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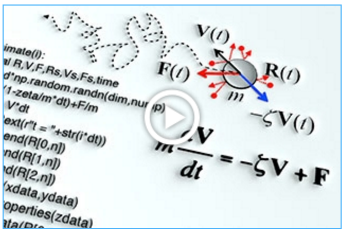

Stochastic Processes: Data Analysis and Computer Simulation

The course deals with how to simulate and analyze stochastic processes, in particular the dynamics of small particles diffusing in a fluid.

京都大学 KYOTO UNIVERSITY

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What you'll learn

- Basic Python programming
- Basic theories of stochastic processes

- Simulation methods for a Brownian particle
- Application: analysis of financial data

Meet the instructors

Ryoichi Yamamoto
Professor, Chemical Engineering
Kyoto University

John J. Molina
Assistant Professor
Kyoto University

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Length:	6 weeks
Effort:	2-3 hours per week
Price:	FREE Add a Verified Certificate for $49
Institution:	KyotoUx
Subject:	Physics
Level:	Intermediate
Languages:	English
Video Transcripts:	English

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Prerequisites
Basic mathematics expected of a 2^{nd} year undergraduate student (differential and integral calculus and linear algebra).

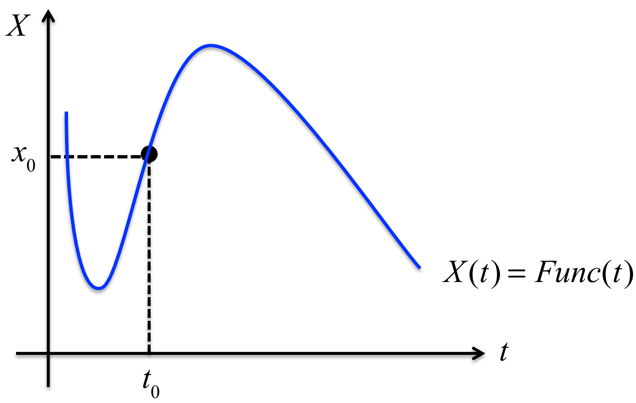
Brownian motion 1: basic theories

Basic knowledge of stochastic process

Stochastic process

A deterministic process:

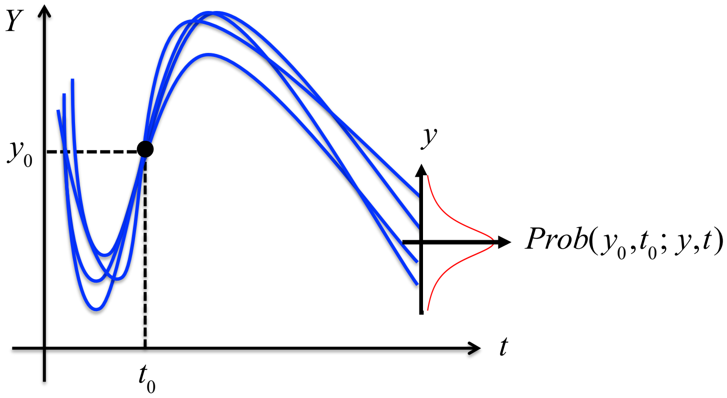
$$X(t) = Func(t)$$



Stochastic process

A stochastic process:

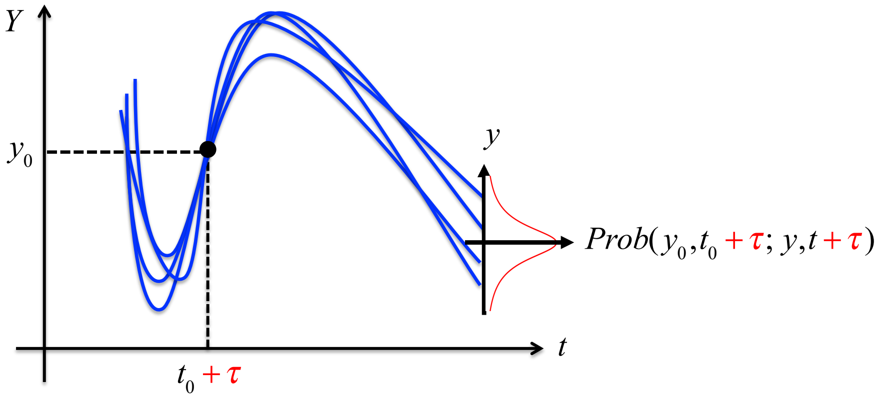
$$Y(t) \neq Func(t) \quad \rightarrow \quad Prob(y_0, t_0; y, t)$$



Stochastic process

A stochastic process:

$$Y(t) \neq Func(t) \quad \rightarrow \quad Prob(y_0, t_0; y, t)$$



A steady stochastic process:

$$Prob(y_0, t_0 + \tau; y, t + \tau) = Prob(y_0, t_0; y, t)$$

Stochastic process

Consider a steady stochastic process $Y(t)$ with its mean $\langle Y(t) \rangle = 0$ and define Fourier transformation

$$\tilde{Y}_T(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} Y_T(t) \qquad (1)$$

and inverse Fourier transformation

$$Y_T(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} \tilde{Y}_T(\omega) \qquad (2)$$

