Lecture 5

The Generalized Langevin Equation

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CONTENTS

I. THE GENERALIZED LANGEVIN EQUATION

Consider a particle of mass M governed by the one-dimensional potential energy function $V(Q) : \Omega \subset \mathbb{R} \to \mathbb{R}$. The dynamics of the particle is fully described by the pair of time-dependent variables $\{Q(t),\, P(t)\}$, where Q denotes the position, and P denotes the moment $P = M\dot{Q}$. Assume that the particle interact with N one-dimensional oscillators of mass m_i, position q_i and momentum p_i, with $i = 1, 2, \ldots, N$, through a potential $0.5k_i(Q - q_i)^2$, where k_i is a spring constant with units [force length^{-1}].

The complete Hamiltonian that describes the dynamics of the system is written as

$$H(Q, P; q_1, p_1; q_2, p_2, \ldots; Q_N, P_N) = \frac{P^2}{2M} + \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(Q) + \frac{1}{2}\sum_{i=1}^{N} k_i(q_i - Q)^2\,, \tag{1}$$

the equations of motion of the particle are

$$\begin{cases} \dot{Q} &= \dfrac{P}{M}\,, \\ \dot{P} &= -\nabla V(Q) - \displaystyle\sum_{i=1}^{N} k_i(Q - q_i)\,, \end{cases} \tag{2}$$

the equations of motion of the oscillators are

$$\begin{cases} \dot{q}_i &= \dfrac{p_i}{m_i}\,, \\ \dot{p}_i &= k_i(Q - q_i)\,, \end{cases} \qquad \forall i = 1...N\,. \tag{3}$$

The entire system of $2N + 2$ equations of motion can be reduced to 2 equations

$$\begin{cases} \dot{Q} = \dfrac{P}{M}\,, \\ \dot{P} = -\nabla V(Q(t)) - \displaystyle\int_0^t ds\, \dot{Q} K(t-s) + R(t)\,, \end{cases} \tag{4}$$

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

$$\int_0^t ds\, \dot{Q} K(t-s)\,, \tag{5}$$

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

$$K(t) = \sum_{i=1}^{N} k_i \cos(\omega_i t)\,; \tag{6}$$

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

$$R(t) = \sum_{i=1}^{N} k_i \left[q_i(0) - Q(0)\right] \cos(\omega_i t) + \frac{k_i}{m_i \omega_i} p_i(0) \sin(\omega_i t)\,. \tag{7}$$

II. THE MEMORY KERNEL

The integral over time from 0 to t in the GLE tells us that the time-evolution of the particle of mass M is influenced by its past. In other words, to know the state $\{Q(t),\, P(t)\}$ of the particle at time t, it is necessary to know the entire time evolution of the particle from 0 to t. How the particle "remembers" its past behavior and how the previous states influence the current state at time t, is described by the memory kernel $K(t)$ whose shape depends on the physical characteristics of the oscillators: the angular frequencies ω_i, the masses m_i and the spring constants k_i $\forall i = 1, 2, \ldots, N$.

In fig. 1, we show three different sets of parameters ω_i, m_i and k_i. In the first row, ω_i, m_i and k_i are equal for all the oscillators. In the second case, the angular frequencies are

