Lecture 6

Derivation of Langevin Dynamics from the Generalized Langevin Equation

CONTENTS

I. THE GENERALIZED LANGEVIN EQUATION

The Kac-Zwanzig model is a system made of a particle of mass M connected to N harmonic oscillators with physical characteristics $\{\omega_i,\, k_i,\, m_i\}$ (respectively, the angular frequencies, the spring constants, and the masses). The complete Hamiltonian function gives rise to $2N+2$ equations of motions, respectively 2 for the position and momentum $\{Q(t),\, P(t)\}$ of the particle, and $2N$ for the positions and the momenta $\{q_i(t),\, p_i(t)\}$ of the oscillators. On the other hand, the system of equations can be rewritten as a system of only two equations for the particle:

$$\begin{cases} \dot{Q} = \dfrac{P}{M}\,, \\ \dot{P} = -\nabla V(Q(t)) - \displaystyle\int_0^t ds\, \dot{Q} K(t-s) + R(t)\,, \end{cases} \tag{1}$$

where the second equation is known as Generalized Langevin Equation (GLE). The GLE is made of three terms: (i) a Markovian term $\nabla V(Q(t))$ that depends only on the state of the system at time t; (ii) a non-Markovian term

$$\int_0^t ds\, \dot{Q} K(t-s)\,, \tag{2}$$

which conserves the story of the particle by means of the memory kernel

$$K(t) = \sum_{i=1}^{N} k_i \cos(\omega_i t)\,; \tag{3}$$

(iii) a noise term that depends on the initial momenta, positions and the physical characteristics of the oscillators

$$R(t) = \sum_{i=1}^{N} k_i \left[q_i(0) - Q(0)\right] \cos(\omega_i t) + \frac{k_i}{m_i \omega_i} p_i(0) \sin(\omega_i t)\,. \tag{4}$$

The choice of physical parameters, positions and initial moments of the oscillators determines the shape of the memory kernel and the noise term. Consider the physical parameters [1]:

$$\begin{cases} \omega_i = N^a u_i \\ k_i = \dfrac{2}{\pi} \dfrac{\alpha^2 M \gamma}{\alpha^2 + \omega_i^2} \Delta\omega \\ m_i = \dfrac{k_i}{\omega_i^2} \end{cases}\,, \tag{5}$$

where $u_i \sim \mathcal{U}[0,1]$ is a random number drawn from the uniform distribution, $a \in [0,1]$, $\alpha > 0$ is a parameter with units $[\mathrm{rad} \cdot \mathrm{time}]^{-1}$, M is the mass of the particle and γ is a friction parameter with units $[\mathrm{time}^{-1}]$ that describes the collision rate between the particle and the oscillators. It follows that $\sum \Delta\omega \xrightarrow{N\to\infty} \int d\omega$ in the memory kernel which is rewritten as inverse Fourier cosine transform:

$$\begin{aligned} K(t) &= \frac{2}{\pi} \int_0^\infty d\omega\, \frac{\alpha^2 M \gamma}{\alpha^2 + \omega_i^2} \cos(\omega_i t) && (6) \\ &= \alpha M \gamma e^{-\alpha t}\,. && (7) \end{aligned}$$

Regarding the noise term, assuming that the oscillators are in thermal equilibrium, we draw the initial positions $q_i(0)$ and the initial momenta $p_i(0)$ from the Boltzmann distribution, and we rewrite $R(t)$ as

$$R(t) = \sqrt{\frac{1}{\beta}} \sum_{i=1}^{N} \sqrt{k_i} \left[\xi_i \cos(\omega_i t) + \eta_i \sin(\omega_i t)\right] , \tag{8}$$

where $\xi, \eta_i \in \mathcal{N}(0,1)$ are random number drawn from the normal distribution, $\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the temperature.

We refer to Lecture Notes 4 and 5 for details about the derivation of the Generalized Langevin Equation, the memory kernel, and the noise term.

II. THE FLUCTUATION-DISSIPATION THEOREM

The non-Markovian term and the noise term in the GLE describe the interaction between the particle and the oscillators, which can occur in two ways. On the one hand we have a force that opposes the motion of the particle. This can be interpreted as a frictional force of the environment, represented by the oscillators in the Kac-Zwanzig model, acting on the particle. On the other hand we have an apparently random force that transfers energy from the environment (the oscillators) to the particle.

