“Stochastic Models for Granular Matter 2”

Stochastic models for
granular liquids and solids

Kuniyasu Saitoh
MSM, CTW
University of Twente

Random variables

Random variable

Its evolution is always fluctuating, i.e. ***stochastic***, around the mean.

e.g.) Velocities of Brownian particles, stock prices, currency JPY/EUR, etc.

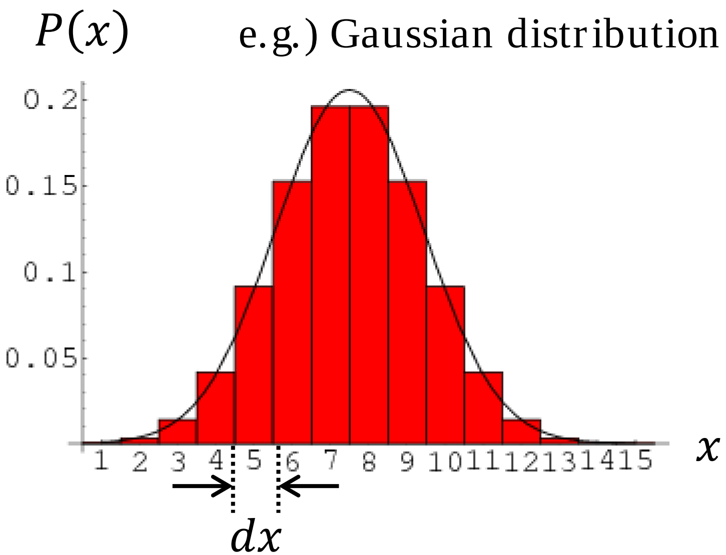
Probability distribution function (PDF)

“The probability that a random variable, x, is found between $x \sim x + dx$” = $P(x)dx$

The sum of probabilities is one, i.e. ***normalized***.

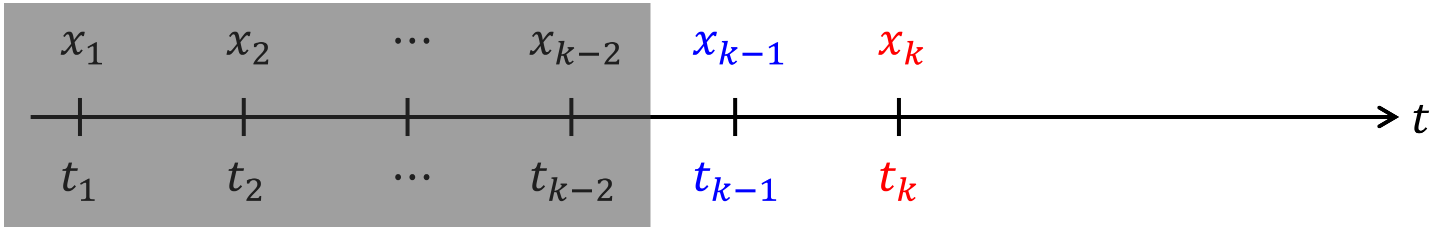
$$\int P(x)dx = 1$$

e.g.) Gaussian distribution



Chapman-Kolmogorov equation

Markov process



Random variables depend *only* on the previous values.
e.g.) x_k at t_k is fully determined from x_{k-1} at t_{k-1}.

Chapman-Kolmogorov eq.

$$P(x_k, t_k) = \int W(x_k | x_{k-1}) P(x_{k-1}, t_{k-1}) dx_{k-1}$$

$W(x_k|x_{k-1})$, **transition probability**:
The probability for x_{k-1} to become x_k

e.g.) Markov-chain

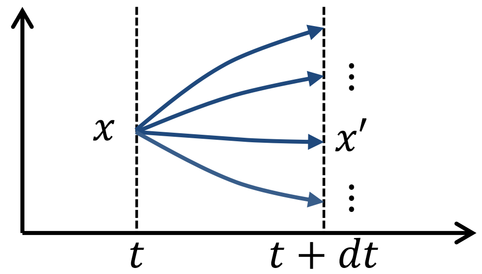
$$P(x_k, t_k) = \int \cdots \int W(x_k|x_{k-1}) W(x_{k-1}|x_{k-2}) \cdots W(x_2|x_1) P(x_1, t_1) dx_{k-1} \cdots dx_1$$