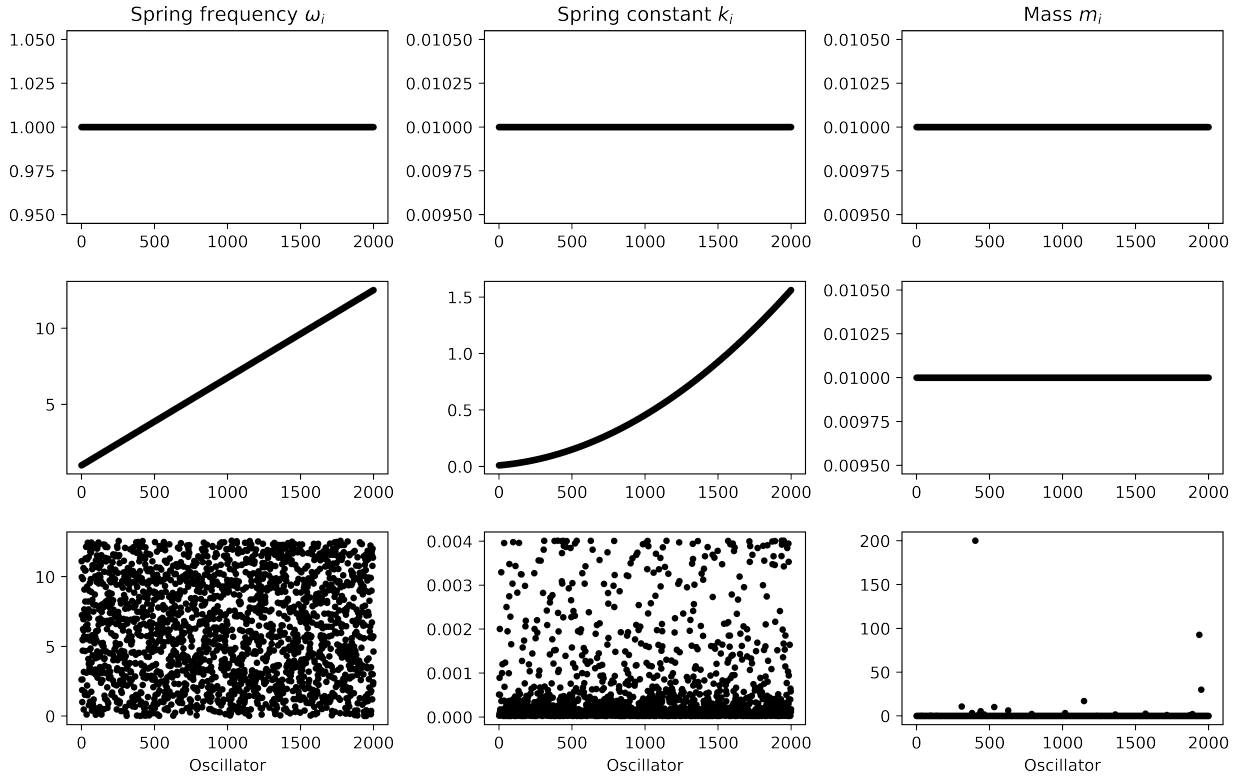

FIG. 1. Three different sets of parameters ω_i, k_i and m_i for $N = 2000$ oscillators.

chosen linearly increasing, the masses are all equal and the spring constants are estimated as $k_i = m_i\omega_i^2$. In the third case, the parameters are chosen as in ref. [1]. Correspondingly, we show in fig. 2 the memory kernel for each set of parameters. While in the first and second case the memory kernel is a sinusoidal function, in the third case the memory kernel is a peaked exponential function. This means that in the first two cases the memory kernel plays an important role in determining the dynamics of the particle, while in the third case it can be neglected. In what follow, we discuss the parameters of the third case proposed in ref. [1].

The angular frequencies of the N oscillators are randomly chosen from a uniform distribution:

$$\omega_i = N^a u_i \,, \tag{8}$$

where $u_i \sim \mathcal{U}[0,1]$ and $a \in [0,1]$. The spring constants are written as

$$k_i = \frac{2}{\pi}\frac{\alpha^2 M\gamma}{\alpha^2+\omega_i^2}\Delta\omega \,, \tag{9}$$

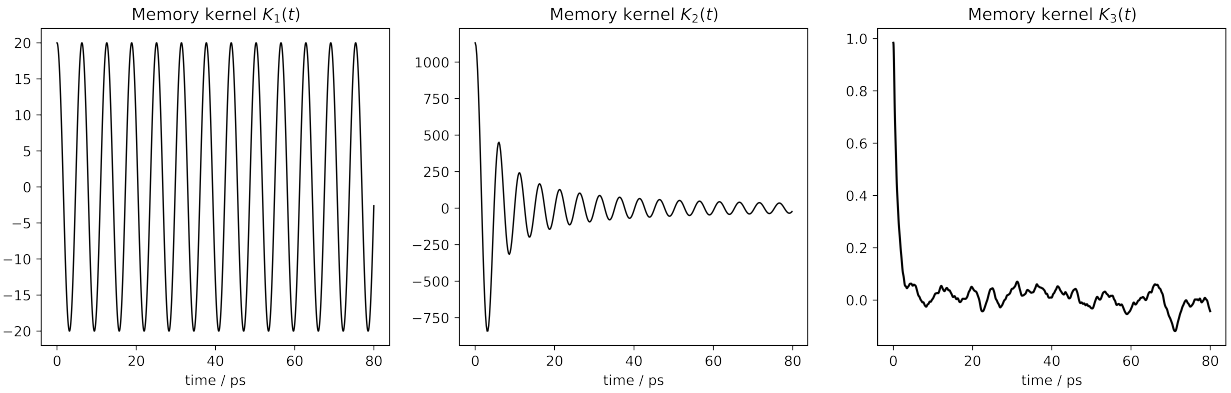

FIG. 2. Three memory kernels corresponding to the sets of parameters of fig. 1.

