Open Quantum Systems: Solutions to Exercise Session 2

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Exercise 1: Brownian Motion in a Harmonic Oscillator Heat Bath

1. The equations of Motion for the combined Hamiltonian $H_s + H_B$ come from the equations of motion for a hamiltonian systems i.e

$$\dot{x} = \frac{\partial H}{\partial p} \ ; \ -\dot{p} = \frac{\partial H}{\partial x}$$

$$\dot{q_j} = \frac{\partial H}{\partial p_j} \ ; \ -\dot{p_j} = \frac{\partial H}{\partial q_j}$$

Therefore the equations of motion for the combined system are

$$\frac{dx}{dt} = \frac{p}{m} \ ; \ \frac{dp}{dt} = -U'(x) + \sum_j \gamma_j (q_j - \frac{\gamma_j}{\omega_j^2} x)$$

$$\frac{dq_j}{dt} = p_j \ ; \ \frac{dp_j}{dt} = -\omega_j^2 q_j + \gamma_j x$$

2. For the bath with position coordinates $\{q_j\}$ we can solve the equations of motion, first by introducing a time dependence on the system with coordinate $x(t)$. Then we integrate the position equations of the using using methods to solve linear first order ordinary differential equations with an inhomogenity of $\gamma_j x$ as well as the Green's function method.
So we get

$$\int_0^t dq_j = \int_0^t p_j dt$$

$$q_j(t) - q_j(0)cos(\omega_j t) = \int_0^t p_j dt$$

Now using the solved equation of motion for the momentum and substituting:

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

Where we have used variation of parameters to find the integral on the end of the equation.

3. Integration by parts of the above answer leads to:

$$\int udv = uv - \int vdu \ ; \ u = x(s), dv = \frac{sin(\omega_j(t-s))}{\omega_j}$$

$$du = \dot{x}(s) = \frac{p(s)}{m}$$

$$v = \int \frac{sin(\omega_j(t-s))}{\omega_j} = \frac{cos(\omega_j(t-s))}{\omega_j^2}$$

Evaluated at the limits gives

$$\frac{x(t)}{\omega_j^2} - \frac{x(0)cos(\omega_j t)}{\omega_j^2} - \int_0^t \frac{cos(\omega_j(t-s))}{\omega_j^2}\dot{x}(s)ds$$

And substituting back in:

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

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

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

4. Put the above equation into dt/dt so that

$$\frac{dp(t)}{dt} = -U'(x(t)) + \sum_j \gamma_j(q_j(t) - \frac{\gamma_j}{\omega_j^2}x(t))$$

Looking at the second term $\sum_j \gamma_j(q_j(t) - \frac{\gamma_j}{\omega_j^2}x(t))$ and subbing in $q_j(t)$

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

The two $\frac{\gamma_j}{\omega_j^2}x(t)$ cancel and it can be rewritten as

$$\sum_j \gamma_j(q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0))cos(\omega_j t) + \sum_j \gamma_j p_j(0)\frac{sin(\omega_j t)}{\omega_j} - \sum_j \gamma_j\gamma_j\frac{1}{\omega_j^2}\int_0^t cos(\omega_j(t-s))\frac{p(s)}{m}ds$$

Now substitute $K(t=s)$ and $F_p(t)$ where

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

And the integral can be rearranged so that

$$\int_0^t cos(\omega_j(t-s))\frac{p(s)}{m}ds = \int_0^t cos(\omega_j s)\frac{p(t-s)}{m}ds$$

So that we get

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

5.

$$\sum_j \rightarrow \int dw(gw)$$

So $K(t)$ becomes a Fourier integral

$$K(t) = \int_0^t dwg(w)\frac{\gamma^2(\omega)}{\omega^2}cos(\omega t)$$

If $g(w) \propto \omega^2$ and $\gamma(\omega) = C$ (equals a constant).
From the fourier integral theorem

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} daf(a)\int_{-\infty}^{\infty} d\omega cos(\omega x - \omega a)$$

Which can be written in the dirac delta function form

$$\delta(x-a) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega cos(\omega x - \omega a)$$

