Universität des Saarlandes
Fakultät 7 – Physik und Mechatronik

Fachrichtung 7.1 – Theoretische Physik
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Blatt 7 zur Theoretischen Physik IV, WS2023/2024

(Abgabe bis 22.12.2023, 8.30 Uhr)

Exercise 1 *Langevin equation* [20 Points]

a) Consider the first-order linear differential equation

$$\frac{\mathrm{d}}{\mathrm{d}x}y(x) + p(x)y(x) = q(x)$$

with the functions p and q. The initial condition is given by $y(x=0) = y_0$. Determine the corresponding solution.
Hint: Assume that the solution has the form $y(x) = z(x)\exp\big(-\int_0^x p(x')\,\mathrm{d}x'\big)$

b) Solve the Newton equation

$$m\frac{\mathrm{d}}{\mathrm{d}t}v(t) + \gamma v(t) = 0,$$

in which the term $-\gamma v$ describes the frictional force, the coefficient of friction $\gamma > 0$, the mass $m > 0$, and the initial condition is given by $v(t=0) = v_0$.

c) Now consider the Langevin equation

$$m\frac{\mathrm{d}}{\mathrm{d}t}v(t) + \gamma v(t) = \zeta(t),$$

in which $\zeta(t)$ represents the so-called white noise, which fulfills the conditions

$$\langle \zeta(t) \rangle = 0, \quad \langle \zeta(t)\zeta(t') \rangle = 2a^2\delta(t-t')$$

Use the solution from part a) to solve this equation and then calculate $\langle v(t) \rangle$ and $\big\langle [v(t)]^2 \big\rangle$ in the limit of great times $t \to \infty$.

d) Determine the relationship between the parameter a and the temperature.
Hint: Use the equipartition theorem in the limit $t \to \infty$.

e) Calculate the mean square deflection $\big\langle [r(t)]^2 \big\rangle$ $\big($where $r(t) = \int_0^t v(s)\,\mathrm{d}s\big)$ and determine the asymptotic behavior of this variable. Here we assume that $r(0) = 0$.

Exercise 2 *Detailed equilibrium* [16 Points]

The master equation of a Markov process in discrete time is

$$P_{t+1}(c) = \sum_{c' \in S} P_t(c') w(c' \to c),$$

where $P_t(c)$ denotes the probability that the system assumes state c at time t and $w(c' \to c)$ denotes the transition probability from state c' to state c. We assume that there is only a finite number of possible states in the state space S. The stationary state is a probability distribution that fulfills the *global balance condition*:

$$P(c) = \sum_{c' \in S} P(c') w(c' \to c).$$

For given transition rates w, it is usually not trivial to find the stationary occupation probabilities $P(c)$. (In this task we assume that there is only one stationary state and that the stationary occupation probability $P(c)$ of each state c is positive). If there is a function f on S such that

$$f(c') w(c' \to c) - f(c) w(c \to c') = 0$$

$\forall c, c' \in S$ applies, *the detailed balance condition* is fulfilled.

a) Show that the condition of detailed equilibrium in the case of two states, i.e . $S = \{A, B\}$, is always fulfilled and find the stationary distribution.

b) Find the restriction that the condition of detailed equilibrium is fulfilled in the case of three states, i.e. $S = \{A, B, C\}$, and find the stationary distribution in this case.
Hint: The restriction can be formulated by a single equation.

In parts c), d) and e) we assume that the condition of detailed equilibrium is fulfilled.

c) Express the stationary probabilities $P(c)$ using the function f.

d) We use the notation $w(a \leftarrow b) = w(b \to a)$. We consider

$$\mathcal{E}(c) = \log \frac{w(o \leftarrow c_1) w(c_1 \leftarrow c_2) \cdots w(c_n \leftarrow c)}{w(o \to c_1) w(c_1 \to c_2) \cdots w(c_n \to c)}$$

with a fixed starting point o, and independent of the described path $c_1, \ldots, c_n$. Express the stationary state with $\mathcal{E}$.

e) Now a process is to be found which, in the stationary state, can fulfill the probability distribution

$$P(c) = \frac{\exp\big(-\beta E(c)\big)}{\sum_{c' \in S} \exp\big(-\beta E(c')\big)}$$

There are many ways to fulfill this property. Show that the following example provides such a process:

$$w(a \to b) = \frac{1}{|S|} \min\Big\{1\,,\, \exp\big(\beta E(a) - \beta E(b)\big)\Big\}.$$

Exercise 3 *Computational task: Simple Monte Carlo integration* [4 Points]

Monte Carlo integration is a numerical technique for approximating integrals, particularly in cases where traditional methods may be difficult or impractical to apply. The basic idea is to use random points to estimate the value of an integral, as it is shown on Fig. 1.

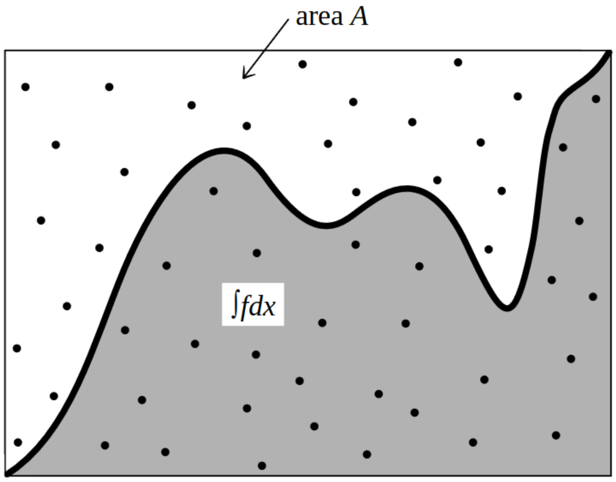

Figure 1: Monte Carlo integration. Random points are chosen within the area A. The integral of the function f is estimated as the area of A multiplied by the fraction of random points that fall below the curve f.[0]

Plot the integral estimation of a Gaussian function

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}$$

as a function of the standard deviation $\sigma \in [0.1; 1]$ for 2 trials. Interpret the tendency. As a guide, there is a Python code in the exercise folder (blatt07_SMCI.py), you can complete it.

[0]Press, William H., Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. 1992. Numerical Recipes in C (2nd Ed.): The Art of Scientific Computing. USA: Cambridge University Press.