Master equation

Chapman-Kolmogorov eq. $P(x,t+\Delta t) = \int W(x|x')P(x',t)dx'$

Transition probabilities are normalized to one:

$$\int W(x'|x)dx' = 1$$



$$P(x,t+\Delta t) - P(x,t) = \int W(x|x')P(x',t)dx' - P(x,t)\int W(x'|x)dx'$$

$$= \int [W(x|x')P(x',t) - W(x'|x)P(x,t)]dx'$$

Transition rate $T(x|x') \equiv \lim_{\Delta t \to 0} \frac{W(x|x')}{\Delta t}$

Master eq.

$$\frac{\partial}{\partial t}P(x,t) = \int [\underbrace{T(x|x')P(x',t)}_{gain} - \underbrace{T(x'|x)P(x,t)}_{loss}]dx'$$

cf.) Note the similarity with the Boltzmann equation!

Fokker-Planck equation

Master eq. $$\frac{\partial}{\partial t}P(x,t) = \int [T(x|x')P(x',t) - T(x'|x)P(x,t)]dx'$$

Multiplied by an arbitrary function, $h(x)$, and integrated over x,

$$\int h(x)\frac{\partial}{\partial t}P(x,t)dx = \iint [h(x)T(x|x')P(x',t) - h(x)T(x'|x)P(x,t)]dxdx'$$

$$= \iint [h(x') - h(x)]T(x'|x)P(x,t)dxdx'$$

Exchange x with x'

Taylor expansion, $\Delta x \equiv x' - x \ll 1$ (cf. *van Kampen's small noise expansion*).

$$h(x') - h(x) = \sum_{n=1}^{\infty} \frac{1}{n!}\frac{\partial^n h}{\partial x^n}\Delta x^n$$

Integrating the right-hand-side by parts,

$$\int h(x)\frac{\partial}{\partial t}P(x,t)dx = \iint \sum_{n=1}^{\infty} \frac{1}{n!}\frac{\partial^n h}{\partial x^n}\Delta x^n\, T(x'|x)P(x,t)dxdx'$$

$$= \iint h(x)\sum_{n=1}^{\infty} \frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}[\Delta x^n T(x'|x)P(x,t)]dxdx'$$

Fokker-Planck equation

The *n*-th moment of transition rate

$$\alpha_n(x) \equiv \int \Delta x^n T(x'|x)dx'$$

$$\int h(x)\frac{\partial}{\partial t}P(x,t)dx = \int h(x)\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}[\alpha_n(x)P(x,t)]dx$$

Because $h(x)$ is arbitrary, the rest of terms should be equal:

Kramers-Moyal expansion

$$\frac{\partial}{\partial t}P(x,t) = \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}[\alpha_n(x)P(x,t)]$$

The expansion truncated at $n = 2$ is the so-called **Fokker-Planck eq.**

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}[\alpha_1(x)P(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[\alpha_2(x)P(x,t)]$$

"Drift" *"Diffusion"*

Fokker-Planck equation

e.g.) Fokker-Planck eq. with time dependent coefficients:

$$\frac{\partial}{\partial t}P(x,t) = -A(t)\frac{\partial}{\partial x}[xP(x,t)] + \frac{B(t)}{2}\frac{\partial^2}{\partial x^2}P(x,t)$$

The solution is a **Gaussian distribution:**

$$P(x,t) = \frac{1}{\sqrt{2\pi\rho}}\exp\left[-\frac{(x-\langle x\rangle)^2}{2\rho}\right]$$

The **mean**, $\langle x\rangle$, and **variance**, $\rho = \langle x^2\rangle - \langle x\rangle^2$, are the solutions of the following equations:

$$\frac{d}{dt}\langle x\rangle = A(t)\langle x\rangle \qquad \frac{d}{dt}\rho = 2A(t)\rho + B(t)$$

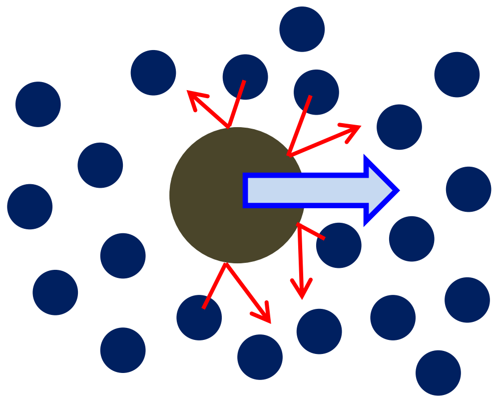
Exercise) Please show that the Gaussian is a solution of the Fokker-Planck eq. with time dependent coefficients.