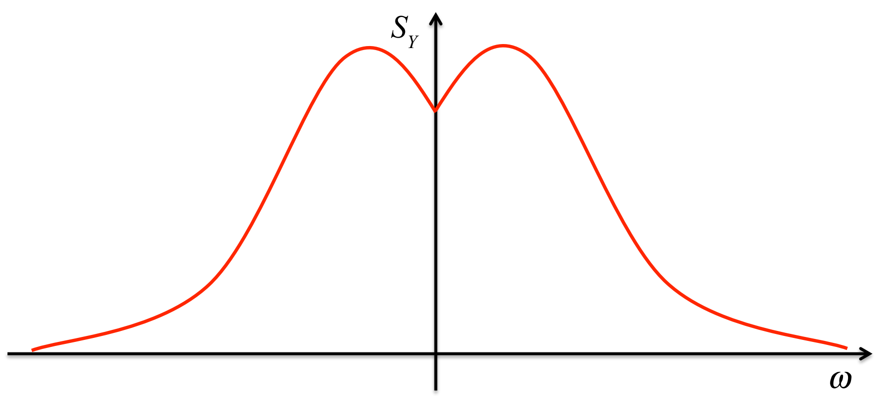
using

$$\begin{aligned} Y_T(t) &= Y(t) \quad (|t| \le T/2) \\ Y_T(t) &= 0 \quad (|t| > T/2) \end{aligned} \qquad (3)$$

Stochastic process

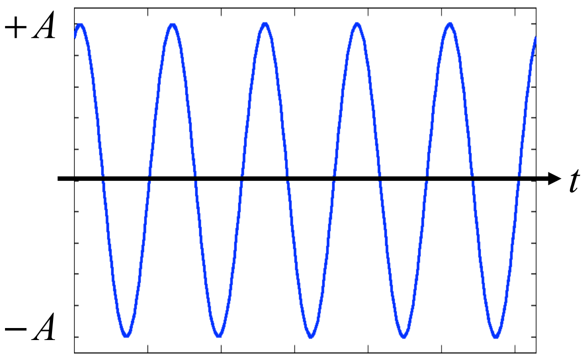
Spectral density / Power spectrum

$$S_Y(\omega) \equiv \lim_{T \to \infty} \frac{1}{T} \left| \tilde{Y}_T(\omega) \right|^2 \qquad (4)$$

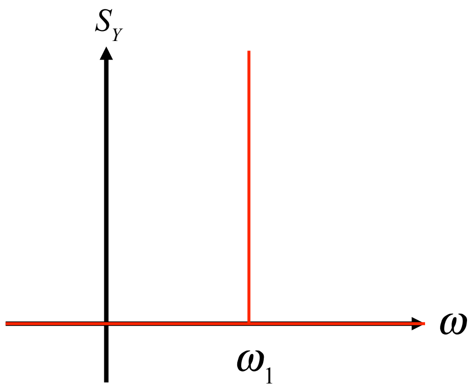


Stochastic process

Case 1: Single cosine wave



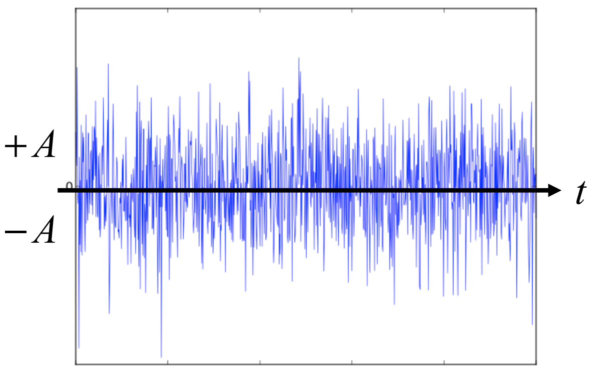
$$Y(t) = A\cos(\omega_1 t) \qquad (5)$$



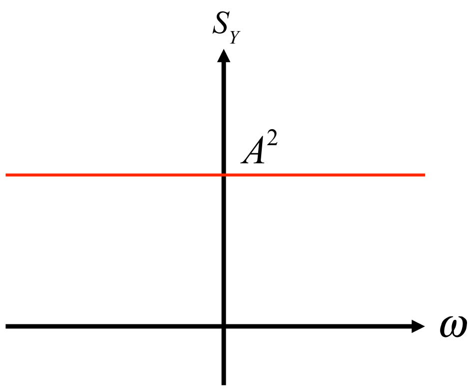
$$S_Y(\omega) = A^2\delta(\omega - \omega_1) \qquad (6)$$