This intuitive fact is formally expressed by the relationship

$$\langle R(0)R(t)\rangle = \frac{1}{\beta} K(t) \,, \tag{9}$$

which connects the memory kernel and the autocorrelation function of the noise term (see Appendix A for details).

Eq. 9, derived and called the second fluctuation-dissipation theorem (FDT) by R. Kubo in 1966 [2], can be understood as a manifestation of the relationship between the memory kernel and the noise term which collectively account for two distinct aspects of the particle's interaction with the surrounding environment (the friction and the random collisions). The FDT requires the oscillators to be in thermal equilibrium but does not require a specific formula for the physical parameters of the oscillators. For example, fig. 1 shows the validity of the FDT for three different choices of physical parameters of the oscillators: (i) $\omega_i = 1$, $k_i = 0.01$, $m_i = 1\ \forall i$; (ii) $\omega_i \propto N$, $k_i = 0.01$, $m_i \propto 1/N^2\ \forall i$; (iii) ω_i, k_i, m_i as in eqs. 5 with $a = 1/3$, $\alpha = 1$, $\gamma = 1.5$, $M = 1$.

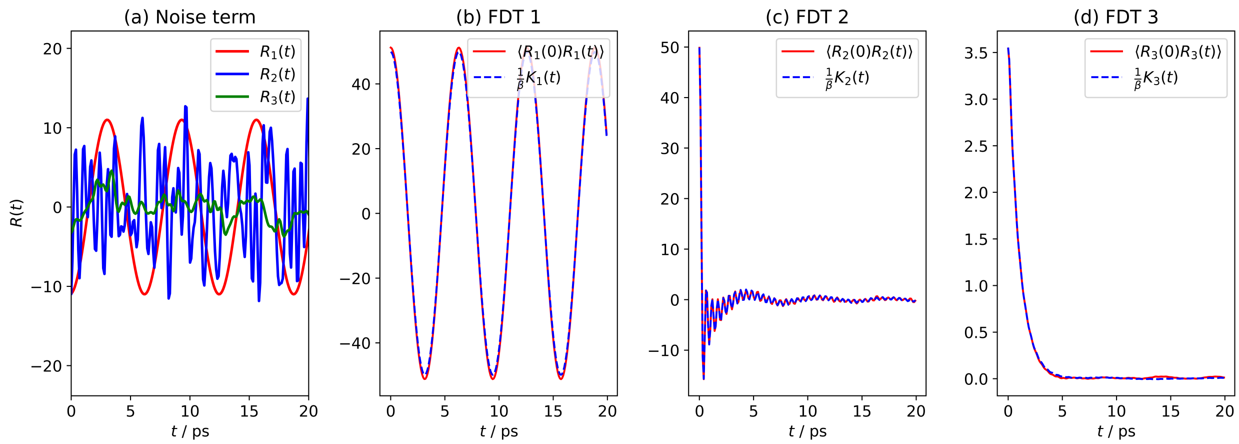

FIG. 1. Noise term (a) and FDT (b,c,d) for three different set of parameters ω_i, k_i, m_i with $N = 2000$ oscillators in thermal equilibrium.

Of particular interest is the third case, where the memory kernel converges to an exponential function (see eq. 7 and Lecture Notes 5 for details) that depends on the α parameter. When $\alpha \to \infty$, the exponential function becomes narrow and peaked (see fig. 2), and it can be approximated as a delta function:

$$K(t) = 2\gamma M \delta(t)\,. \tag{10}$$

Consequently, the FDT (eq. 11) becomes

$$\langle R(0)R(t)\rangle = \frac{2\gamma M}{\beta}\delta(t)\,, \tag{11}$$

which is known as first fluctuation-dissipation theorem.

