1. Part I: Numerical integration of Langevin equations (10 points, until 2009/05/20)

Implement the Euler algorithm described in problem 2 of problem set 11 for the numerical integration of the one-dimensional Langevin equation

$$\dot{\hat{x}} = a(\hat{x}, t) + \sqrt{2D}\,\hat{\xi}(t)\,, \tag{1}$$

where $\hat{\xi}(t)$ is Gaussian white noise with $\langle \hat{\xi}(t) \rangle = 0$ and $\langle \hat{\xi}(t)\hat{\xi}(t') \rangle = \delta(t - t')$. Use Gaussian random numbers for the ζ_k, which you generate using the Box-Muller algorithm described in problem 2 of problem set 3. Use a uniform random number generator of your choice.

- Plot a couple of sample trajectories for the case of free diffusion $a(x, t) = 0$ and $\hat{x}(0) = 0$ for varying time-step h.
- Check the result $\langle [\hat{x}(t)]^2 \rangle = 1$ for the Ornstein-Uhlenbeck type process with $a(x, t) = -x$, $D = 1$ and $\hat{x}(0) = 1$: Plot the difference of the mean from the given analytical result for a final time $t = 1$ and the standard deviation of this difference obtained by averaging over $N = 10000$ realizations for different time steps $h = 0.0001, 0.001, 0.01, 0.1$.

Note that in many cases, the Langevin equation (1) comes from a model for the motion of a particle in the presence of a time-dependent force $F(x, t)$:

$$m\,\ddot{\hat{x}} + \eta\,\dot{\hat{x}} = F(\hat{x}, t) + \sqrt{2\eta k_{\mathrm{B}} T}\,\hat{\xi}(t)\,, \tag{2}$$

which is approximated in the overdamped limit $m \to 0$.[1] Then, we can identify $a(x, t) = (1/\eta)F(x, t)$ and $D = k_{\mathrm{B}}T/\eta$.

2. Part II: Applications (10 points, until 2009/05/27)

The following examples demonstrate some important phenomena that triggered substantial research efforts in the field of stochastic processes in physics during the last years. They all are particular examples of the stochastic dynamics of the form (1), or equivalently

$$\dot{\hat{x}} = -\frac{\partial}{\partial x} V(\hat{x}, t) + \sqrt{2D}\,\hat{\xi}(t) \tag{3}$$

for a time-dependent "potential" $V(x, t)$.

[1] This is usually a good approximation for the dynamics on small distances, where damping effects play a dominant role.

For every example, a reference is provided, which contains more information about the importance of the model. Reasonable model parameters and/or parameter ranges are always given, but part of the exercise is to play around with the various parameters to identify particularly interesting and surprising behaviour.

Select one of the four alternatives! Shortly present your results during the last exercise class on May 27th.

Alternative 1: Flashing ratchet

See, e.g., D. Astumian, *Thermodynamics and Kinetics of a Brownian Motor*, Science **276**, 917 (1997).

Consider the stochastic dynamics (3) in the spatially periodic but asymmetric, time-dependent potential

$$V(x) = \sin x + \frac{1}{4}\sin(2x) - F\,x$$
$$V(x,t) = V(x)\left\{1 + A\,\mathrm{sign}\big[\sin(\Omega t)\big]\right\}.$$

- Plot $V(x)$ for both $F = 0$ and $F = 1$ as well as $V(x,t)$ for $F = 0$ and $A = 1$ for $t = \pi/2\Omega$ and $t = 3\pi/2\Omega$.
- Plot some sample trajectories (with initial condition $\hat{x}(0) = 0$) for $A = \Omega = D = 1$ and $F = 0$.
- Plot the particle current averaged over one driving period $\mathcal{T} = 2\pi/\Omega$

  $$\overline{\langle\dot{\hat{x}}(t)\rangle} := \frac{1}{\mathcal{T}}\int_t^{t+\mathcal{T}} \mathrm{d}t'\,\langle\dot{\hat{x}}(t')\rangle \tag{4}$$

  in the long-time limit $t \to \infty$ as a function of the tilting force F (in the interval $[-1,1]$) for $A = \Omega = D = 1$ and as a function of A for $F = 0$ and $D = \Omega = 1$. Hint: Use that, provided that the stationary solution (t very large) fulfils $\langle\dot{\hat{x}}(t)\rangle_{\mathrm{s}} = \langle\dot{\hat{x}}(t+\mathcal{T})\rangle_{\mathrm{s}}$,

  $$\langle\dot{\hat{x}}\rangle_{\mathrm{s}} := \lim_{t\to\infty}\overline{\langle\dot{\hat{x}}(t)\rangle} = \lim_{t\to\infty}\frac{\langle\hat{x}(t)\rangle}{t}. \tag{5}$$

  Why? Note that $\hat{x}(t)$ is ergodic and thus already

  $$\langle\dot{\hat{x}}\rangle_{\mathrm{s}} = \lim_{t\to\infty}\frac{\hat{x}(t)}{t} \tag{6}$$

  for (almost) all realizations of the stochastic process $\hat{x}(t)$. Verify this by numerically calculating the standard deviation of the limit on the right-hand side. Discuss the result for the current as a function of the tilting force. Why is it surprising? Is the driving-amplitude dependence of the current as you would expect it from general laws of thermodynamics?

