

Stat. Phys. IV: Lecture 3

Spring 2024

Note on the Fourier transform and spectral densities

The definition of the Fourier transform alters in different references, here we consider (Risken's definition):

Fourier transform

$$\tilde{X}(\omega) = \int_{-\infty}^{\infty} X(t) e^{-i\omega t} dt$$
$$X(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{X}(\omega) e^{i\omega t} d\omega$$

- $1/2\pi$ factor can also be moved to the other side as done in Gardiner and Zoller.
- $2\pi\delta(\omega - \omega') = \int_{-\infty}^{\infty} e^{-i(\omega-\omega')t} dt$
- For a real valued signal: $\tilde{X}(\omega) = \tilde{X}^*(-\omega)$
- Real signals from measurements are limited in time (T). For these signals gated Fourier transform is defined by:

Gated Fourier transform

$$\tilde{X}_T(\omega) = \int_0^T X(t) e^{-i\omega t} dt$$

Stochastic processes

Autocorrelation (For Ergodic processes)

$$C_{XX}(\tau) = \langle X(t)X(t + \tau) \rangle$$

$$\begin{aligned}\langle \tilde{X}(\omega)\tilde{X}^*(\omega') \rangle &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle X(t)X(t + \tau) \rangle e^{-i(\omega-\omega')t} e^{-i\omega\tau} dt d\tau = \\ &= 2\pi\delta(\omega - \omega') \int_{-\infty}^{\infty} C_{XX}(\tau) e^{-i\omega\tau} d\tau\end{aligned}$$

Wiener-Khinchin theorem

$$2\pi\delta(\omega - \omega') S_{XX}(\omega) = \langle \tilde{X}(\omega)\tilde{X}^*(\omega') \rangle$$

$$S_{XX}(\omega) = \int_{-\infty}^{\infty} C_{XX}(\tau) e^{-i\omega\tau} d\tau$$

Power spectral density with gated Fourier transform

We can define the power of a stochastic process $X(t)$ as:

$$P = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle |X(t)|^2 \rangle dt = \int_{-\infty}^{+\infty} \underbrace{\lim_{T \rightarrow \infty} \frac{\langle |\tilde{X}_T(\omega)|^2 \rangle}{T}}_{S_{XX}(\omega)} d\omega$$

Power spectral density with gated Fourier transform

$$S_{XX}(\omega) = \lim_{T \rightarrow \infty} \frac{\langle |\tilde{X}_T(\omega)|^2 \rangle}{T}$$

Another approach is to define gated Fourier transform as: $\tilde{X}'_T(\omega) = \frac{1}{\sqrt{T}} \int_0^T X(t) e^{-i\omega t} dt$.
In this case we can define power spectral density as:

$$S_{XX}(\omega) = \lim_{T \rightarrow \infty} \langle |\tilde{X}'_T(\omega)|^2 \rangle$$

Two-force hypothesis (molecular impingement model)¹

Langevin equation

$$m \frac{dv}{dt}(t) = -\gamma v(t) + f\Gamma(t) \text{ with } f = \sqrt{2\gamma k_B T} \text{ (from equipartition)}$$

- γ : drag coefficient; $\Gamma(t)$: Gaussian white noise.
- This equation can be derived by considering velocity of a particle as a Markov jump process (also called a continuous-time random walk) in 1D
- for $P(v, t)$ (probability of the particle having velocity v at time t) we can derive (by invoking Boltzmann distribution):

Fokker-Planck equation

$$\partial_t P(v, t) = \frac{\gamma}{m} \partial_v [v P(v, t)] + \frac{\gamma k_B T}{m^2} \partial_v^2 P(v, t)$$

- it can be shown using the Kramers-Moyal expansion that this is equivalent to the Langevin-equation

¹D. T. Gillespie. "Fluctuation and dissipation in Brownian motion". In: *Am. J. Phys.* 51.1077 (1993).

A molecular impingement model of Brownian motion²

Jumping probabilities:

$$W_+(v) = B(1 - v/A) \text{ and } W_-(v) = B(1 + v/A)$$

Leading to the Fokker-Planck equation:

Fokker-Planck equation

$$\frac{\partial}{\partial t} P(v, t) = C_1 \frac{\partial}{\partial v} [v P(v, t)] + C_2 \frac{\partial^2}{\partial v^2} P(v, t)$$

$$\text{where } C_1 = \lim_{N \rightarrow \infty} \frac{2B}{N} \text{ and } C_2 = \lim_{N \rightarrow \infty} \frac{BA^2}{N^2}$$

Note: as $N \rightarrow \infty$, also $A \rightarrow \infty$ in a way that $\Delta = \frac{A}{N} \rightarrow 0$