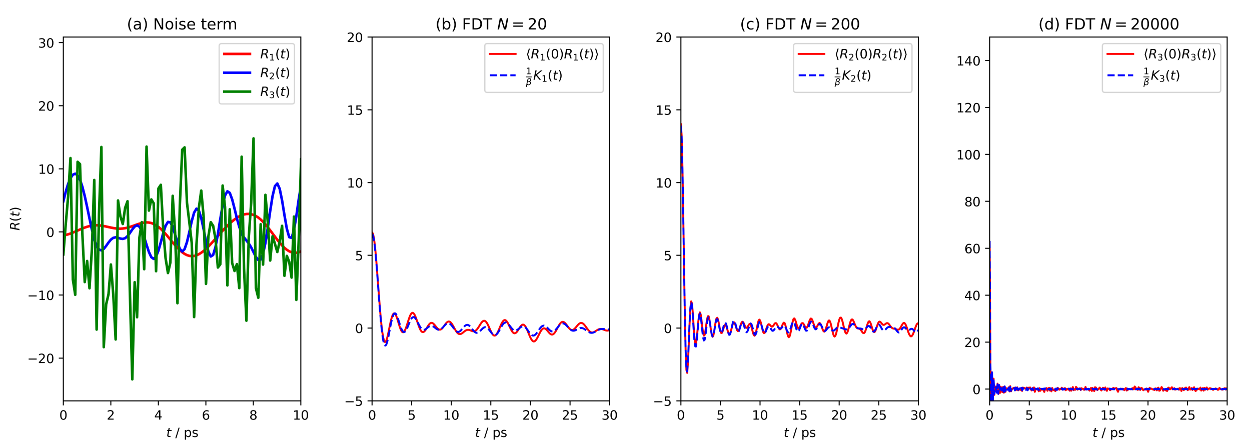

FIG. 2. Noise term (a) and FDT (b,c,d) for $N = 20$, 200, 20000 oscillators in thermal equilibrium.

III. SPECTRAL ANALYSIS OF NOISE TERM

The function defined in eq. 4 expresses the noise term as the sum of sinusoidal functions that depend on the angular frequencies of the oscillators of the system. The Fourier transform, then allows the noise term to be expressed as a function of the angular frequencies of the oscillators:

$$\hat{R}(\omega) = \int_{-\infty}^{\infty} dt\, R(t)\; e^{-i\omega t}\,. \tag{12}$$

To know which frequencies contribute most to the signal, we can then calculate the power spectrum

$$S(\omega) = \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} |\hat{R}_t(\xi)|^2\,, \tag{13}$$

where $\mathcal{T}$ is the length of the signal. For more details about the Fourier transform and the spectral analysis, see Appendix B.

In fig. 3), we report the power spectrum of the noise term for $N = 20,\, 200,\, 20000$ oscillators. We observe that by increasing the number of oscillators, the range of frequencies widens. This is because we have defined frequencies as a function of the number of oscillators (see eq. 4 and fig. 4). Additionally, if $N \to \infty$, then the power spectrum converges to the power spectrum of the white noise, which is constant over the entire domain of the frequencies.

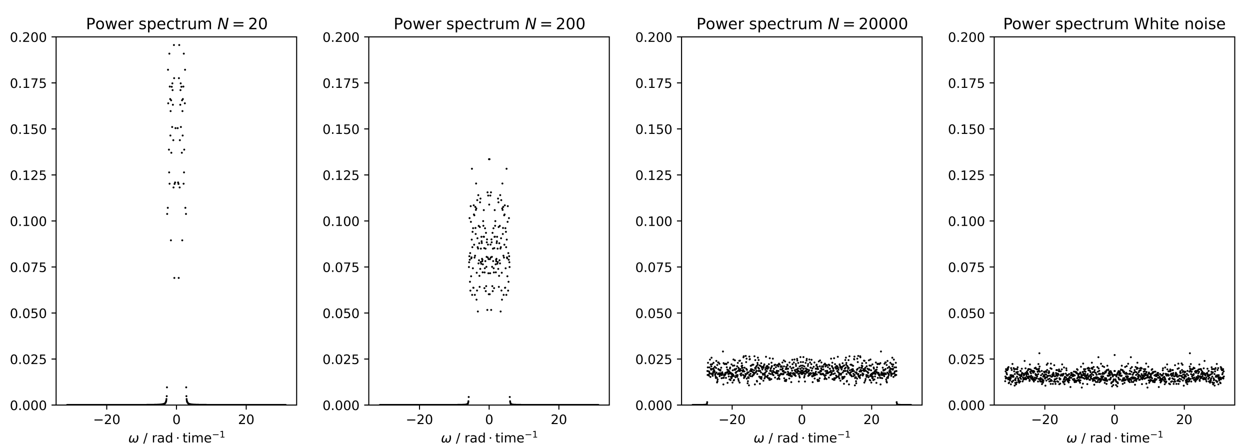

FIG. 3. Power spectrum of the noise term with $N = 20,\, 200,\, 20000$ oscillators in thermal equilibrium (a,b,c) and power spectrum of the white noise (d).

