Open Quantum Systems: Exercise Session 2

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Exercise 1: Brownian Motion in a Harmonic Oscillator Heat Bath

We are considering a harmonic oscillator in contact with a bath of harmonic oscillators. The single harmonic oscillator, which we also refer to as the *system*, has momentum coordinate p and position coordinate x. The system has Hamiltonian

$$H_s = \frac{p^2}{2m} + U(x).$$

The bath has momentum coordinates $\{p_j\}$ and position coordinates $\{q_j\}$, the bath and interaction Hamiltonian is

$$H_B = \sum_j \left(\frac{p_j^2}{2} + \frac{1}{2}\omega_j^2 \left(q_j - \frac{\gamma_j}{\omega_j^2} x \right)^2 \right)$$

1. Write down the equations of motion for the system and bath harmonic oscillators *1pt*

2. Show that the bath position equations are solved by

$$q_j(t) = q_j(0)\cos(\omega_j t) + p_j(0)\frac{\sin(\omega_j t)}{\omega_j} + \gamma_j \int_0^t ds\, x(s) \frac{\sin(\omega_j (t-s))}{\omega_j}$$

2pts

3. Show that the above expression can be rewritten as

$$q_j(t) - \frac{\gamma_j}{\omega_j^2} x(t) = \left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right) \cos(\omega_j t) + p_j(0)\frac{\sin(\omega_j t)}{\omega_j} - \gamma_j \int_0^t ds\, \frac{p(s)}{m} \frac{\cos(\omega_j (t-s))}{\omega_j^2}$$

1pt

4. Use the above equation to obtain the differential equation for the system momentum

$$\frac{dp(t)}{dt} = -U'(x(t)) - \int_0^t ds\, K(s) \frac{p(t-s)}{m} + F_p(t)$$

where

$$K(t) = \sum_j \frac{\gamma_j^2}{\omega_j^2} \cos \omega_j t$$

and

$$F_p(t) = \sum_j \gamma_j P_j(0) \frac{\sin \omega_j t}{\omega_j} + \sum_j \gamma_j \left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right) \cos \omega_j t$$

1pt

5. Let us now take the continuum limit, which means we replace the discrete sums by integrals as $\sum_j \to \int d\omega \, g(\omega)$, where $g(\omega)$ is the density of states. In this way, we can write $K(t)$ as

$$K(t) = \int_0^\infty d\omega \, g(\omega) \frac{\gamma^2(\omega)}{\omega^2} \cos \omega t.$$

Show that if $g(\omega) \propto \omega^2$ and $\gamma(\omega) = C$ then $K(t) \propto \delta(t)$. *1pt*

6. Assume that the bath initial conditions are taken from the distribution

$$f(p, q) = \frac{\exp(-H_B/k_B T)}{Z}, \tag{1}$$

where k_B is the Boltzmann constant and Z a normalisation constant. Show that taking the expected value E of the following functions with respect to (1) gives

$$\mathsf{E}\left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right) = 0, \quad \mathsf{E}(p_j(0)) = 0$$

and

$$\mathsf{E}\left(\left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right)^2 \right) = \frac{k_B T}{\omega_j^2}, \quad \mathsf{E}(p_j^2(0)) = k_B T.$$

Show that there no correlations between different js. *2pts*

7. Show that $\mathsf{E}(F_p(t) F_p(t')) = k_B T K(t - t')$. This equality is called a fluctuation-dissipation relation. *1pt*

Exercise 2: Stochastic integration

In ordinary calculus, integrals are defined by

$$\int_a^b dt f(t) = \lim_{N \to \infty} \sum_{k=0}^{N} (t_{k+1} - t_k) f(\theta_k)$$

where $t_k = k(a - b)/N$ and

$$\theta_k = s t_{k+1} + (1 - s) t_k$$

for $0 \leq s \leq 1$. In ordinary calculus the choice of s is free in the definition of the integral.