Langevin equation

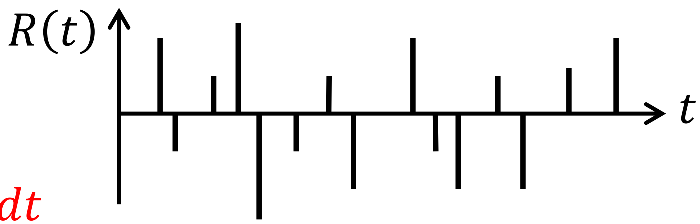
"**Brownian particle** (a macroscopic sphere immersed into liquid)" is a physical model of stochastic process which can be described by the **Langevin eq.**:

$$m\frac{d}{dt}\mathbf{v}(t) = -m\gamma\mathbf{v}(t) + \mathbf{R}(t)$$

Drag force (macro) *Random force (micro)*



Uncorrelated "white noise"



- *Mean value is zero,* $\langle \mathbf{R}(t) \rangle = 0$
- *Correlation-time is zero,* $\langle \mathbf{R}(t) \cdot \mathbf{R}(0) \rangle = 2R_0\delta(t)$
- *Integrating over* $t = 0 \sim \infty$, $R_0 = \int_0^{\infty} \langle \mathbf{R}(t) \cdot \mathbf{R}(0) \rangle dt$
- *Uncorrelated with previous velocities,* $\langle \mathbf{R}(t) \cdot \mathbf{v}(0) \rangle = 0$

The solution is

$$\mathbf{v}(t) = \left[\mathbf{v}(0) + \frac{1}{m}\int_0^t e^{\gamma t'}\mathbf{R}(t')dt'\right]e^{-\gamma t}$$

e.g.) Velocity autocorrelation *decays exponentially*

$$\frac{\langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle}{\langle \mathbf{v}(0) \cdot \mathbf{v}(0) \rangle} = e^{-\gamma t}$$

Langevin equation

Squaring the solution and taking an statistical (ensemble) average,

$$\langle \mathbf{v}(t)^2 \rangle = \langle \mathbf{v}(0)^2 \rangle e^{-2\gamma t} + \frac{2e^{-2\gamma t}}{m} \int_0^t e^{\gamma t'} \langle \mathbf{R}(t') \cdot \mathbf{v}(0) \rangle dt' + \frac{e^{-2\gamma t}}{m^2} \iint_0^t e^{\gamma (t'+t'')} \langle \mathbf{R}(t') \cdot \mathbf{R}(t'') \rangle dt' dt''$$
$$= \langle \mathbf{v}(0)^2 \rangle e^{-2\gamma t} + \frac{R_0}{m^2\gamma}(1 - e^{-2\gamma t})$$

Thermal equilibrium:

$$\frac{m}{2}\langle v(t)^2 \rangle = \frac{m}{2}\langle v(0)^2 \rangle = \frac{3}{2} k_B T$$

$$\therefore \langle v(t)^2 \rangle = \langle v(0)^2 \rangle = \frac{3k_B T}{m}$$

$$\frac{3k_B T}{m} = \frac{3k_B T}{m} e^{-2\gamma t} + \frac{R_0}{m^2\gamma}(1 - e^{-2\gamma t}) \rightarrow \frac{R_0}{m^2\gamma} \quad (t \rightarrow \infty)$$

Fluctuation-dissipation theorem (FDT)

$$\gamma = \frac{R_0}{3mk_B T} = \frac{1}{3mk_B T} \int_0^\infty \langle \mathbf{R}(t) \cdot \mathbf{R}(0) \rangle dt$$

Langevin equation

Multiplying the Langevin eq. by $\mathbf{r}(t)$ and taking a statistical (ensemble) average,

$$m\left\langle \mathbf{r}(t)\cdot\frac{d}{dt}\mathbf{v}(t)\right\rangle = -m\gamma\langle \mathbf{r}(t)\cdot\mathbf{v}(t)\rangle + \langle \mathbf{r}(t)\cdot\mathbf{R}(t)\rangle$$

$$\mathbf{r}\cdot\frac{d}{dt}\mathbf{v} = \frac{1}{2}\frac{d^2}{dt^2}\mathbf{r}^2 - \mathbf{v}^2$$

$$\mathbf{r}\cdot\mathbf{v} = \frac{1}{2}\frac{d^2}{dt^2}\mathbf{r}^2$$

Random force is space-independent!