Stochastic process

Case 2: White noise



$$Y(t) = A\xi(t) \qquad (7)$$

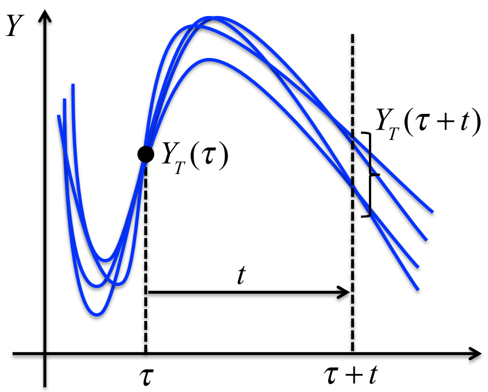


$$S_Y(\omega) = A^2 \qquad (8)$$

Stochastic process

Auto-correlation function

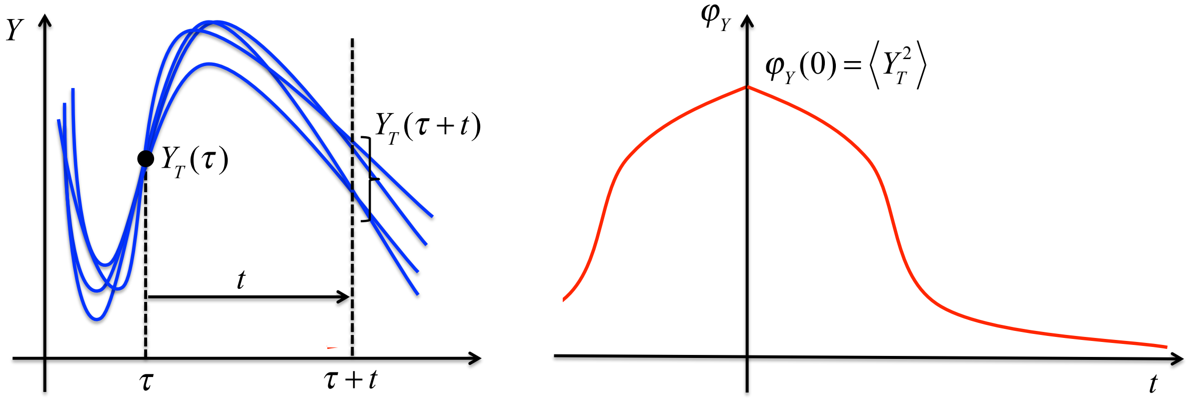
$$\varphi_Y(t) \equiv \lim_{T\to\infty} \frac{1}{T} \int_{-\infty}^{\infty} d\tau \, Y_T(\tau) Y_T(\tau + t) \equiv \langle Y(\tau) Y(\tau + t) \rangle_\tau \qquad (9)$$



Stochastic process

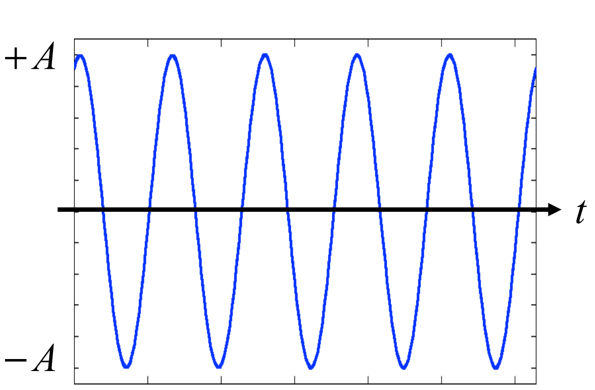
Auto-correlation function

$$\varphi_Y(t) \equiv \lim_{T\to\infty} \frac{1}{T} \int_{-\infty}^{\infty} d\tau \, Y_T(\tau) Y_T(\tau + t) \equiv \langle Y(\tau) Y(\tau + t) \rangle_\tau \qquad (9)$$

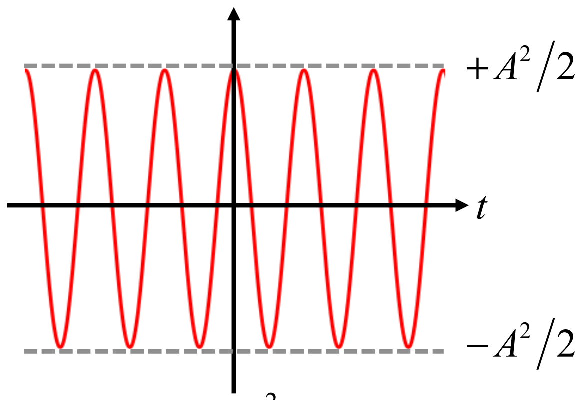


Stochastic process

Case 1: Single cosine wave



$$Y(t) = A\cos(\omega_1 t) \qquad (10)$$



$$\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t) \qquad (11)$$

Stochastic process

$$\varphi_Y(t) = \lim_{T\to\infty}\frac{A^2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \cos(\omega_1\tau)\cos(\omega_1(\tau+t))$$

$$= \lim_{T\to\infty}\frac{A^2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \sin\left(\omega_1\tau+\frac{\pi}{2}\right)\sin\left(\omega_1(\tau+t)+\frac{\pi}{2}\right)$$

$$= \lim_{T\to\infty}\frac{A^2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \sin\left(\omega_1\tau+\frac{\pi}{2}\right)\left[\sin\left(\omega_1\tau+\frac{\pi}{2}\right)\cos(\omega_1 t)+\cos\left(\omega_1\tau+\frac{\pi}{2}\right)\sin(\omega_1 t)\right]$$

