Problem Sheet 4

1. Exercise 7.10 on page 223 of the Lecture Notes.

2. Exercise 7.11 on pages 223-224 of the Lecture Notes.

3. Exercise 8.3 on page 265 of the Lecture Notes.

4. Exercise 8.14 on page 267 of the Lecture Notes.

5. Consider the generalized Langevin equation with friction kernel $\kappa(\tau) = \exp(-2\tau)$ for $\tau \in [0, \infty)$. Calculate the Laplace transform of the friction kernel $\kappa(\tau)$ and use equation (8.53) to find the velocity autocorrelation function $\chi(\tau)$.

6. Consider the probability distribution $p(\omega) = \dfrac{C}{2 + \omega^2}$, where $\omega \in (0, \infty)$ and C is a constant.

(a) Find the value of the normalization constant C, i.e. find C such that $\displaystyle\int_0^\infty p(\omega)\, \mathrm{d}\omega = 1$.

(b) Find the cummulative distribution function $F(\omega) = \displaystyle\int_0^\omega p(\eta)\, \mathrm{d}\eta$. Explain how you can sample random numbers ω_i from this distribution.

(c) Show that the mean of the probability distribution $p(\omega)$ is undefined.

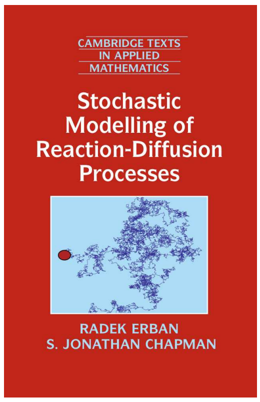
(d) Modify equation (8.72) so that all spring constants k_i, $i = 1, 2, \ldots, N$, are equal to the same value $k = 2\, m_p/N$. Show that equation (8.73) then reads as follows

$$\kappa(\tau) = 2 \int_0^\infty \cos(\omega\tau)\; p(\omega)\, \mathrm{d}\omega. \tag{8.73*}$$

(e) Use equation (8.73)* to find the friction kernel $\kappa(\tau)$.

(f) Calculate the Laplace transform of the friction kernel $\kappa(\tau)$ and use equation (8.53) to find the velocity autocorrelation function $\chi(\tau)$. Use equation (8.60) to find the diffusion coefficient D.

(g) [OPTIONAL] Write a computer code which implements this model for $N = 10^4$ oscillators. Estimate the velocity autocorrelation function $\chi(\tau)$ and diffusion coefficient D from your simulations and compare your computational results with your theoretical results obtained in part (f).



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The online version is available to everyone at all times through SOLO (Search Oxford Libraries Online). College libraries also have physical copies.

Students wishing to further practise material covered in Lectures 13, 14, 15 and 16 can also solve Exercises 7.1-7.9 on pages 222 and 223, Exercise 7.12 on page 224 and all remaining exercises in the Lecture Notes which accompany Chapter 8 (exercises on pages 265-267).

Example Exam Question: students could solve Question 2 in the 2019 exam paper (Honour School of Mathematics Part B: Paper B5.1 & Honour School of Mathematics and Statistics Part B: Paper B5.1, Trinity Term 2019). Question 2 in this exam can be solved by a variant of a method studied in Chapter 8, which is also practiced in Exercise 8.3 (included above in Problem Sheet 4).