In Lecture 3 the concept of Stochastic differentials $d\chi_t$ was introduced. An important difference between ordinary calculus and stochastic calculus is that the choice of s does matter for the resulting integral. For example, let w_t be the Wiener process, in general,

$$\lim_{N\to\infty}\sum_{k=0}^{N}(w_{t_{k+1}}-w_{t_k})f(w_{t_k}) \neq \lim_{N\to\infty}\sum_{k=0}^{N}(w_{t_{k+1}}-w_{t_k})f\left(w_{\frac{t_{k+1}+t_k}{2}}\right)$$

To illustrate this fact, in this exercise we will calculate the stochastic integral

$$\int_0^t w_s^{(\theta)}dw_s \equiv \lim_{N\to\infty}\sum_{k=0}^{N-1}(w_{t_{k+1}}-w_{t_k})w_{\theta_k} = \frac{w_t^2-(1-2s)t}{2} \tag{2}$$

which clearly shows a dependence on the choice of s.

1. Show that we can write

   $$\sum_{k=0}^{N-1} w_{\theta_k}(w_{t_{k+1}}-w_{t_k})$$
   $$=\sum_{k=0}^{N-1}\frac{w_{t_{k+1}}^2-w_{t_k}^2}{2}+\sum_{k=0}^{N-1}\frac{(w_{\theta_k}-w_{t_{k+1}})+(w_{\theta_k}-w_{t_k})}{2}(w_{t_{k+1}}-w_{t_k})$$

   1pt

2. Show that the first sum on the right hands side, given that $w_0=0$, becomes

   $$\sum_{k=0}^{N-1}\frac{w_{t_{k+1}}^2-w_{t_k}^2}{2}=\frac{w_t^2}{2}.$$

   1pt

3. Show that we can rewrite the second sum as

   $$\sum_{k=0}^{N-1}\frac{(w_{\theta_k}-w_{t_{k+1}})+(w_{\theta_k}-w_{t_k})}{2}(w_{t_{k+1}}-w_{t_k})$$
   $$=-\frac{1}{2}\sum_{k=0}^{N-1}[(w_{\theta_k}-w_{t_{k+1}})^2-(w_{\theta_k}-w_{t_k})^2]$$

   1pt

4. Now we calculate the average, denoted by E, of the right hand side of the above equation. Show that the average of the first part is

   $$\mathsf{E}\sum_{k=0}^{N-1}(w_{\theta_k}-w_{t_{k+1}})^2=(1-s)t \tag{3}$$

   and the second part

   $$\mathsf{E}\sum_{k=0}^{N-1}(w_{\theta_k}-w_{t_k})^2=st \tag{4}$$

   (*Hint: Perhaps at this time it is good to remember, or learn, that for a Wiener process* $\mathsf{E}((w_t-w_s)^2)=|t-s|$) *2pts*

Additionally, it is possible to show that as $N\to\infty$ the sums (3) and (4) converge to their average value. As such we have proven equation (2).

Exercise 3: Ito vs Stratonovich

Notice that by choosing $s = 1/2$ in equation (2), the result of the integral looks like the result coming from ordinary integration. In fact, for the choice $s = 1/2$, it is in general true that

$$\int_a^b \frac{df^{(\theta)}(w_t)}{dw_t} dw_t = f(w_b) - f(w_a).$$

The special $s = 1/2$ case is called the Stratonovich differential while the $s = 0$ case is the Ito differential. Let $f(t, \chi_t)$ be a function and χ_t be a stochastic process. We define the notation for the Ito prescription

$$f(\chi_t)d\chi_t = f(\chi_t)(\chi_{t+dt} - \chi_t)$$

and for the Stratonovich prescription

$$f(\chi_t) \circ d\chi_t = f(\chi_t + d\chi_t/2)(\chi_{t+dt} - \chi_t).$$

Let the differential of χ_t in the Ito description be $d\chi_t = b(\chi_t)dt + A(\chi_t)\, dw_t$. It is then important to note that, although they look similar

$$b(\chi_t)dt + A(\chi_t)\, dw_t \neq b(\chi_t)dt + A(\chi_t) \circ\, dw_t,$$

but instead

$$d\chi_t = b(\chi_t)dt + A(\chi_t)\, dw_t = b(\chi_t)dt - \frac{A(\chi_t)(\partial_{\chi_t} A(\chi_t))}{2} dt + A(\chi_t) \circ\, dw_t. \quad (5)$$