where $\alpha > 0$ is a parameter with units $[\text{rad} \cdot \text{time}]^{-1}$, γ is a physical quantity with units $[\text{time}]^{-1}$ that denotes the friction between the particle of mass M and the heat bath, $\Delta\omega = {}^{N^a}/_{N}$. The choice of the parameters guarantees that the units of k_i are [force length^{-1} = mass time^{-2}]. Finally, the masses of the oscillators are calculated as

$$m_i = \frac{k_i}{\omega_i^2}\,. \tag{10}$$

Inserting eq. 9 into eq. 6 yields

$$K(t) = \sum_{i=1}^{N} \frac{2}{\pi} \frac{\alpha^2 M\gamma}{\alpha^2 + \omega_i^2}\, \Delta\omega\, \cos(\omega_i t)\,. \tag{11}$$

If $N \to \infty$, $\Delta\omega \to d\omega$ because $a \in [0, 1]$, then the sum in eq. 11 can be replaced by the integral

$$K(t) = \int_0^\infty d\omega\, \frac{2}{\pi} \frac{\alpha^2 M\gamma}{\alpha^2 + \omega_i^2}\, \cos(\omega_i t)\,. \tag{12}$$

We now observe that the eq. 12 is the inverse Fourier cosine transform (see Appendix A) of the function

$$f(t) = \alpha M\gamma e^{-\alpha t}\,. \tag{13}$$

Then

$$K(t) = \frac{2}{\pi} \int_0^\infty d\omega\, \frac{\alpha^2 M\gamma}{\alpha^2 + \omega_i^2}\, \cos(\omega_i t) \tag{14}$$

$$= \alpha M\gamma e^{-\alpha t}\,. \tag{15}$$

Fig. 3 shows the validity of eq. 15.

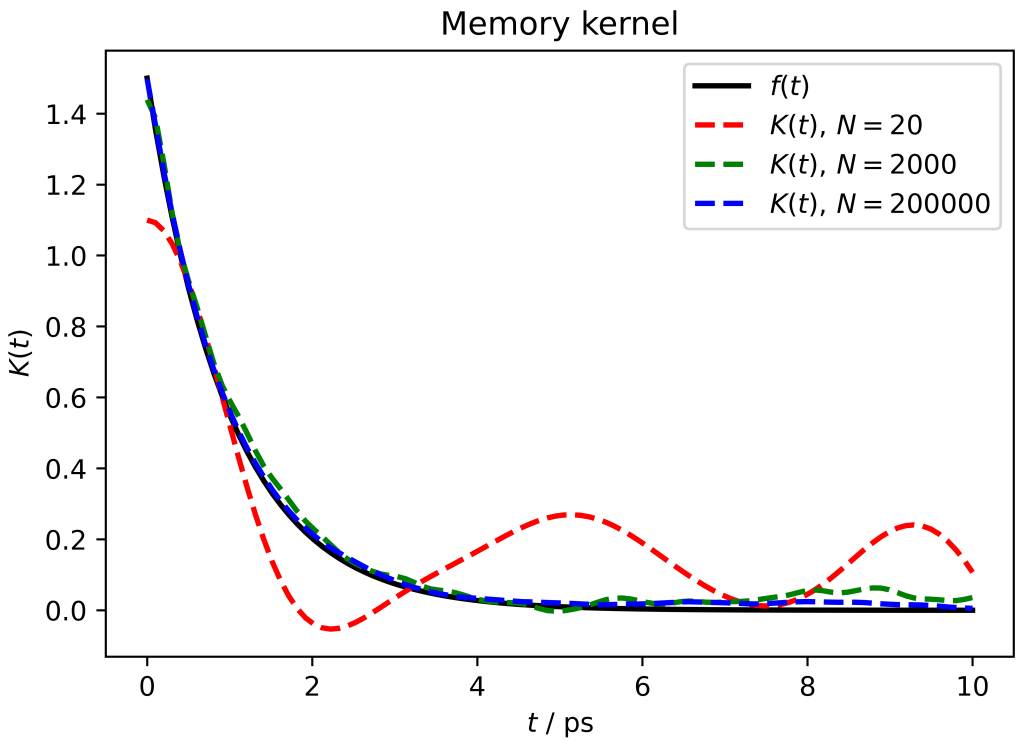

FIG. 3. Memory kernel: $\alpha = 1$, $\gamma = 1.5\,\mathrm{ps}^{-1}$, $N = 20$, 2000, 200000, $a = 0.333$.