So $K(t)$ can be written as

$$K(t) \propto \int_0^{\infty} d\omega C^2 cos(\omega t)$$

Which is like the dirac delta function with $a = 0$ and $x = t$

$$\therefore K(t) \propto \delta(t)$$

6. The distribution looks pretty similar to a Gibbs distribution which is a form of gaussian distribution.

$$E(q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0)) = \frac{1}{Z}\int_{-\infty}^{\infty} (q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0)) \exp(\frac{-H_B}{k_bT})dq_j(0)$$

Noticing that this is of the form

$$\frac{1}{Z}\int_{-\infty}^{\infty} q_j(0)P(q_j(0)^2)dq_j(0)$$

Where P is the probability distrbution function. Because this is a guassian distribution we can see that is is an odd function and the integral will equal 0. The same can be said for $E(p_j(0))$.
$-H_B$ relates to $q_j(0)^2$ due to the fact that we are using the baths initial conditions and that the q_j part of the baths hamiltonian is of second order. Essentially we can only consider the q_j or p_j terms in the respective expectation values.

3.1

7. For the fluctuation-dissipation relation we can use the answers to the second moment expectation values and some trig indentities to solve.

$$< F_p(t)F_p(t') >= \frac{1}{Z}\int F_p(t)F_p(t')\exp(\frac{-H_B}{k_bT})dq_j(0)dp_j(0)$$

$$= \frac{1}{Z}\int \Big[\sum_j \gamma_j p(0)\frac{sin(\omega_j t)}{\omega_j} + \sum_j (q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0))cos(\omega_j t)\Big]\cdot\ldots$$

$$\Big[\sum_j \gamma_j p(0)\frac{sin(\omega_j t')}{\omega_j} + \sum_j (q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0))cos(\omega_j t')\Big]\cdot\exp(\frac{-H_B}{k_bT})dq_j(0)dp(0)$$

Using the answers in the previous question

$$= \sum_j \Big[\gamma_j^2\frac{k_BT}{\omega_j^2}cos(\omega_j t)cos(\omega_j t') + \gamma_j^2\frac{k_BT}{\omega_j^2}sin(\omega_j t)sin(\omega_j t')\Big]$$

Using the identity

$$cos(a)cos(b) + sin(a)sin(b) = cos(a-b)$$

4.1

We get

$$= k_BT\sum_j \frac{\gamma_j^2}{\omega_j^2}cos(\omega_j(t-t'))$$

Which, using the K from before equals

$$= k_BTK(t-t')$$

Exercise 2: Stochastic integration

1.

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

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

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

Factorising

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

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

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

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

2.
$$\sum_{k=0}^{N-1} \frac{w_{t_{k+1}}^2 - w_{t_k}^2}{2}$$
Evaluate the first term and add that onto the summation
$$\frac{w_t^2 - 0^2}{2} + \sum_{k=1}^{N-1}$$
$$= \frac{w_t^2}{2} + 0$$
$$= \frac{w_t^2}{2}$$

3.
$$\sum_{k=0}^{N-1} \frac{(w_{\theta_k} - w_{t_{k+1}}) + (w_{\theta_k} - w_{t_k})}{2}(w_{t_{k+1}} - w_{t_k})$$
$$= \frac{1}{2}\sum_{k=0}^{N-1}((w_{\theta_k} - w_{t_{k+1}}) + (w_{\theta_k} - w_{t_k}))(w_{t_{k+1}} - w_{t_k})$$
$$\frac{1}{2}\sum_{k=0}^{N-1}[2w_{\theta_k}w_{t_{k+1}} - 2w_{\theta_k}w_{t_k} - w_{t_{k+1}}^2 + w_{t_k}^2]$$
$$= -\frac{1}{2}\sum_{k=0}^{N-1}[(w_{\theta_k} - w_{t_{k+1}})^2 - (w_{\theta_k} - w_{t_k})^2]$$
5.1

4. Not answered

Exercise 3: Ito vs Stratonovich

1. We expand the equation using a Taylor expansion up to order 2
$$f(a) + \frac{f'(a)}{1!}(x - a)$$
5.2

So that we get
$$f(\chi_t) \circ d\chi_t = \frac{\partial f(\chi_t)}{2}\partial t + f(\chi_t)d\chi_t$$
5.3