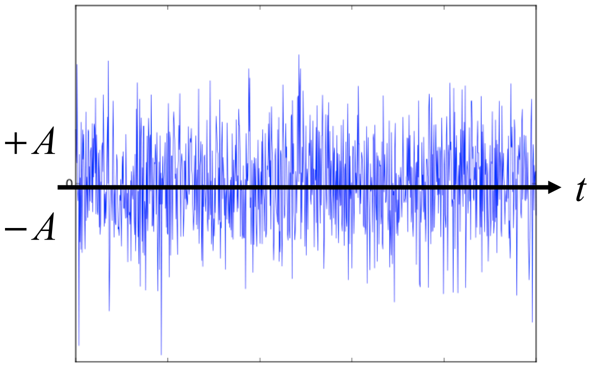
$$= \lim_{T\to\infty}\frac{A^2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \left[\sin^2\left(\omega_1\tau+\frac{\pi}{2}\right)\cos(\omega_1 t)+\sin\left(\omega_1\tau+\frac{\pi}{2}\right)\cos\left(\omega_1\tau+\frac{\pi}{2}\right)\sin(\omega_1 t)\right]$$

$$= \cos(\omega_1 t)\lim_{T\to\infty}\frac{A^2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \sin^2\left(\omega_1\tau+\frac{\pi}{2}\right) + \sin(\omega_1 t)\lim_{T\to\infty}\frac{A^2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \sin\left(\omega_1\tau+\frac{\pi}{2}\right)\cos\left(\omega_1\tau+\frac{\pi}{2}\right)$$

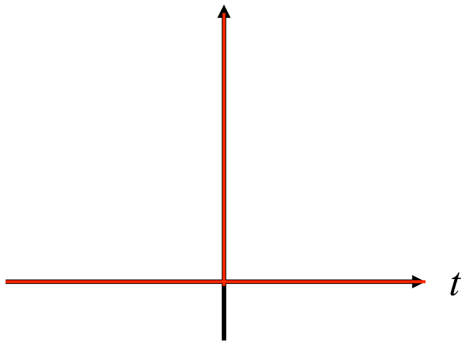
$$= \frac{A^2}{2}\cos(\omega_1 t) + 0 \quad \cdots \quad \text{Eq.}(11)$$

Stochastic process

Case 2: White noise



$$Y(t) = A\xi(t) \qquad (12)$$



$$\varphi_Y(\omega) = A^2\delta(t) \qquad (13)$$

Stochastic process

From Eq.(9),

$$\varphi_Y(t) = \lim_{T\to\infty}\frac{1}{T}\int_{-\infty}^{\infty} d\tau\left[Y_T(\tau)\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega(\tau+t)}\tilde{Y}_T(\omega)\right]\right]$$

$$= \lim_{T\to\infty}\frac{1}{2\pi T}\int_{-\infty}^{\infty} d\omega\left[e^{-i\omega t}\tilde{Y}_T(\omega)\int_{-\infty}^{\infty} d\tau\left[e^{-i\omega\tau}Y_T(\tau)\right]\right]$$

$$= \lim_{T\to\infty}\frac{1}{2\pi T}\int_{-\infty}^{\infty} d\omega\left[e^{-i\omega t}\tilde{Y}_T(\omega)\tilde{Y}_T^*(\omega)\right]$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\left[\lim_{T\to\infty}\frac{1}{T}\left|\tilde{Y}_T(\omega)\right|^2\right] = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} S_Y(\omega) \qquad (14)$$

Stochastic process

And also,

$$S_Y(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \varphi_Y(t) \tag{15}$$

Wiener-Khintchine theorem:

$$\varphi_Y(t) \underset{\text{Foulier Eq.(15)}}{\overset{\text{inverse Foulier Eq.(14)}}{\rightleftharpoons}} S_Y(\omega)$$

Sum rules:

$$\varphi_Y(0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, S_Y(\omega) \tag{16}$$

$$S_Y(0) = \int_{-\infty}^{\infty} dt\, \varphi_Y(t) \tag{17}$$

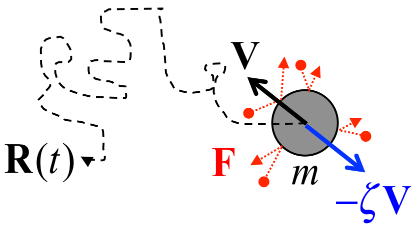
Brownian motion 1: basic theories

Brownian motion and the Langevin equation

Brownian motion and the Langevin equation

Equation of motion of a Brownian particle:

Particle radius:	a
Particle mass:	m
Solvent viscosity:	η
Friction constant:	$\zeta = 6\pi\eta a$
Particle position:	$\mathbf{R}(t)$
Particle velocity:	$\mathbf{V}(t) = d\mathbf{R}/dt$
Friction force:	$-\zeta\mathbf{V}(t)$
Random force:	$\mathbf{F}(t)$



