1. Problem: Noisy harmonic oscillator (10 points)

The equation of motion for a classical harmonic oscillator is given by

$$m\,\ddot{\hat{x}}(t)+\eta\,\dot{\hat{x}}(t)+k\,\hat{x}(t)=\sqrt{2\eta k_B T}\;\hat{\xi}(t),$$

where $\hat{\xi}(t)$ describes Gaussian white noise with mean value $\langle\hat{\xi}(t)\rangle = 0$ and $\langle\hat{\xi}(t)\hat{\xi}(t')\rangle = \delta(t-t')$.

If we restrict ourselves to the stationary case, it is advantageous to consider the Fourier transform $\hat{x}(\omega)=\int \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\ \hat{x}(t)$ of the process. Derive an equation for $\hat{x}(\omega)$.

1.1. Mean value and autocorrelation function

Calculate the mean value $\langle\hat{x}(t)\rangle$ and the autocorrelation function $\langle\hat{x}(t)\hat{x}(t')\rangle$ for the stationary process for the underdamped case $\gamma=\eta/m<2\,\omega_0$ where $\omega_0^2=k/m$.

2. Problem: Numerical integration of SDEs (no points)

2.1. Introduction

The numerical integration of stochastic differential equations relies on the same ideas as those of ordinary differential equations: One replaces the exact dynamics by an approximate time-discrete one, thereby making an error which scales with the size of the time-step size h. The introduction of random variables makes the situation more complicated, though. First, the Wiener process introduces errors already on the order of $h^{1/2}$. Second, the size of the error depends on the type of convergence (e.g. for moments or in the mean-square sense) one is interested in. Third, being a Monte-Carlo simulation, the maximal error also depends on the number of realizations one generates.

2.2. Expansion of the SDE for short times

Let us consider the one-dimensional stochastic differential with additive noise of strength D:

$$\dot{\hat{x}}=a(\hat{x},t)+\sqrt{2D}\,\xi(t)\quad\text{or}\quad \mathrm{d}\hat{x}=a(\hat{x},t)\,\mathrm{d}t+\sqrt{2D}\,\mathrm{d}\hat{W}(t)\,. \tag{1}$$

In order to find an approximation for the dynamics for small time steps h, integrate this equation from t to $t+h$ and insert this solution again in the resulting expression to find

$$\hat{x}(t+h) = \hat{x}(t) + \sqrt{2D}\,\Delta\hat{W}_h(t) + a(\hat{x}(t),t)\,h + \sqrt{2D}\,a'(\hat{x}(t),t)\,\hat{F}_h(t) + \mathcal{O}(h^2)\,, \tag{2}$$

where $a'(x,t)$ denotes the partial derivative with respect to the first argument, and we have introduced the increment of the Wiener process and its time integral:

$$\Delta\hat{W}_h(t) := \hat{W}(t+h) - \hat{W}(t) \tag{3a}$$

$$\hat{F}_h(t) := \int_t^{t+h} \mathrm{d}t'\,\Delta\hat{W}_{t'-t}(t)\,. \tag{3b}$$

Calculate the first and second moments of the random processes (3).

Of what order in h are, thus, the second and fourth term on the right-hand side?

2.3. Approximation for expectation values

If we are interested in a numerical approximation to an expectation value $\langle f(\hat{x}(t),t)\rangle$ of a function of the original process $\hat{x}(t)$, we can replace the exact dynamics (1) by the approximate one in discrete time $t = t_0 + kh$, $k = 0, 1, \ldots$ defined by

$$\check{x}(t+h) = \check{x}(t) + a(\check{x}(t),t)\,h + \sqrt{2Dh}\,\hat{\zeta}_k \tag{4}$$

and $\check{x}(t_0) = \hat{x}(t_0)$. Here, we have introduced random numbers $\hat{\zeta}_k$ with

$$\langle\hat{\zeta}_k\rangle = \langle\hat{\zeta}_k^3\rangle = 0 \quad \text{and} \quad \langle\hat{\zeta}_k\,\hat{\zeta}_{k'}\rangle = \delta_{kk'}\,. \tag{5}$$

Note that these variables do not necessarily have to be independent Gaussians.

Derive from Eq. (2) that this procedure yields an approximation for the expectation value after one time step up to second order in h:

$$\langle f(\hat{x}(t_0+h))\rangle = \langle f(\check{x}(t_0+h))\rangle + \mathcal{O}(h^2) \tag{6}$$

What is the order of the total error after $K = T/h$ time-steps, if T is the total integration time?