Alternative 2: Rocking ratchet

See, e.g., D. Astumian, *Thermodynamics and Kinetics of a Brownian Motor*, Science **276,** 917 (1997).

Consider the stochastic dynamics (3) in the spatially periodic but asymmetric, time-dependent potential

$$V(x) = \sin x + \frac{1}{4}\sin(2x) - F\,x$$
$$V(x,t) = V(x) - A\sin(\Omega t)\,x\,.$$

- Plot $V(x)$ for $F = 0$ and $F = 1$ as well a $V(x,t)$ for $F = 0$ and $A = 1$ for $t = 0$ and $t = \pi/2\Omega$.
- Plot some sample trajectories (with initial condition $\hat{x}(0) = 0$) for $A = \Omega = D = 1$ and $F = 0$.
- Plot the long-time limit of the time-averaged particle current $\langle\dot{\hat{x}}\rangle_{\rm s}$ (see Eq. (5)) as a function of the tilting force F (in the interval $[-1,1]$) for $A = \Omega = D = 1$ and as a function of A for $F = 0$ and $D = \Omega = 1$. Also check the ergodicity as discussed after Eq. (6). Discuss the result for the current as a function of the tilting force. Why is it surprising? Is the driving-amplitude dependence of the current as you would expect it from general laws of thermodynamics?

Alternative 3: Stochastic resonance

See, e.g., L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, *Stochastic Resonance*, Rev. Mod. Phys. **70**, 223 (1998).

Consider the stochastic dynamics (3) in the time-dependent double-well potential

$$V(x,t) = -\frac{1}{2}\,x^2 + \frac{1}{4}\,x^4 - A\sin(\Omega t)\,x\,.$$

- Plot $V(x,t)$ for $A = 0.25$ for $t = 0$ and $t = 0$, $t = \pi/2\Omega$, $t = \pi/\Omega$, and $t = 3\pi/2\Omega$.
- Plot some sample trajectories (with initial condition $\hat{x}(0) = 1$) for $A = 0.1$, $\Omega = 0.01$ and $D = 0.01$, 0.1, 1 over a couple of driving periods.
- Plot the stationary (i.e., for large t) solution $\langle\hat{x}(t)\rangle_{\rm s}$ for $\Omega = 0.01$, two driving amplitudes $A = 0.01$, $A = 0.1$ and $D = 0.1$. Check that it is $\mathcal{T}$-periodic and approximately of the form $\langle\hat{x}(t)\rangle_{\rm s} = \bar{x}\sin(\Omega t - \bar{\phi})$. The latter approximation becomes exact in the linear-response limit, i.e., for $A \to 0$.
- Plot the spectral amplification $S := (\bar{x}/A)^2$, which characterizes the response of the system to the sinusoidal driving, as a function of the noise strength D in the interval $[0.01, 0.5]$ for $\Omega = 0.01$ and $A = 0.1$: Calculate $\bar{x}$ as the maximum of $\langle\hat{x}(t)\rangle_{\rm s}$ within one driving period. What do you observe?

Alternative 4: Stochastic synchronization

See, e.g., L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, *Stochastic Resonance*, Rev. Mod. Phys. **70**, 223 (1998).

Consider the stochastic dynamics (3) in the time-dependent double-well potential

$$V(x,t) = -\frac{1}{2}\,x^2 + \frac{1}{4}\,x^4 - A\sin(\Omega t)\,x$$

with initial condition $\hat{x}(0) = 1$.

- Plot $V(x,t)$ for $A = 0.25$ for $t = 0$ and $t = 0$, $t = \pi/2\Omega$, $t = \pi/\Omega$, and $t = 3\pi/2\Omega$.
- Plot some sample trajectories (with initial condition $\hat{x}(0) = 1$) for $A = 0.25$, $\Omega = 0.01$ and $D = 0.01$, 0.1, 1 over a couple of driving periods.
- Introduce a stochastic discrete-phase process $\hat{\phi}(t)$ as follows: At initial time $t = 0$: $\hat{\phi}(0) = 0$. This value is kept until $\hat{x}(t)$ becomes smaller than -0.75. From this time instance on, we set $\hat{\phi}(t) = \pi$. We increase this value to $\hat{\phi}(t) = 2\pi$, when for the next time $\hat{x}(t)$ becomes larger than 0.75, and so on.[2] Plot this discrete-phase process together with the sample trajectories for $\hat{x}(t)$.
- Define an average phase velocity (frequency) in the long-time limit $\omega := \lim_{t\to\infty}\langle\hat{\phi}(t)\rangle/t$. Check the ergodicity of this quantity (see alternative 1). Plot this frequency as a function of the noise strength D in the interval $[0, 0.2]$ for fixed $A = 0.25$ and $\Omega = 0.01$. What do you observe, especially, if you compare the result to the frequency Ω?

[2] More precisely, one should use the instantaneous minima of the potential $V(x,t)$ as "trigger" positions. If you prefer doing so, you can find these minima and implementing this improved variant.