Langevin Equation:

$$m\frac{d\mathbf{V}}{dt} = -\zeta\mathbf{V} + \mathbf{F} \qquad (21)$$

Brownian motion and the Langevin equation

Random force:

$$\mathbf{F}(t) = \left(F_x(t), F_y(t), F_z(t)\right)$$

White noise:

$$\left\langle F_\alpha(t) \right\rangle = 0 \qquad (22)$$

$$\varphi_F(t) \equiv \left\langle F_\alpha(\tau) F_\beta(\tau + t) \right\rangle = 2\tilde{D}\delta_{\alpha\beta}\delta(t) \qquad (23)$$

where $\alpha, \beta \in x, y, z$, and

$$\delta_{\alpha\beta} = 1 \quad (\alpha = \beta), \quad \delta_{\alpha\beta} = 0 \quad (\alpha \neq \beta)$$

$$\delta(t) = \infty \quad (t = 0), \quad \delta(t) = 0 \quad (t \neq 0)$$

Brownian motion and the Langevin equation

Power spectrum of random force $\mathbf{F}(t)$:

$$S_F(\omega) = \lim_{T \to \infty} \frac{1}{T} \left| \tilde{\mathbf{F}}_T(\omega) \right|^2$$

$$= \int_{-\infty}^{\infty} dt \varphi_F(t) e^{i\omega t}$$

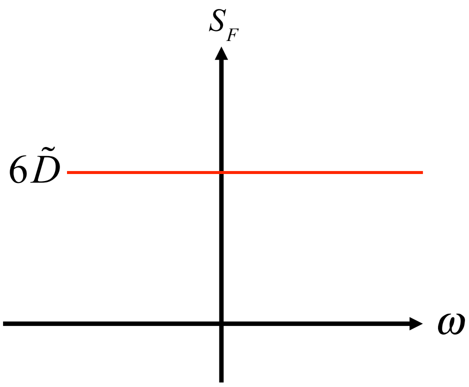
$$= \int_{-\infty}^{\infty} dt \left\langle \mathbf{F}(\tau) \bullet \mathbf{F}(\tau + t) \right\rangle e^{i\omega t}$$

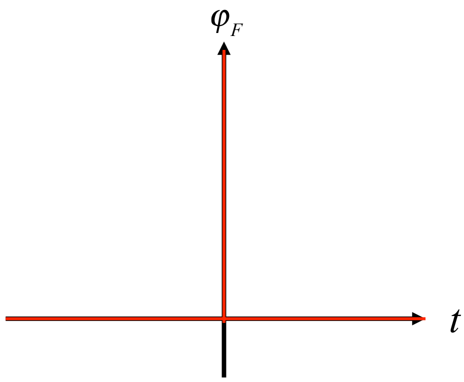
$$= \int_{-\infty}^{\infty} dt 6\tilde{D}\delta(t) e^{i\omega t}$$

$$= 6\tilde{D} \qquad (24)$$

Brownian motion and the Langevin equation

Property of random force $\mathbf{F}(t)$:





$$S_F(\omega) = 6\tilde{D} \qquad \varphi_F(t) = 6\tilde{D}\delta(t)$$

Brownian motion and the Langevin equation

Fourier transform Eq.(1)

$$-i\omega m\tilde{\mathbf{V}}_T(\omega) = -\zeta\tilde{\mathbf{V}}_T(\omega) + \tilde{\mathbf{F}}_T(\omega)$$

$$\tilde{\mathbf{V}}_T(\omega) = \frac{\tilde{\mathbf{F}}_T(\omega)}{-i\omega m + \zeta}$$

Power Spectrum of particle velocity $\mathbf{V}(t)$:

$$S_V(\omega) = \lim_{T\to\infty}\frac{1}{T}\left|\tilde{\mathbf{V}}_T(\omega)\right|^2$$

$$= \lim_{T\to\infty}\frac{1}{T}\left|\tilde{\mathbf{F}}_T(\omega)\right|^2 \frac{1}{m^2\omega^2+\zeta^2} = \frac{6\tilde{D}}{m^2\omega^2+\zeta^2} \qquad (25)$$

Brownian motion and the Langevin equation

Auto-correlation function of particle velocity $\mathbf{V}(t)$:

Using Winner-Khintchine theorem and Eq.(6)

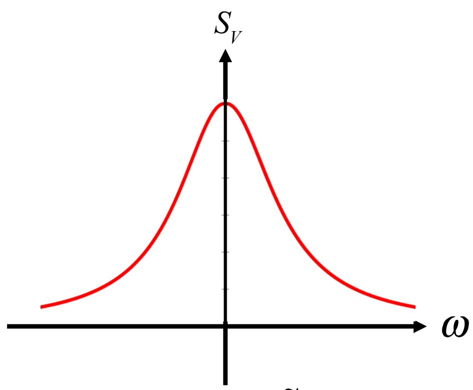
$$\varphi_V(t) \equiv \langle \mathbf{V}(\tau)\cdot\mathbf{V}(\tau+t)\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega S_V(\omega) e^{-i\omega t}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{6\tilde{D}}{m^2\omega^2+\zeta^2} e^{-i\omega t}$$