Under these considerations, we can now rewrite the memory kernel as

$$K(t) = \alpha M \gamma e^{-\alpha t}\,, \tag{16}$$

and we observe that as the parameter $a \to \infty$, the memory kernel becomes a peaked function with a high value at $t = 0$, and zeros values at $t > 0$ (fig. 4).

Consequently, the integral in the GLE (eq. 4) can be approximated as

$$\int_0^t ds\, \dot{Q} K(t-s) = \int_0^t ds\, \dot{Q}\, \alpha M \gamma e^{-\alpha(t-s)} \tag{17}$$

$$\approx M\gamma \dot{Q} \tag{18}$$

$$= \gamma \dot{P}\,. \tag{19}$$

Alternatively, we can approximate the memory kernel with the δ-function (see Appendix B):

$$K(t-s) \approx 2M\gamma\delta(t-s) \tag{20}$$

where the factor 2, which is cancelled after integrating from 0 to t, takes into account that

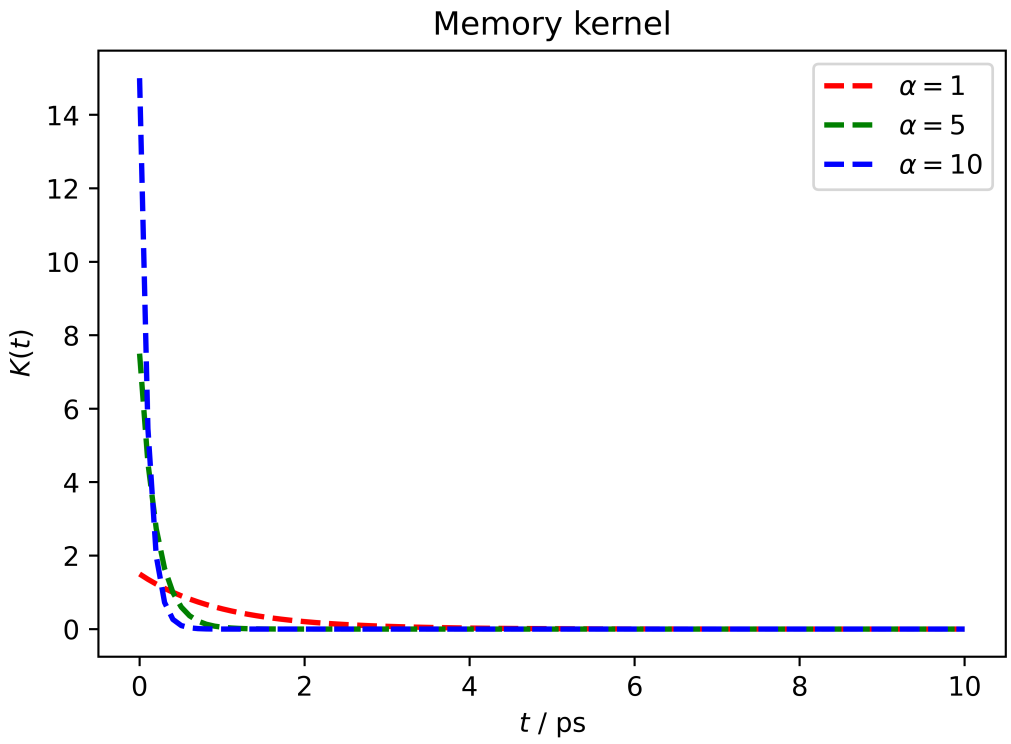

FIG. 4. Memory kernel: $\alpha = 1,\ 5,\ 10$, $\gamma = 1.5\,\mathrm{ps}^{-1}$.

the function $f(t)$ (eq. 13) approximates half δ-function:

$$\int_0^t ds\,\dot{Q}K(t-s) \approx 2\gamma M \int_0^t ds\,\dot{Q}\delta(t-s) \tag{21}$$

$$= M\gamma\dot{Q} \tag{22}$$

$$= \gamma\dot{P}\,. \tag{23}$$

III. THE NOISE TERM

The noise term (eq. 7)

$$R(t) = \sum_{i=1}^{N} k_i\left[q_i(0) - Q(0)\right]\cos(\omega_i t) + \frac{k_i}{m_i\omega_i}p_i(0)\sin(\omega_i t)\,, \tag{24}$$

depends on the choice of the initial momenta, positions and physical characteristics of the oscillators. This term is deterministic in the GLE (eq. 4), however, it can be replaced by a white noise process under specific conditions.