Observe that for a function $f(\chi_t)$, one finds the in the Ito prescription that

$$\begin{aligned} df(\chi_t) =& f(\chi_t + d\chi_t) - f(\chi_t) \\ =& f(\chi_t) + \partial_{\chi_t} f(\chi_t) d\chi_t + \frac{1}{2}\partial^2_{\chi_t} f(\chi_t) d\chi_t d\chi_t - f(\chi_t) \\ =& \partial_{\chi_t} f(\chi_t) d\chi_t + \frac{1}{2}\partial^2_{\chi_t} f(\chi_t) d\chi_t d\chi_t \end{aligned} \quad (6)$$

1. We now want to express the differential $df(\chi_t)$ in the Stratonovich description. To do so, expand both $f(\chi_t + d\chi_t)$ and $f(\chi_t)$ around $\chi_t + d\chi_t/2$ up to second order in $d\chi_t$ to find that

   $$df(\chi_t) = \partial_{\chi_t} f(\chi_t) \circ d\chi_t = (\partial_x f(x))|_{x=\chi_t + d\chi_t/2} d\chi_t \quad (7)$$

   2pts

2. Consider the process $\chi_t = w_t^2$. Show that in the Ito representation

   $$d\chi_t = 2w_t dw_t + dt$$

   and in the Stratonovic representation

   $$d\chi_t = 2w_t \circ dw_t$$

   1pt

3. Consider now the lognormal process ξ_t its differential in the Ito sense is given by
$$d\xi_t = \mu\xi_t dt + \sigma\xi_t dw_t. \tag{8}$$
This stochastic process is an elementary example of capital growth in the stock market. In this exercise we will show that it is a clear example that one should take care with the discretisation, as getting getting it wrong might lead from riches to rags.
Using the result of point 1, convert the lognormal process (8) to the Stratonovich description. *1pt*

4. As mentioned above, Stratonovic differential equations obey the usual rules of calculus. Integrate the Stratonovich differential equation to find the solution. *1pt*

5. We can also find the solution of the lognormal process directly from the Ito description. Suppose that $\xi_t = f(w_t, t)$, writing the Ito differential gives
$$d\xi_t = \partial_{w_t} f\, dw_t + \left(\partial_t + \frac{1}{2}\partial^2_{w_t}\right) f dt.$$
Comparing the above equation to (8), we get the set of equations
$$\begin{cases} \partial_{w_t} f(w_t) = \sigma f(w_t) \\ \left(\partial_t + \frac{1}{2}\partial^2_{w_t}\right) f = \mu f. \end{cases}$$
Show that the above set of equations gives the same solution as that obtained by the Stratonovich differential equation. *1pt*
From the solution you should be able to see that care has to be taken with the Ito description. For $0 < \mu\frac{\sigma^2}{2}$, naively integrating the Ito process would lead to $\xi_t = e^{\mu t + \sigma w_t}$, such that
$$\mathsf{E}(\ln \xi_t) = \mu t \xrightarrow{t\uparrow\infty} +\infty$$
while the actual solution gives
$$\mathsf{E}(\ln \xi_t) \xrightarrow{t\uparrow\infty} -\infty$$

Exercise 4: Ornstein-Uhlenbeck Process

The Ornstein-Uhlenbeck process is given by the Ito differential
$$d\xi_t = \theta(\mu - \xi_t)dt + \sigma dw_t \tag{9}$$
for σ, θ positive numbers.

1. Write the Ornstein-Uhlenbeck process in the Stranotovic hform and show that the solution can be written as
$$\xi_t = \mu(\xi_0 - \mu)e^{-\theta t} + \sigma \int_0^t e^{-\theta(t-s)} dw_s$$
(*Hint: It could be convenient to use the result of the Appendix of Lecture 3) 2pts*

2. Calculate the Ito differential of the above equation and show that you get (9). *1pt*