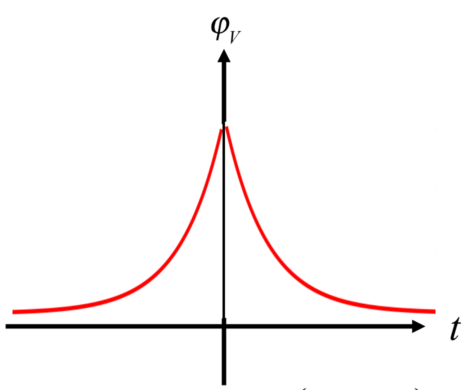
$$= \frac{3\tilde{D}}{\zeta m}\exp\left(-\frac{\zeta}{m}|t|\right) \quad (26)$$

Brownian motion and the Langevin equation

Property of particle velocity $\mathbf{V}(t)$:



$$S_V = \frac{6\tilde{D}}{m^2\omega^2+\zeta^2}$$



$$\varphi_V = \frac{3\tilde{D}}{\zeta m}\exp\left(-\frac{\zeta}{m}|t|\right)$$

Brownian motion and the Langevin equation

From Eq.(26) $\varphi_V(t=0) = \langle \mathbf{V}^2 \rangle = \dfrac{3\tilde{D}}{\zeta m}$

Equipartition of energy $\langle \mathbf{V}^2 \rangle = \dfrac{3k_B T}{m}$

$$\therefore \frac{3\tilde{D}}{\zeta m} = \frac{3k_B T}{m} \quad \rightarrow \quad \boxed{\tilde{D} = k_B T \zeta} \tag{29}$$

Fluctuation-dissipation theorem

Brownian motion and the Langevin equation

Displacement: $\Delta\mathbf{R}(t) \equiv \mathbf{R}(t) - \mathbf{R}(0) = \int_0^t \mathbf{V}(t_1)\,dt_1$

Mean square displacement:

$$\left\langle \left|\Delta\mathbf{R}(t)\right|^2 \right\rangle = \int_0^t dt_1 \int_0^t dt_2 \left\langle \mathbf{V}(t_1)\cdot\mathbf{V}(t_2) \right\rangle$$

$$= \int_0^t dt_1 \int_0^t dt_2 \frac{3\tilde{D}}{\zeta} \exp\left(-\frac{\zeta}{m}\left|t_2 - t_1\right| \right)$$

$$= 2\int_0^t dt_1 \int_{t_1}^t dt_2 \frac{3\tilde{D}}{\zeta} \exp\left(-\frac{\zeta}{m}\left(t_2 - t_1\right) \right) = \frac{6\tilde{D}}{\zeta^2} t + Cons.$$

Brownian motion and the Langevin equation

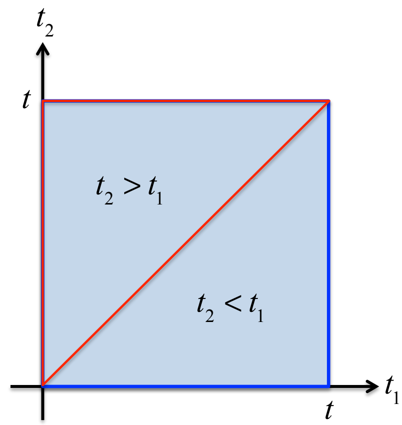
Displacement: $\Delta\mathbf{R}(t) \equiv \mathbf{R}(t) - \mathbf{R}(0) = \int_0^t \mathbf{V}(t_1)\,dt_1$

Mean square displacement:

$$\left\langle \left|\Delta\mathbf{R}(t)\right|^2 \right\rangle = \int_0^t dt_1 \int_0^t dt_2 \left\langle \mathbf{V}(t_1)\bullet\mathbf{V}(t_2)\right\rangle$$

$$= \int_0^t dt_1 \int_0^t dt_2 \frac{3\tilde{D}}{\zeta}\exp\left(-\frac{\zeta}{m}\left|t_2 - t_1\right|\right)$$

$$= 2\int_0^t dt_1 \int_{t_1}^t dt_2 \frac{3\tilde{D}}{\zeta}\exp\left(-\frac{\zeta}{m}\left(t_2 - t_1\right)\right) = \frac{6\tilde{D}}{\zeta^2}t + Cons.$$



Brownian motion and the Langevin equation

Self diffusion constant:

$$D \equiv \lim_{t\to\infty} \frac{\left\langle \left|\Delta\mathbf{R}(t)\right|^2 \right\rangle}{6t} = \frac{\tilde{D}}{\zeta^2} \qquad (30)$$

Einstein relation: (from Eq.(29) and (30))

$$D = \frac{k_B T}{\zeta} \qquad (31)$$

Stokes-Einstein relation: (from Eq.(31) and Stokes law $\zeta = 6\pi a\eta$)

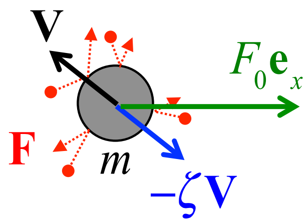
$$D = \frac{k_B T}{6\pi a\eta} \qquad (32)$$

Brownian motion 1: basic theories

Linear response theory and the Green-Kubo formula

Linear response theory and the G-K formula

A Brownian particle under the external force $\mathbf{F}_{ext} = F_0 \mathbf{e}_x$