First of all, we rewrite eq. 24 as

$$R(t) = \sqrt{\frac{1}{\beta}} \sum_{i=1}^{N} \sqrt{k_i} \left[\sqrt{k_i \beta} \left(q_i(0) - Q(0) \right) \cos(\omega_i t) + p_i(0) \sqrt{\frac{\beta}{m_i}} \sin(\omega_i t) \right] , \tag{25}$$

where we multiplied and divided eq. 24 by $\sqrt{\beta}$ and we used

$$\frac{k_i}{m_i \omega_i} = \frac{\sqrt{k_i}}{\sqrt{k_i}} \frac{k_i}{m_i \omega_i} \tag{26}$$

$$= \sqrt{k_i} \frac{\sqrt{k_i}}{m_i \omega_i} \tag{27}$$

$$= \sqrt{k_i} \frac{\sqrt{m_i \omega_i^2}}{m_i \omega_i} \tag{28}$$

$$= \sqrt{k_i} \frac{1}{\sqrt{m_i}} . \tag{29}$$

The term $\beta = 1/k_B T$ is a thermodynamic quantity, where k_B is the Boltzmann constant and T is the temperature of the system.

We now assume that the oscillators are in thermal equilibrium at time $t = 0$, i.e. their positions and momenta are distributed according to the Boltzmann distribution:

$$\begin{cases} \pi_q(q_i(0)) = \dfrac{1}{Z_{q_i}} \exp\left(-\beta \dfrac{k_i}{2} (q_i(0) - Q(0))^2 \right) \\ \pi_p(p_i(0)) = \dfrac{1}{Z_{p_i}} \exp\left(-\beta \dfrac{p_i(0)^2}{2 m_i} \right) \end{cases} , \tag{30}$$

where Zq_i and Zp_i are two normalization constants. The two Boltzmann distributions are exponential functions with quadratic arguments. Comparing these two functions with the Gaussian function

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2} \frac{(x - x(0))^2}{\sigma^2} \right) , \tag{31}$$

we conclude that $q_i(0)$ and $p_i(0)$ are distributed according to a Gaussian function. Then, drawing random positions and momenta from the Boltzmann distribution is equivalent to drawing random positions and momenta from a properly scaled normal distribution:

$$\begin{cases} q_i(0) = Q(0) + \xi_i \sqrt{\dfrac{1}{\beta k_i}} \\ p_i(0) = \eta_i \sqrt{\dfrac{m_i}{\beta}} \end{cases} , \tag{32}$$

where $\xi, \eta_i \in \mathcal{N}(0, 1)$. Then, eq. 25 is rewritten as

$$R(t) = \sqrt{\frac{1}{\beta}} \sum_{i=1}^{N} \sqrt{k_i} \left[\xi_i \cos(\omega_i t) + \eta_i \sin(\omega_i t) \right] , \tag{33}$$