And the 2nd order and replace f with $\partial_{\chi_t} f$
$$\partial_{\chi_t} f(\chi_t) \circ d\chi_t = \frac{\partial^2_{\chi_t} f(\chi_t)}{2}\partial t + \partial_{\chi_t} f(\chi_t)d\chi_t$$
Using the chain rule we see that
$$\frac{\partial^2_{\chi_t} f(\chi_t)}{2}\partial t + \partial_{\chi_t} f(\chi_t)d\chi_t = df(\chi_t)$$
So
$$df(\chi_t) = \partial_{\chi_t} f(\chi_t) \circ d\chi_t$$
Which is equivalent to
$$\partial_x f(x)|_{x=\chi_t + d\chi_t/2} d\chi_t$$

2.

$$d\chi_t = b(\chi_t)dt + A(\chi_t)dw_t$$

So in the case that $\chi_t = w_t^2$

$$b(\chi_t) = 0 \; ; \;\; A(\chi_t) = 1$$

From equation (5) on the sheet we have then

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

Recognising that $dw_{t_i} \cdot dw_{t_j} = \delta_{ij}dt = dt$
For the Statonovic representation we have

$$d\chi_t = dt\{b - \frac{A}{2}\partial_{x_t}A\} + dw_t \circ A$$

So

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

3. A log-normal distrbution is of the form

$$X = e^{\mu+\sigma Z}$$

$$df(\chi_t) = \partial_{x_t}f(\chi_t) \circ d\chi_t$$

$$d\xi_t = \mu\xi_t dt + \sigma\xi_t dw_t$$

$$d\xi_t = \left\{\mu - \frac{\sigma^2}{2}\right\}\xi_t dt + \sigma\xi_t dw_t$$

4.

$$d\xi_t = \left\{\mu - \frac{\sigma^2}{2}\right\}\xi_t dt + \sigma\xi_t dw_t$$

To solve this lets multiply by $1/\xi_t$. So we have

$$\frac{1}{\xi_t}d\xi_t = \frac{1}{\xi_t}\left\{\mu - \frac{\sigma^2}{2}\right\}\xi_t dt + \frac{1}{\xi_t}\sigma\xi_t dw_t$$

$$= \frac{1}{\xi_t}d\xi_t = \left\{\mu - \frac{\sigma^2}{2}\right\}dt + \sigma dw_t$$

Now use Ito's lemma where

$$\frac{\partial f}{\partial x}(\xi_t, t) = \frac{1}{\xi_t}$$

so

$$f(x,t) = ln(x)$$

We have

$$d(ln\xi_t) = 0dt + \frac{1}{\xi_t}d\xi_t - \frac{1}{2}\frac{1}{\xi_t}d < \xi_t >$$

Where $d < \xi_t >$ is the quadratic variation

$$d < \xi_t >= \sigma^2\xi_t^2$$

Solving for $\frac{1}{\xi_t} d\xi_t$ we set

$$\frac{1}{\xi_t} d\xi_t = d(ln\xi_t) + \frac{1}{2}\frac{1}{\xi_t^2} d < \xi_t >$$

So that

$$d(ln\xi_t) = \Big\{\mu - \frac{\sigma^2}{2}\Big\}dt + \sigma dw_t$$

$$d(ln\xi_t) + \frac{1}{2}\frac{1}{\xi_t}\sigma\xi_t^2 = \Big\{\mu - \frac{\sigma^2}{2}\Big\}dt + \sigma dw_t$$

Cancelling and simplfying gives

$$ln\xi_t = ln\xi_0 + \int_0^t \Big[\mu - \frac{\sigma^2}{2} - \frac{\sigma^2}{2}\Big]dt + \int_0^t \sigma dw_t$$

$$\xi_t = \xi_0 exp\Big[\int_0^t \mu - \sigma^2 dt + \int_0^t \sigma dw_t\Big]$$

7.1

5. Not answered

Exercise 4: Ornstein-Uhlenbeck Process

1.