Langevin Equation:

$$m \frac{d\mathbf{V}}{dt} = -\zeta \mathbf{V} + \mathbf{F} + F_0 \mathbf{e}_x \qquad (41)$$

Linear response theory and the G-K formula

Steady state average under external force, $\lim_{t\to\infty}\langle\cdots\rangle_{ext}$

$$\lim_{t\to\infty}\left\langle\frac{d\mathbf{V}}{dt}\right\rangle_{ext}=(0,0,0)$$

$$\lim_{t\to\infty}\langle\mathbf{V}\rangle_{ext}=\left(\lim_{t\to\infty}\langle V_x\rangle_{ext},0,0\right)$$

$$\lim_{t\to\infty}\langle\mathbf{F}\rangle_{ext}=(0,0,0)$$

$$\lim_{t\to\infty}\langle F_0\mathbf{e}_x\rangle_{ext}=(F_0,0,0)$$

Linear response theory and the G-K formula

Thus, the steady drift velocity:

$$\lim_{t\to\infty}\langle V_x\rangle_{ext}=\frac{F_0}{\zeta}=\frac{DF_0}{k_BT} \qquad (42)$$

Here we used the Einstein relation Eq. (31) and finally:

$$D=\lim_{t\to\infty}\langle V_x\rangle_{ext}\frac{k_BT}{F_0} \qquad (43)$$

Linear response theory and the G-K formula

The linear response theory (LRT):

References:
- Barrat and Hansen "Basic concepts for simple and complex liquids" (Cambridge, 2003)
- Zwanzig "Non-equilibrium statistical mechanics" (Oxford, 2001)

Linear response theory and the G-K formula

The linear response theory (LRT):

References:
- Barrat and Hansen "Basic concepts for simple and complex liquids" (Cambridge, 2003)
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H_0 : Equilibrium Hamiltonian

$H_0 + H'(t)$: Hamiltonian under external force $F(t)$ conjugate with A , $H'(t) \equiv -AF(t)$

Linear response theory and the G-K formula

The linear response theory (LRT):

References:
- Barrat and Hansen "Basic concepts for simple and complex liquids" (Cambridge, 2003)
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H_0 : Equilibrium Hamiltonian

$H_0 + H'(t)$: Hamiltonian under external force $F(t)$ conjugate with A, $H'(t) \equiv -AF(t)$

$\langle B(t) \rangle_{H_0} \equiv B_0$: Average value of B at equilib. under H_0

$\langle B(t) \rangle_{H_0+H'(t)} \equiv B_0 + \langle \Delta B(t) \rangle_{H_0+H'(t)}$

: Average value of B at t under $H_0 + H'(t)$

Linear response theory and the G-K formula

For a small external force with $H'(t) = -AF(t)$, the time evolution of B is determined within LRT as:

$$\langle \Delta B(t) \rangle_{H_0+H'} = \int_{-\infty}^{t} ds\, \Phi_{BA}(t-s) F(s) \quad (44)$$

Here $\Phi_{BA}(t)$ is the response function, which is defined as the cross correlation function of $\dot{A} \equiv \frac{dA}{dt}$ and B at equilibrium:

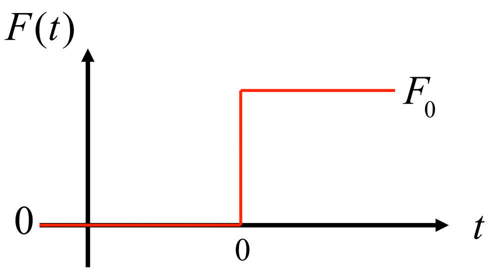
$$\Phi_{BA}(t) = \frac{1}{k_B T} \langle B(\tau + t) \dot{A}(\tau) \rangle_{H_0} \quad (45)$$

Linear response theory and the G-K formula

Apply LRT to define self-diffusion constant D using equilibrium correlation function. We assume:

$$A(t) \equiv R_x(t)\,, \quad B(t) \equiv V_x(t)$$

$$F(t) = \Theta(t)\,, \quad H'(t) = -AF(t) = -R_x F_0 \Theta(t)$$



Linear response theory and the G-K formula

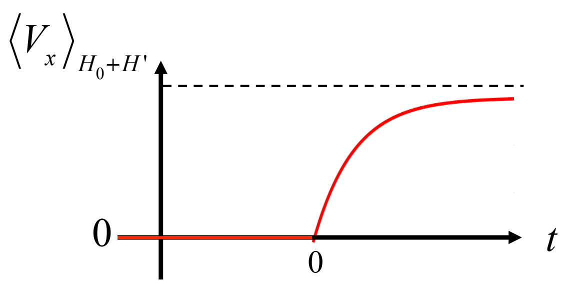
From LRT Eqs. (44) and (45):

$$\left\langle \Delta B(t) \right\rangle_{H_0+H'} = \left\langle V_x(t) \right\rangle_{H_0+H'} = \frac{F_0}{k_B T} \int_0^t ds \left\langle V_x(\tau + t - s) V_x(\tau) \right\rangle_{H_0}$$