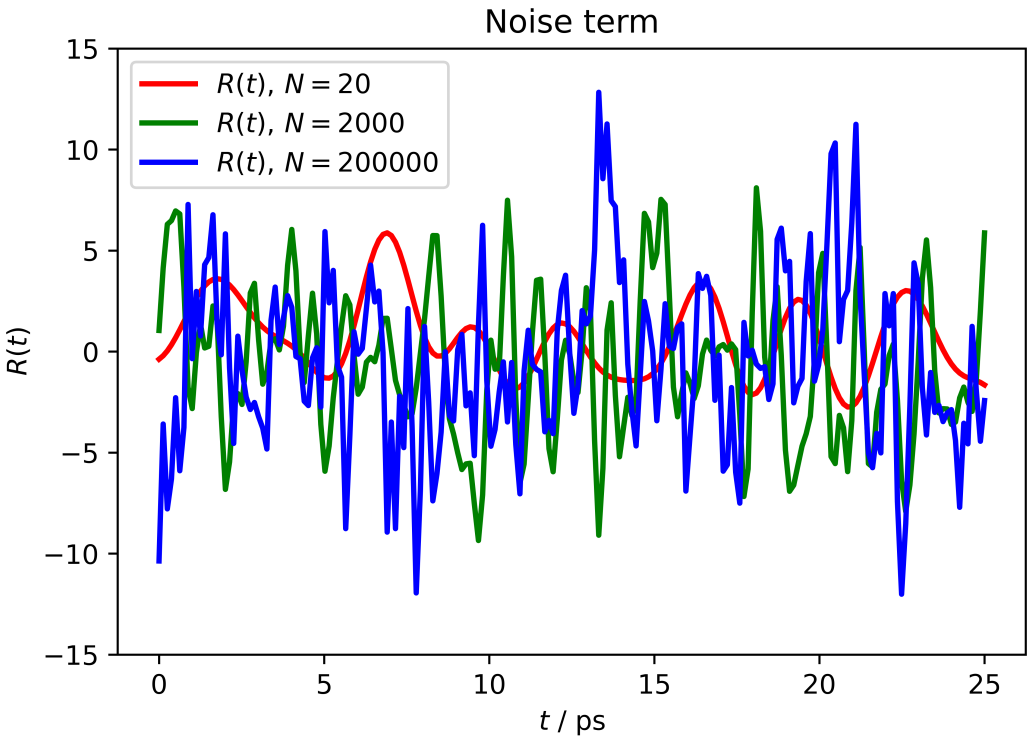

FIG. 5. Memory kernel: $\alpha = 5$, $\gamma = 1.5\,\mathrm{ps}^{-1}$, $N = 20$, 2000, 200000, $a = 0.333$.

Appendix A: Fourier cosine transform

Given a real- or complex-valued function $f(t) : \mathbb{R}^+ \to \mathbb{C}$, the Fourier cosine transform of $f(t)$ is defined as

$$\hat{f}(\omega) = \int_0^\infty dx\, f(t) \cos(\omega t)\,, \tag{A1}$$

where $\omega > 0$. The inverse Fourier cosine transform of $\hat{f}(\omega)$ is defined as

$$f(t) = \frac{2}{\pi} \int_0^\infty dt\, \hat{f}(\omega) \cos(\omega t)\,. \tag{A2}$$

In eq. 15, we used the Fourier cosine transform

$$\hat{f}(\omega) = \int_0^\infty dx\, \alpha M \gamma e^{-\alpha t} \cos(\omega t) \tag{A3}$$

$$= \frac{\alpha^2 M \gamma}{\alpha^2 + \omega^2}\,, \tag{A4}$$

Appendix B: δ-function

The δ-function can be heuristically written as

$$\delta(t) = \begin{cases} \infty & t = 0 \\ 0 & t \neq 0 \end{cases} . \tag{B1}$$

The δ-function satisfies the property

$$\int_{-\infty}^{\infty} dt\, \delta(t) = 1\,. \tag{B2}$$

Additionally, given an arbitrary function $f(t)$:

$$\int_{-\infty}^{\infty} dt\, f(t)\delta(t) = f(0)\,, \tag{B3}$$

and

$$\begin{aligned} \int_{-\infty}^{\infty} ds\, f(s)\delta(s-t) &= \int_{-\infty}^{\infty} ds\, f(s)\delta(t-s) && \text{(B4)} \\ &= f(t)\,. && \text{(B5)} \end{aligned}$$

The integral over a subset of the domain is

$$\begin{aligned} \int_{-t}^{t} ds\, f(s)\delta(s-t) &= \int_{-t}^{t} ds\, f(s)\delta(t-s) && \text{(B6)} \\ &= \int_{-\infty}^{\infty} ds\, \chi_{[-t,\,t]}\, f(s)\delta(t-s) && \text{(B7)} \\ &= \chi_{[-t,\,t]}(t)\, f(t) && \text{(B8)} \\ &= \frac{f(t)}{2} \quad \forall\, t > 0\,, && \text{(B9)} \end{aligned}$$

where we used the half maximum convention to define the indicator function

$$\chi_{[-t,\,t]}(s) = \begin{cases} 0 & s < -t \\ 1/2 & s = -t \,\wedge\, s = t \\ 0 & s > t \end{cases} \quad \forall\, t > 0. \tag{B10}$$

Likewise, integrating over $[0,\, t]$ yields

$$\begin{aligned} \int_{0}^{t} ds\, f(s)\delta(s-t) &= \int_{0}^{t} ds\, f(s)\delta(t-s) && \text{(B11)} \\ &= \int_{-\infty}^{\infty} ds\, \chi_{[0,\,t]}\, f(s)\delta(t-s) && \text{(B12)} \\ &= \chi_{[0,\,t]}(t)\, f(t) && \text{(B13)} \\ &= \frac{f(t)}{2} \quad \forall\, t > 0\,, && \text{(B14)} \end{aligned}$$

[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).