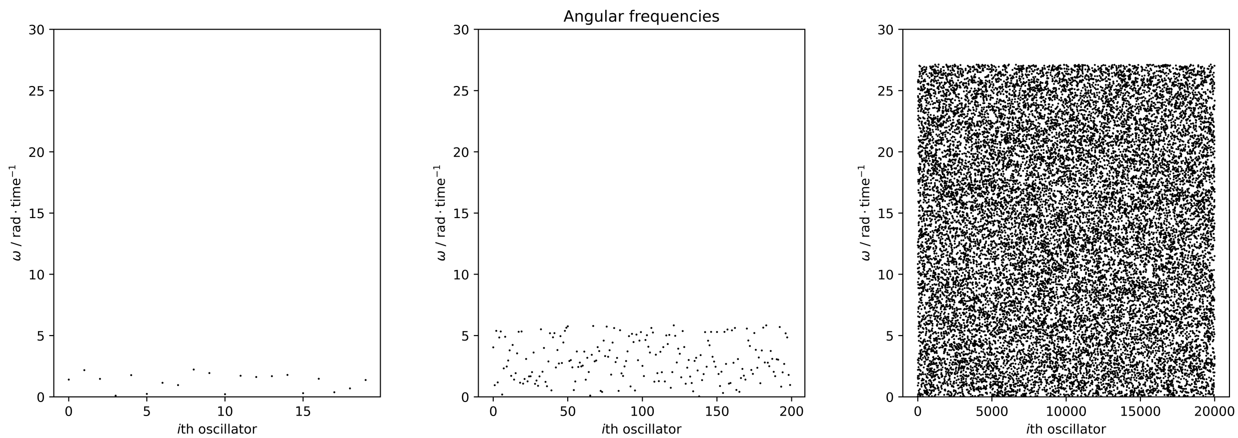

FIG. 4. Angular frequencies corresponding generated by eq. 5, corresponding to the power spectra in fig. 3.

IV. LANGEVIN DYNAMICS

The GLE (eq. 1), can be reduced to the equation of the Langevin Dynamics

$$\dot{P} = -\nabla V(Q) - \gamma P(t) + \sigma\eta(t)\,, \tag{14}$$

where we used eq. 10 in the non-Markovian term

$$\begin{aligned} \int_0^t ds\, \dot{Q} K(t-s) &\approx 2\gamma M \int_0^t ds\, \dot{Q}\delta(t-s) && (15) \\ &= M\gamma\dot{Q} && (16) \\ &= \gamma P\,, && (17) \end{aligned}$$

and the noise term has been replaced by a white noise process with properties

$$\begin{cases} \langle \eta(t) \rangle = 0\,, \\ \langle \eta(t),\, \eta(t') \rangle = \delta(t-t')\,, \end{cases} \tag{18}$$

multiplied by the variance

$$\sigma^2 = \frac{2\gamma M}{\beta}\,, \tag{19}$$

derived by eq. 11.

Appendix A: Autocorrelation function

In eq. 9, we introduced the autocorrelation function of a time-dependent variable $f(t)$

$$\begin{aligned} C(t) &= \langle f(0) f(t) \rangle && \text{(A1)} \\ &= \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} ds\, f(s) f(s+t)\,, && \text{(A2)} \end{aligned}$$

where $\mathcal{T}$ is an arbitrary large time value. In case the timeline is discretized into N equally spaced time intervals of length Δt, eq. (A2) is approximated as:

$$\begin{aligned} C(t) &= \langle f(0) f(\tau) \rangle && \text{(A3)} \\ &\approx \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \sum_k^N f(t_k) f(t_{k+n}) \Delta t && \text{(A4)} \\ &= \lim_{N\to\infty} \frac{1}{N} \sum_i^N f(t_k) f(t_{k+n})\,, && \text{(A5)} \end{aligned}$$

where we used $\mathcal{T} = N\Delta t$ and $t = n\Delta t$. Note that in practical applications, where time $\mathcal{T}$ is a finite number, eq. A5 is further approximated as

$$\begin{aligned} C(t) &= \langle R(0) R(\tau) \rangle && \text{(A6)} \\ &\approx \frac{1}{N-n} \sum_k^{N-n} f(t_k) f(t_{k+n})\,. && \text{(A7)} \end{aligned}$$