$$\langle \mathbf{r}(t)\cdot\mathbf{R}(t)\rangle = 0$$

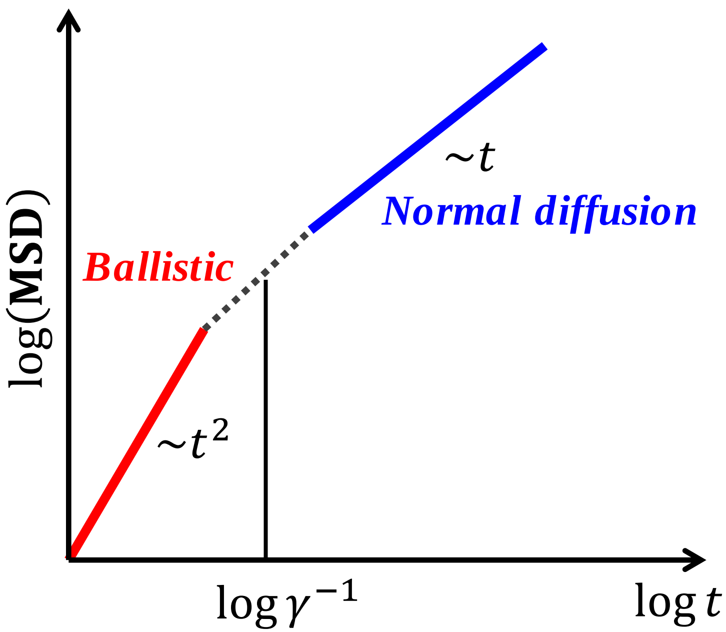
Differential equation of $\langle r(t)^2\rangle$

$$\frac{d^2}{dt^2}\langle \mathbf{r}(t)^2\rangle + \gamma\frac{d}{dt}\langle \mathbf{r}(t)^2\rangle = 2\langle \mathbf{v}(t)^2\rangle = \frac{6k_BT}{m}$$

Mean-square displacement (MSD)

$$\therefore \langle \mathbf{r}(t)^2\rangle = \frac{6k_BT}{m\gamma}\left(t - \frac{1}{\gamma} + \frac{1}{\gamma}e^{-\gamma t}\right)$$

$$\approx \begin{cases} \dfrac{3k_BT}{m}t^2 & (\text{short time scale}, \gamma t \ll 1) \\ \dfrac{6k_BT}{m\gamma}t & (\text{long time scale}, \gamma t \gg 1) \end{cases}$$



Langevin equation

Diffusion coefficient

$$D \equiv \lim_{t\to\infty} \frac{\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2\rangle}{6t} = \frac{k_B T}{m\gamma}$$

$$\mathbf{r}(0) = \mathbf{0}$$

$$\langle \mathbf{r}(t)^2\rangle \approx \frac{6k_B T}{m\gamma} t$$

Time-integral of the velocity autocorrelation function

$$\int_0^\infty \langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle dt = \langle \mathbf{v}(0)^2\rangle \int_0^\infty e^{-\gamma t} dt = \frac{3k_B T}{m\gamma}$$

Green-Kubo formula

$$D = \frac{1}{3}\int_0^\infty \langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle dt$$

Note the similarity with the FDT!
Both are given by time-integrals of autocorrelation!

cf.) Green-Kubo formula for transport coefficients:

Shear viscosity $\eta = \lim_{|\mathbf{k}|\to 0} \frac{1}{k_B T V}\int_0^\infty \langle \boldsymbol{\sigma}_{\mathbf{k}}{}^{\perp}(t)\cdot\boldsymbol{\sigma}_{\mathbf{k}}{}^{\perp}(0)\rangle dt$

cf.) **Long-time tails**

$\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle \sim t^{-d/2}$ (in a long-time limit, in d-dimension)

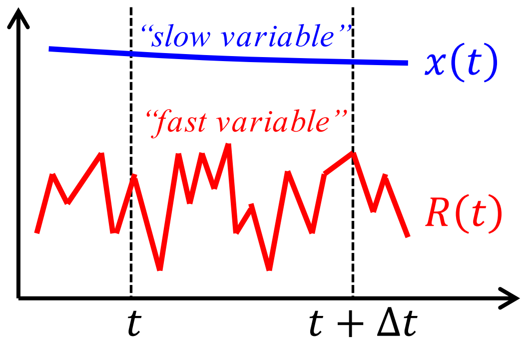
Langevin equation

Langevin equation (1-dimension)

$$\frac{d}{dt}x = -\gamma x + R(t)$$

$$\therefore \Delta x \approx -\gamma x \Delta t + \int_t^{t+\Delta t} R(t')dt'$$