We remark that when one is interested in the mean-square convergence of the sample path, i.e., a small $\langle\big[\hat{x}(t+h) - \check{x}(t+h)\big]^2\rangle$, the use of Gaussians with the properties (4) is required to obtain an approximation to order h^2.

Finally, note that in order to obtain the expectation value $\langle f(\check{x}(T))\rangle$, we have to generate many, say a number $N \gg 1$, realizations of the discret dynamics (4) and then use the average over the indvidual results as estimation for the expectation value. The corresponding error will be of the order of $1/\sqrt{N}$. The total time M(i.e., the number of operations) needed for obtaining the approximate result is $M = NK = TN/h$. Obviously, for fixed T and M, either N or h can be still chosen freely, provided that their ratio remains the same. The optimal choice would be to make both the statistical error (due to finite N) and the one due to the time discretization (due to finite h) equal.[1] Show that if the error due to time-discretization scales as h^α (for the method described above, we have $\alpha = 1$) the total error E scales in this "optimal case" as $M^{-\alpha/(2\alpha+1)}$ with an α-dependent prefactor.

3. Problem: Chain rule for Stratonovich SDE (no points)

The chain rule for the Itô calculus, i.e., Itô's formula [for t-independent $f(\hat{x}(t), t) = f(\hat{x}(t))$]

$$\mathrm{d}f(\hat{x}(t)) = \left\{ a_{\mathrm{I}}(\hat{x}(t), t) f'(\hat{x}(t)) + \frac{1}{2}[b_{\mathrm{I}}(\hat{x}(t), t)]^2 f''(\hat{x}(t)) \right\} \mathrm{d}t + b_{\mathrm{I}}(\hat{x}(t), t)\, f'(\hat{x}(t))\, \mathrm{d}\hat{W}(t) \quad (7)$$

contains a second order derivative with respect to x. Here, $\hat{x}(t)$ has to obey the Itô SDE

$$\mathrm{d}\hat{x}(t) = a_{\mathrm{I}}(\hat{x}(t), t)\, \mathrm{d}t + b_{\mathrm{I}}(\hat{x}(t), t)\, \mathrm{d}\hat{W}(t) \quad (8)$$

We will now demonstrate that the chain rule for the Stratonovich calculus is more straightforwardly given by the common chain rule of differential algebra,

$$\mathrm{d}f(\hat{x}(t)) = \left\{ a_{\mathrm{S}}(\hat{x}(t), t)\mathrm{d}t + b_{\mathrm{S}}(\hat{x}(t), t) \circ \mathrm{d}\hat{W}(t) \right\} f'(\hat{x}(t)) = \mathrm{d}\hat{x}(t)\, f'(\hat{x}(t))\,, \quad (9)$$

where $\hat{x}(t)$ has to fulfill the Stratonovich SDE implicitely defined by the second equality sign, i.e., Eq. (10) below.

3.1. Transformation

Show for the one-dimensional case that the Stratonovich SDE

$$\mathrm{d}\hat{x}(t) = a_{\mathrm{S}}(\hat{x}(t), t)\, \mathrm{d}t + b_{\mathrm{S}}(\hat{x}(t), t) \circ \mathrm{d}\hat{W}(t) \quad (10)$$

is equivalent to the Itô SDE

$$\mathrm{d}\hat{x}(t) = \left[a_{\mathrm{S}}(\hat{x}(t), t) + v^{(\frac{1}{2})}(\hat{x}(t), t) \right] \mathrm{d}t + b_{\mathrm{S}}(\hat{x}(t), t)\, \mathrm{d}\hat{W}(t)\,, \quad (11)$$

where the noise-induced drift is given by

$$v^{(\frac{1}{2})}(x, t) = \frac{1}{2}\, b_{\mathrm{S}}(x, t)\, \frac{\partial}{\partial x}\, b_{\mathrm{S}}(x, t)\,. \quad (12)$$

[1] Note that "parallelizing" the Monte-Carlo runs is trivially possible, while this is not the case for the dynamics of a single realization, which might change this assumption.

3.2. Chain rule

Using Itô's formula (7) show that the chain rule for the Stratonovich calculus (9) is exactly the same as for the ordinary calculus.

Hint: Convert the Stratonovich SDE into the Itô SDE for which the chain rule is known. Define a new function $y = f(x)$ with the inverse $x = g(y)$ and write down the Itô's formula for dy in terms of $g(y)$. How are df/dx and dg/dy related? Are you able to convert back the resulting Itô SDE to the Stratonovich SDE?