Appendix B: Fourier transform and spectral analysis

Consider a continuous integrable time-dependent function $f(t) : \mathbb{R} \to \mathbb{C}$, the Continuous Fourier transform (CFT) is written as

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} dt\, f(t)\; e^{-2\pi i\, \xi t}\,, \tag{B1}$$

where ξ are ordinary frequencies with units [time^{-1}]. Note that if the function $f(x)$ is defined on a space-domain (i.e. it is a function of some variable with [length] units), the frequencies ξ are called wavenumbers and the units are [length^{-1}].

Alternatively, we introduce the angular frequencies $\omega = 2\pi\xi$ with units [rad $\cdot$ time^{-1}], and the Fourier transform is written as

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} dt\, f(t)\; e^{-i\omega t}\,. \tag{B2}$$

The corresponding inverse Fourier transforms are written as

$$f(t) = \int_{-\infty}^{\infty} d\xi \, \hat{f}(\xi) \; e^{-2\pi i \, \xi t} \,, \tag{B3}$$

and

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \, \hat{f}(\omega) \; e^{-i\omega t} \,. \tag{B4}$$

The idea behind the Fourier transform is that a function in the time-domain (or space-domain or other-variable-domain), can be decomposed as a sum of complex exponential functions that depend on certain frequencies. The transform and its inverse therefore allow to transform a function defined on the time-domain into a function defined on the frequency-domain, and vice versa.

1. Fourier transform with numpy.fft.fft()

Consider a discrete time-dependent variable $f(t)$ evaluated on N discrete points $t_0, \, t_1, \, \dots, \, t_{N-1}$. Then the CFT is approximated by the Discrete Fourier Transform (DFT)

$$\hat{f}(\xi) := \hat{f}(m\Delta\xi) \tag{B5}$$

$$\approx \sum_{n=0}^{N-1} f(t_0 + n\Delta t) \exp\left[-2\pi i \,(t_0 + n\Delta t)\, m\Delta\xi\right] \, \Delta t \,, \tag{B6}$$

where we used $\xi = m\Delta\xi$ and $t = t_0 + n\Delta t$. Inserting the frequency resolution $\Delta\xi = {}^{1}\!/_{N\Delta t}$ into eq. B6 and rearranging the equation yields

$$\hat{f}(m\Delta\xi) \approx \exp\left(2\pi i \, t_0 \, m\Delta\xi\right) \, \Delta t \sum_{n=0}^{N-1} f(t_0 + n\Delta t) \exp\left(-2\pi i \frac{nm}{N}\right) \tag{B7}$$

$$= \exp\left(2\pi i \, t_0 \, m\Delta\xi\right) \, \Delta t \bar{f}(\xi) \,. \tag{B8}$$

In applications, the function $\bar{f}(\xi)$ can be approximated using the Fast Fourier Transform (FFT) algorithm. With Python and NumPy, it can be estimated as

$$\bar{f}(\xi) = \mathsf{numpy.fft.fft(f)} \tag{B9}$$

where f is a numpy array containing the values $f(t_0), \, f(t_1), \, \dots, \, f(t_{N-1})$. Note that, if $t_0 = 0$, then

$$\hat{f}(m\Delta\xi) \approx \Delta t \bar{f}(\xi) \;. \tag{B10}$$

To produce the array of the ordinary frequencies, it is possible to use the function

$$\mathsf{xi} = \mathsf{numpy.fft.fftfreq(Nsteps,\ dt)}\ , \tag{B11}$$

which can be converted in angular frequencies:

$$\mathsf{omega} = 2 * \mathsf{numpy.pi} * \mathsf{xi}\,. \tag{B12}$$

2. The power spectrum

Signal processing theory introduces the concept of energy carried by a signal $f(t)$ (not to be confused with physical energy in [Joule] units), defined as

$$E = \int_{-\infty}^{\infty} dt\, |f(t)|^2 \tag{B13}$$

$$= \int_{-\infty}^{\infty} d\xi\, |\hat{f}(\xi)|^2\,. \tag{B14}$$

where we applied Parseval's theorem in the second equality. The integrand of eq. B14 is the energy spectral density

$$\bar{S}(\xi) = |\hat{f}(\xi)|^2\,, \tag{B15}$$

which describes which frequencies contribute most to the transport of energy.