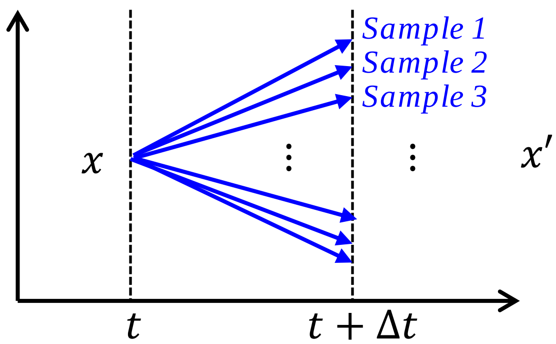
NOT $R(t)\Delta t$!



The *n*-th moment

$$\alpha_n(x) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int \Delta x^n W(x'|x)dx' = \lim_{\Delta t \to 0} \frac{\langle \Delta x^n \rangle}{\Delta t}$$

Take an average over all possible x'



e.g.)

$$\alpha_1(x) = \lim_{\Delta t \to 0} \frac{\langle \Delta x \rangle}{\Delta t} = \lim_{\Delta t \to 0} \left[-\gamma x + \frac{1}{\Delta t} \int_t^{t+\Delta t} \langle R(t') \rangle dt' \right] = -\gamma x$$

$\langle \cdots \rangle$ does not work on x

$$\alpha_2(x) = \lim_{\Delta t \to 0} \frac{\langle \Delta x^2 \rangle}{\Delta t} = \lim_{\Delta t \to 0} \left[(\gamma x)^2 \Delta t - 2\gamma x \int_t^{t+\Delta t} \langle R(t') \rangle dt' + \frac{1}{\Delta t} \iint_t^{t+\Delta t} \langle R(t')R(t'') \rangle dt' dt'' \right] = R_0$$

Fokker-Planck eq.

$$\frac{\partial}{\partial t} P(x,t) = \gamma \frac{\partial}{\partial x} [xP(x,t)] + \frac{R_0}{2} \frac{\partial^2}{\partial x^2} P(x,t)$$

Generalized Langevin equation

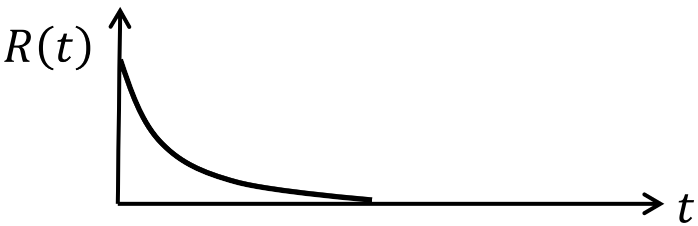
$$m\frac{d}{dt}\mathbf{v}(t) = -m\int_0^t \gamma(t-t')\mathbf{v}(t')dt' + \mathbf{R}(t)$$

Viscosity coefficient has ***"memory"***

Correlated "colored noise"

$$\langle \mathbf{R}(t)\cdot\mathbf{R}(0)\rangle = mk_BT\gamma(t)$$

i.e. Correlation time is finite



Multiplying the generalized Langevin eq. by $\mathbf{v}(0)$ and taking statistical average, the velocity autocorrelation function obeys

$$\frac{d}{dt}\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle = \int_0^t \gamma(t-t')\langle \mathbf{v}(t')\cdot\mathbf{v}(0)\rangle dt'$$