$$= \frac{F_0}{k_B T} \int_t^0 dt' \frac{ds}{dt'} \left\langle V_x(\tau + t') V_x(\tau) \right\rangle_{H_0} = \frac{F_0}{k_B T} \int_0^t dt' \left\langle V_x(\tau + t') V_x(\tau) \right\rangle_{H_0}$$

$$= \frac{F_0}{3 k_B T} \int_0^t dt' \left\langle \mathbf{V}(\tau + t') \cdot \mathbf{V}(\tau) \right\rangle_{H_0}$$

$$(t' \equiv t - s)$$



Linear response theory and the G-K formula

From Eqs. (43) and (46):

$$D = \lim_{t\to\infty} \left\langle V_x(t) \right\rangle_{H_0 + H'(t)} \frac{k_B T}{F_0}$$

$$= \frac{1}{3} \int_0^\infty dt' \left\langle \mathbf{V}(\tau + t') \bullet \mathbf{V}(\tau) \right\rangle_{H_0}$$

$$\boxed{D = \frac{1}{3} \int_0^\infty dt \varphi_V(t)} \qquad (47)$$

(Green-Kubo formula for D)

Homework 3

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Homework 3-1

1.0 point possible (graded)

Calculate the auto-correlation function $\varphi_Y(t)$ for a dynamic process $Y(t) = A\sin(\omega_1 t + \pi)$. Choose the correct answer from the following choices.

- $\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t)$
- $\varphi_Y(t) = \frac{A^2}{2}\sin(\omega_1 t)$
- $\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t + \pi)$
- $\varphi_Y(t) = \frac{A^2}{2}\sin(\omega_1 t + \pi)$

Submit You have used 0 of 2 attempts

Homework 3-2

1.0 point possible (graded)

Calculate the auto-correlation function $\varphi_Y(t)$ for a dynamic process $Y(t) = A\cos(\omega_1 t) + B\xi(t)$, where $\xi(t)$ is the White noise introduced in Part 1. Choose the correct answer from the following choices.

- $\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t) + AB\sqrt{\cos(\omega_1 t)\delta(t)} + B^2\delta(t)$
- $\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t) + AB\sqrt{2\cos(\omega_1 t)\delta(t)} + B^2\delta(t)$
- $\varphi_Y(t) = \frac{A^2B^2}{2}\cos(\omega_1 t)\delta(t)$
- $\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t) + B^2\delta(t)$
- $\varphi_Y(t) = \frac{A^2}{2}\cos(\omega_1 t) - B^2\delta(t)$

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Homework 3-3

2.0 points possible (graded)

Estimate the diffusion constant D of spherical particles with radius $a = 1\mu$m immersed in water at $T = 300$K using the Stokes-Einstein relation (Eq.(32))

$$D = \frac{k_B T}{6\pi a \eta}$$

and the following parameters

- Viscosity of water at room temperature: $\eta = 0.85 \times 10^{-3}$ Pa·s
- The Boltzmann constant: $k_B = 1.38064852 \times 10^{-23}$ J·K^{-1}

Choose the value closest to your answer from the following choices.

- 2.6×10^{-7} m^2·s^{-1}
- 2.6×10^{-13} m^2·s^{-1}
- 2.6×10^{-19} m^2·s^{-1}
- 2.6×10^{-7} m^{-2}·s
- 2.6×10^{-13} m^{-2}·s
- 2.6×10^{-19} m^{-2}·s

Submit You have used 0 of 2 attempts

Homework 3-4

1.0 point possible (graded)

Calculate the right-hand-side of Eq.(47) using the correlation function given in Eq.(26).

$$\varphi_V(t) = \frac{3\tilde{D}}{\zeta m} \exp\left(-\frac{\zeta}{m}|t|\right)$$

$$D = \frac{1}{3}\int_0^\infty \mathrm{d}t\, \varphi_V(t)$$

Choose the correct result for D from the following choices.

- $\tilde{D}$
- $6\tilde{D}t$
- $\frac{\tilde{D}}{k_B T \zeta}$
- $\frac{m\tilde{D}}{\zeta}$
- $\frac{\tilde{D}}{\zeta^2}$

Submit You have used 0 of 2 attempts

Homework 3-5

2.0 points possible (graded)

Replace $F_0 \to 2F_0$ in Eq.(41), then redo all the calculations to derive the equation corresponding to equation Eq.(47). Choose the correct equation, relating the diffusion constant D to the velocity auto-correlation funciton $\varphi_V(t)$, from the following choices.

- $D = \frac{2}{3} \int_0^\infty \mathrm{d}t\ \varphi_V(t)$
- $D = \frac{\sqrt{2}}{3} \int_0^\infty \mathrm{d}t\ \varphi_V(t)$
- $D = \frac{1}{3} \int_0^\infty \mathrm{d}t\ \varphi_V(t)$
- $D = \frac{1}{3\sqrt{2}} \int_0^\infty \mathrm{d}t\ \varphi_V(t)$
- $D = \frac{1}{6} \int_0^\infty \mathrm{d}t\ \varphi_V(t)$

Submit You have used 0 of 2 attempts