Likewise, we introduce the concept of power of the signal $f(t)$ of length $\mathcal{T}$:

$$P = \lim_{T\to\infty} \frac{1}{\mathcal{T}} \int_{t_0-\mathcal{T}/2}^{t_0+\mathcal{T}/2} dt\, |f(t)|^2\,, \tag{B16}$$

and the power spectrum in ordinary frequencies is defined as

$$S(\xi) = \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} |\hat{f}_t(\xi)|^2\,, \tag{B17}$$

or, in angular frequencies, as

$$S(\omega) = \lim_{\mathcal{T}\to\infty} \frac{1}{2\pi\mathcal{T}} |\hat{f}(\omega)|^2\,, \tag{B18}$$

where the factor $1/2\pi$ guarantees that

$$\mathrm{var}(f(t)) = \langle f(t)^2 \rangle = \int_{-\infty}^{\infty} d\xi\, S(\xi) = \int_{-\infty}^{\infty} d\omega\, S(\omega)\,. \tag{B19}$$

according to the Wiener–Khinchin theorem.

In fig. 5, we report the power spectrum of the Gaussian white noise.

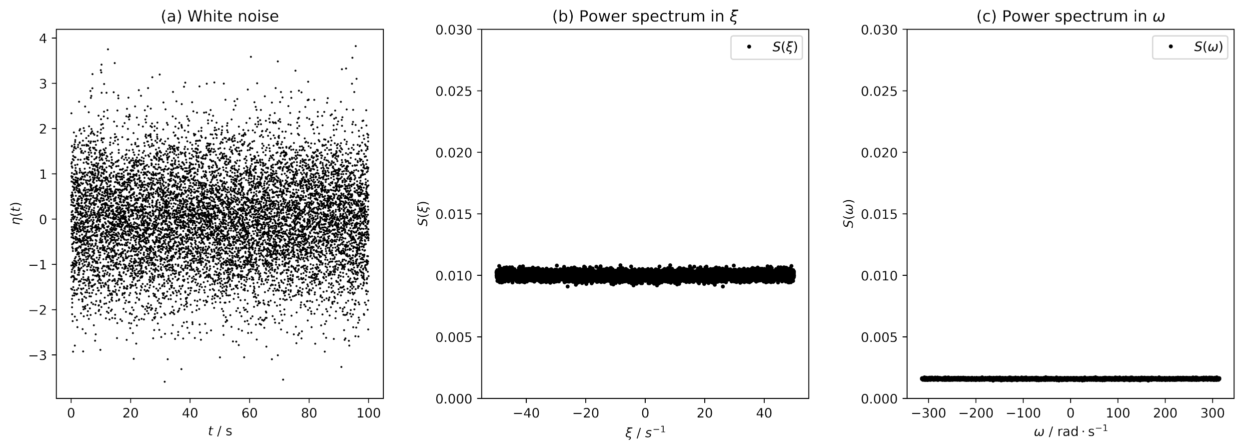

FIG. 5. Example of white noise (a) and power spectrum (b,c) with ordinary and angular frequencies.

3. The Wiener–Khinchin theorem

The Wiener–Khinchin theorem states that

$$\langle f(0)f(t)\rangle = \int_{-\infty}^{\infty} d\xi\, S(\xi) e^{2\pi i\,\xi t}\,, \tag{B20}$$

and

$$S(\xi) = \int_{-\infty}^{\infty} dt\, \langle f(0)f(t)\rangle\; e^{-2\pi i\,\xi t}\,. \tag{B21}$$

[1] R. Kupferman, A. M. Stuart, J. R. Terry, and P. F. Tupper, Long-term behaviour of large mechanical systems with random initial data, Stochastics and Dynamics **02**, 533 (2002).

[2] R. Kubo, The fluctuation-dissipation theorem, Rep. Prog. Phys. **29**, 255 (1966).