e.g.) $\gamma(t) = \gamma(0)e^{-t/\tau}$

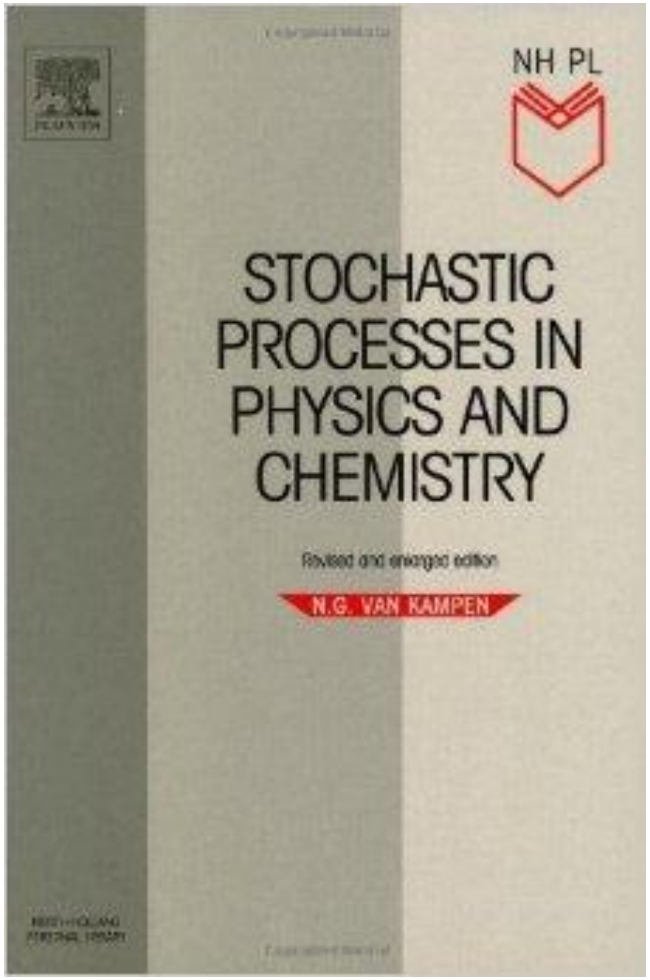
$$\frac{\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle}{\langle \mathbf{v}(0)\cdot\mathbf{v}(0)\rangle} = \frac{\gamma_1 e^{-\gamma_2 t} - \gamma_2 e^{-\gamma_1 t}}{\gamma_1-\gamma_2}$$

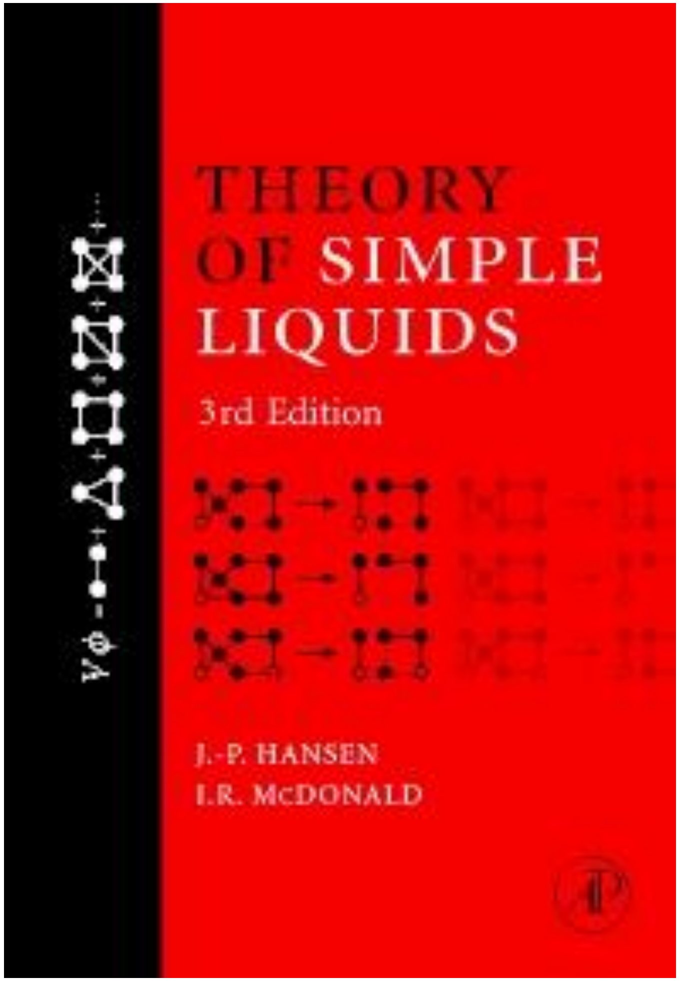
Mixing two relaxation time scales, ${\gamma_1}^{-1}$ and ${\gamma_2}^{-1}$

References

1. N.G. van Kampen, “Stochastic Processes in Physics and Chemistry”, the 3rd edition.

2. J.-P. Hansen and I.R. McDonald, “Theory of Simple Liquids”, the 3rd edition.





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