5.162}$$

□□□.□□□数□□□□□□□□□□□□□, $|r|$□□□□力学□□$|r|$□□□□□□□□, □□□□□□□分□□□□□□□□□□□.□方□θ□□□□□常□□定□□□度□動□□□□□□□□□□□□□□□□□.

$|r|$□□□□力学□□, □□□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□

$$\frac{d|r|}{dt} = \lambda|r| - |r|^3 := f_\lambda(|r|) \tag{5.163}$$

$$\frac{d\theta}{dt} = 1, \tag{5.164}$$

□□□□□□.□□□□, $f_\lambda(|r|^{(i)*}) = 0$□□□□□, □□□□$|r|$□□□□力学□□□定□□, $|r| \leq 0$□□□□□□□□□, $|r|^{(1)*} = 0$□, $\lambda > 0$□□□□$|r|^{(2)*} = \sqrt{\lambda}$□□□□□存□□□.□□□, $|r|^{(1)*} = 0$□$dz/dt = 0$□□□□□z□□□□力学□□□□定□□□□□方□, $\lambda > 0$□□$|r|^{(2)*} = \sqrt{\lambda}$□$dz/dt \neq 0$□□□, □定□□□度1□□□□□□□□□, z□□□□力学□□□□定□□□□□□□□□□□□□□.□□□□□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□□□,

$$\mathsf{J}_{11}(|r|) = \partial_{|r|} f_\lambda(|r|) = \lambda - 2|r|^2, \tag{5.165}$$

□□, □定□$|r|^{(1)*}$□□□□□$f_\lambda(|r|^{(1)*}) = \lambda$□□□□□, $\lambda < 0$□□安定□□定□□□□, □□$\lambda = 0$□□$d|r|/dt < 0$□□安定□□定□□□□□□対□, $\lambda > 0$□□□安定□□定□□□□.□方□, □定□$|r|^{(2)*}$□□□□□$f_\lambda(|r|^{(2)*}) = -\lambda$□□□, $\lambda > 0$□安定□□定□□□□.□□□, λ□□□□□□□□□□動□□□□□□, $\lambda \leq 0$□□$|r| = 0$□安定□□定□□□□□□□□□□□□□□□□□平面□□$x = y = 0$□□□□□□□□□, $\lambda > 0$□□$|r| = \sqrt{\lambda}$□□$d\theta/dt = 1$□□□□□□□□, □□□□$x = \sqrt{\lambda}\cos(t+\theta_0)$, $y = \sqrt{\lambda}\sin(t+\theta_0)$□□□□□□安定□□□.□□□$\theta_0$□定数□□□. $x = \sqrt{\lambda}\cos(t+\theta_0)$, $y = \sqrt{\lambda}\sin(t+\theta_0)$□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□, □□□□□分□□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□.□□□□□□□□□□□□□□□□□□□□□分□□□□□□□□□□□□□□□分□□, □□□□□□□□□□□□□□分□□□□□□□□□.

□□□

$$\frac{d|r|}{dt} = \lambda|r| + |r|^3 + O(|r|^4) \tag{5.166}$$

$$\frac{d\theta}{dt} = 1, \tag{5.167}$$

□□□□□表□□□□□□分□□□□□□□□□□□□□□□分□□□□.□□□□□□□□□□□□□□□□□□□□□□分□□□□□

$$\frac{d|r|}{dt} = \lambda|r| + |r|^3 - |r|^5 := f_\lambda(|r|), \tag{5.168}$$

$$\frac{d\theta}{dt} = 1, \tag{5.169}$$

□□□□□□□□□□□□□□□.z□力学□□□□□□□□□□□□□□,

$$\frac{dz}{dt} = (\lambda + i)z + z|z|^2 - z|z|^4, \tag{5.170}$$

□□□□□.□□□□□$|r|$□□□□力学□□□□$f_\lambda(|r|^{(i)*}) = 0$□□□□□定□□, $|r| \geq 0$□□□□□, $|r|^{(1)*} = 0$, $-1/4 < \lambda < 0$□$|r|^{(2)*} = \sqrt{(1-\sqrt{1+4\lambda})/2}$, $-1/4 \leq$

λ□$|r|^{(3)*} = \sqrt{(1+\sqrt{1+4\lambda})/2}$□□□□存□□□. □□安定□□□□□□□□□□□□□
□□□□□□□□□□□分□□□□□, $|r|^{(1)*}$□$\lambda < 0$□安定□□$\lambda \geq 0$□□安定□□□,
$|r|^{(2)*}$□□安定□□□, $|r|^{(3)*}$□$\lambda = -1/4$□□安定□□$\lambda > -1/4$□安定□□定□□□□.
□□□□λ□□□□□□□□□□□□□□行□□□□□□定□□□□□□$|r|^{(1)*}$□□□□
□$\lambda = 0$□□安定□□□,$|r|^{(3)*}$□□□□□□□□□□□□□□□□□□□□□, λ□□□□□
□□□□□□□□行□□□□$|r|^{(3)*}$□□□□□□□□□□□□□□□$\lambda < -1/4$□□□
□□□□□□□, 安定□□定□□□□$|r|^{(1)*}$□□□□□□□□□□□□□□□□□□□□
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