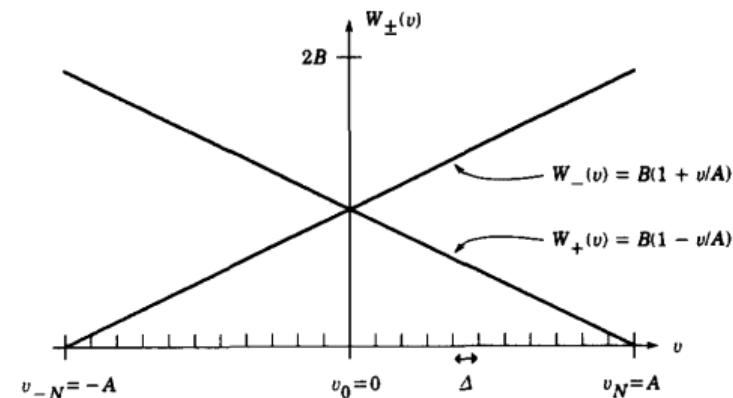


Fig. 2. Graphs of the stepping functions $W_{\pm}(v)$ in Eqs. (31).

²See "Fluctuation and dissipation in Brownian motion" by Gillespie

Wiener increment, Itō's lemma

- given a stochastic process $X(t)$ which obeys

$$dX = A(X(t), t)dt + \sqrt{D(X(t), t)}dW$$

- $dW = \Gamma(t)dt = \lim_{dt \rightarrow \infty} \left[\mathcal{N}(0, 1)/\sqrt{dt} \right] dt$: Wiener increment
- What does the increment look like for $f(X(t))$?

Itō's lemma

$$df = \left(A(X(t), t)f' + \frac{1}{2}D(X(t), t)f'' \right) dt + \sqrt{D(X(t), t)}f'dW$$

Summary of Fluctuation dissipation theorems

Langevin approach to Brownian motion → Einstein relation:

$$D = \int_0^\infty \langle v(t)v(t+t') \rangle dt' = \frac{k_B T}{m\gamma}$$

Case of Johnson noise in an electric circuit:

$$R^{-1} = \frac{1}{k_B T} \int_0^\infty \langle I(t)I(t+t') \rangle dt'$$

Generally the damping can be frequency dependent³. For the equation of motion:

$$\dot{v}(t) = - \int_0^t \gamma(t-s)v(s)ds + \frac{F(t)}{m} , \quad (1)$$

we can prove the Generalised Fluctuation Dissipation Theorem (GFDT).

Generalised Fluctuation Dissipation Theorem

$$m\gamma[\omega] = \frac{1}{k_B T} \int_0^\infty \langle F(t_0)F(t_0+t) \rangle e^{-i\omega t} dt$$

³Herbert B. Callen and Theodore A. Welton. "Irreversibility and Generalized Noise". In: *Physical Review*

Proof of GFDT⁴

We start with equation (1) and define the susceptibility as $\chi[\omega] = \frac{1}{m(i\omega + \gamma[\omega])}$, so that $v[\omega] = \chi[\omega]F[\omega]$. We then have to prove: Lemma I:

$$\langle v(t)v(0) \rangle = k_B T \chi(t) ,$$

Lemma II:

$$\int_{-\infty}^{\infty} \langle F(t)F(0) \rangle e^{-i\omega t} dt = 2k_B T \operatorname{Re}\{\chi^{-1}[\omega]\} .$$

With these two steps we can prove the GFDT

Generalised Fluctuation Dissipation Theorem

$$m\gamma[\omega] = \frac{1}{k_B T} \int_0^{\infty} \langle F(t_0)F(t_0 + t) \rangle e^{-i\omega t} dt$$

⁴R. Kubo. "The fluctuation-dissipation theorem". en. In: *Reports on Progress in Physics* 29.1 (1966), p. 255. ISSN: 0034-4885.

GFDT in the quantum limit⁵

$$\langle V^2 \rangle = \frac{2}{\pi} \int_0^\infty R(\omega) \left(\frac{1}{2} \hbar \omega + \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} \right) d\omega$$

reducing in the classical limit to

$$\langle V^2 \rangle \approx \frac{2}{\pi} k_B T \int_0^\infty R(\omega) d\omega$$

- V : fluctuating force
- $R(\omega)$: real part of impedance $Z(\omega)$
- $Z(\omega)$: impedance defined as $V = Z(\omega) \dot{Q}$ with response \dot{Q}

⁵Herbert B. Callen and Theodore A. Welton. "Irreversibility and Generalized Noise". In: *Physical Review* 83.1 (July 1951), pp. 34–40.