$$d\xi_t = \theta(\mu - \xi_t)dt + \sigma dw_t$$

Multiply both sides by an integrating factor $e^{-\theta t}$ and using the chain rule given by:

$$d(e^{-\theta t}\xi_t) = e^{-\theta t}d\xi_t + \xi_t d(e^{-\theta t})$$
$$= e^{-\theta t}d\xi_t - \theta e^{-\theta t}\xi_t dt$$

And multplying by the integration factor gives

$$e^{-\theta t}d\xi_t = e^{-\theta t}\theta(\mu - \xi_t)dt + e^{-\theta t}\sigma dw_t$$

Using the chain rule:

$$d(e^{-\theta t}\xi_t) = e^{-\theta t}\theta(\mu - \xi_t)dt + e^{-\theta t}\sigma dw_t + \xi_t d(e^{-\theta t})$$
$$= e^{-\theta t}\theta(\mu - \xi_t)dt + e^{-\theta t}\sigma dw_t - \theta e^{-\theta t}\xi_t dt$$
$$= e^{-\theta t}(\theta\mu - \theta\xi_t)dt + e^{-\theta t}\sigma dw_t - \theta e^{-\theta t}\xi_t dt$$
$$= (e^{-\theta t}\theta\mu - e^{-\theta t}\theta\xi_t)dt + e^{-\theta t}\sigma dw_t - \theta e^{-\theta t}\xi_t dt$$
$$= e^{-\theta t}\theta\mu dt - e^{-\theta t}\theta\xi_t dt + e^{-\theta t}\sigma dw_t - \theta e^{-\theta t}\xi_t dt$$
$$d(e^{-\theta t}\xi_t) = \theta e^{-\theta t}\mu dt - 2\theta e^{-\theta t}\xi_t dt + e^{-\theta t}\sigma dw_t$$

Integrating:

$$e^{-\theta t}\xi_t - \xi_0 = -\mu e^{-\theta t} + 2\xi_t e^{-\theta t} + \sigma\int e^{-\theta(t-s)}dw_s$$

Where variation of parameters method has been used

$$\xi_t = \theta(\xi_0 - \mu)e^{-\theta t} + \sigma\int_0^t e^{-\theta(t-s)}dw_s$$

2.

$$\xi_t = \mu(\xi_0 - \mu)e^{-\theta t} + \sigma \int_0^t e^{-\theta(t-s)} dw_s$$

We can say that

$$\sigma \int_0^t e^{-\theta(t-s)} dw_s = e^{-\theta t} \cdot \sigma \int_0^t e^{-\theta s} dw_s = Z_t$$

Due to being a gaussian integral we can write

$$\xi_t = \mu(\xi_0 - \mu + Z_t)e^{-\theta t} = f(t, Z_t)$$

With $dZ_t = \sigma e^{-\theta t} dw_t$
From Ito lemma then we have:

$$d\xi_t = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial Z_t} dZ_t +]frac12 \frac{\partial^2 f}{\partial Z^2} < dZ_t, dZ_t >$$

$$= -\theta\mu(\xi_0 - \mu + Z_t)e^{-\theta t} dt + e^{-\theta t} dZ_t + \frac{1}{2} \cdot 0$$

$$= -\theta\mu(\xi_0 - \mu + Z_t)e^{-\theta t} dt + \sigma dw_t$$

$$= \theta\mu dt - \theta(\mu(\xi_0 - \mu)e^{-\theta t} + \sigma \int_0^t e^{-\theta(t-s)} dw_s) dt + \sigma dw_t$$

As you can see the part inside the brackets is equal to ξ_t so we have

$$d\xi_t = \theta(\mu - \xi_t) dt + \sigma dw_t$$

8.1

Index of comments

1.1 where does this cos come from?

1.2 I am a bit confused what is going on here
1/2

3.1 you are a bit short here, but I think you understood what is going on

4.1 9/9

5.1 3/5

5.2 where is the second order term?

5.3 I don't understand this

6.1 is this Stratonovich? Remember to use the right notation

6.2 use the right notation for the Strat. differential!

6.3 why are you using Ito's lemma? You could straightforwardly integrate the Strat. eq

7.1 2.5/5

8.1 3/3