Alternative formulations of the GFDT⁶⁷

We take the example of a damped harmonic oscillator so that the displacement $\delta x[\omega]$ is related to the Langevin force by:

$$\delta x[\omega] = \chi[\omega] F_T[\omega] \text{ with } \chi[\omega] = \frac{1}{M(\omega_M^2 - \omega^2 - i\omega_M^2 \phi[\omega])} \quad (2)$$

In this formulation we can write the fluctuation dissipation theorem as (S_{F_T} is the spectrum of the langevin force):

$$S_{F_T}[\omega] = -\frac{2k_B T}{\omega} \text{Im} \left\{ \frac{1}{\chi[\omega]} \right\}$$

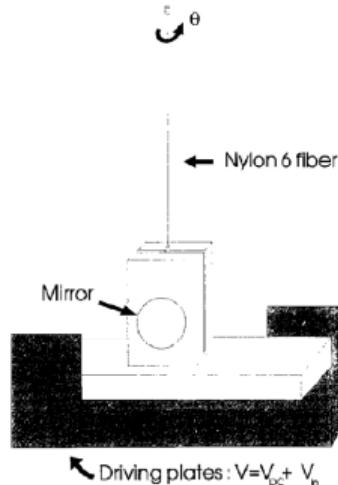
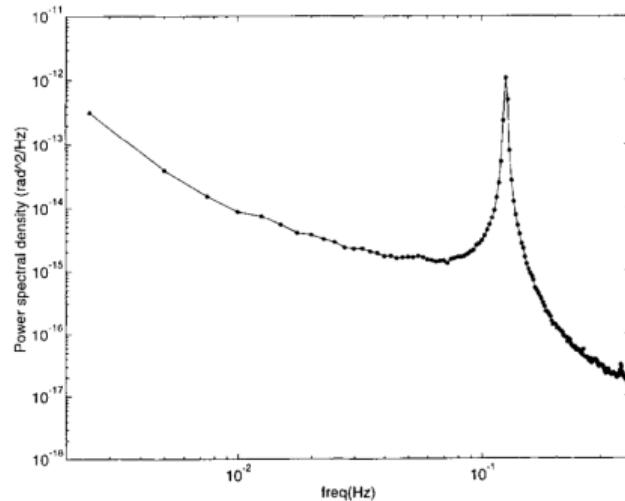
In this formulation $\phi[\omega]$ is the imaginary part of Hooke's law responsible for internal damping in materials:

$$F_{\text{Hooke}} = -M\omega_M^2(1 - i\phi[\omega])\delta x$$

⁶M. Pinard et al. "Full mechanical characterization of a cold damped mirror". In: *Physical Review A* 63.1 (Dec. 2000). arXiv: quant-ph/0008004. ISSN: 1050-2947, 1094-1622.

⁷Peter R. Saulson. "Thermal noise in mechanical experiments". In: *Physical Review D* 42.8 (Oct. 1990), pp. 2437–2445.

Structural damping in solid state resonators⁸



- Phenomenologically, in solid state resonators (from macro- to micro- scale) the loss angle $\phi[\omega]$ is weakly frequency dependent
- This is in contrast to an oscillator with viscous damping, where $\phi[\omega] = \gamma\omega/\omega_M^2$, i.e. increases linearly with frequency

⁸Peter R. Saulson. "Thermal noise in mechanical experiments". In: *Physical Review D* 42.8 (Oct. 1990), pp. 2437–2445.

Simulation of stochastic process using Python



Simulation

We simulate the Ornstein–Uhlenbeck process using the formula

$$V[k + 1] = V[k] + \gamma V[k] \Delta t + \sqrt{c} N \sqrt{\Delta t},$$

for the velocity.

```
[15]: V = np.zeros([N, N_step])
V[:,0] = v0

Normal = np.random.normal(0,1,[N,N_step])

for i in range(N):
    for j in range(N_step-1):
        V[i,j+1] = V[i,j] - gamma * V[i,j] * dt + np.sqrt(c) * Normal[i,j] * np.sqrt(dt)
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Brownian Motion Simulation

March 2019

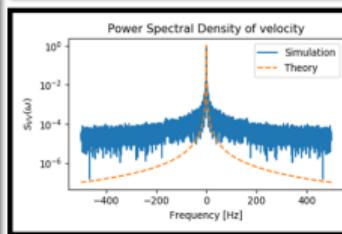
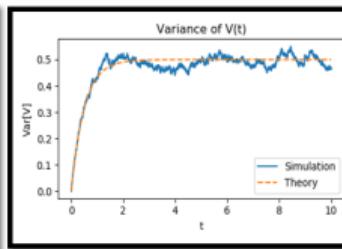
Dynamics of a continuous Markov process $V(t)$ (e.g. velocity of a particle moving in a fluid) is given by an update formula with the form

$$V(t + dt) = V(t) + A(V(t), t)dt + \sqrt{D(V(t), t)}N(t)\sqrt{dt}, \quad (1)$$

where $A(V(t), t)$ and $D(V(t), t)$ are two smooth functions and $N(t)$ is a temporally uncorrelated unit normal random variable

$$N(t) \sim \mathcal{N}(0, 1).$$

This dynamics can be also expressed as a stochastic differential equation

$$\frac{dV}{dt} = A(V(t), t) + \sqrt{D(V(t), t)}\Gamma(t), \quad (2)$$


Questions for paper presentation

- Explain briefly how LIGO is used to detect gravitational wave.
- What are the possible noise sources in an interferometer?
- What is the normal mode analysis and when does it fail? How does the normal mode analysis allow one to compute the noise?
- Explain various dissipation mechanisms in mechanical resonators, and how they are modeled?
- Explain the difference between the scaling of the bulk damping and the surface damping.

