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.

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

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.

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

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

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

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

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

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

4. Not answered

Exercise 3: Ito vs Stratonovich

1. We expand the equation using a Taylor expansion up to order 2

$$f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \ldots$$

So that we get

$$f(\chi_t) \circ d\chi_t = \frac{\partial f(\chi_t)}{2}\partial t + f(\chi_t)d\chi_t$$

And the 2nd order and replace f with $\partial_{\chi_t} f$

$$\partial_{\chi_t} f(\chi_t) \circ d\chi_t = \frac{\partial_{\chi_t}^2 f(\chi_t)}{2}\partial t + \partial_{\chi_t} f(\chi_t)d\chi_t$$

Using the chain rule we see that

$$\frac{\partial_{\chi_t}^2 f(\chi_t)}{2}\partial t + \partial_{\chi_t} f(\chi_t)d\chi_t = df(\chi_t)$$

So

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

Which is equivalent to

$$\partial_x f(x)|_{x=\chi_t+d\chi_t/2} d\chi_t$$

Better more correct and more succinct way of completing question 1.

$$f(\chi_0) = f(\chi_t + d\chi_{t/2}) - \partial_{\chi_t} f(\chi_t + d\chi_{t/2})\frac{d\chi_t}{2}$$

$$+\frac{1}{2}\partial^2_{\chi_t} f(\chi_t - d\chi_{t/2})\frac{d^2\chi_t}{4} + \dots$$

$$f(\chi_t + d\chi_t) = f(\chi_t + d\chi_{t/2}) + \partial_{\chi_t} f(\chi_t + d\chi_{t/2})\frac{d\chi_t}{2}$$

$$+\frac{1}{2}\partial^2_{\chi_t} f(\chi_t + d\chi_{t/2})\frac{d^2\chi_t}{4} + \dots$$

Now

$$\begin{aligned} df(\chi_t) &= f(\chi_t + d\chi_t) - f(\chi_t) \\ &= \partial_{\chi_t} f(\chi_t + d\chi_{t/2}) d\chi_t \\ &= \partial_{\chi_t} f(\chi_t) \circ d\chi_t \end{aligned}$$

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

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

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

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

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

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

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

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

Cancelling and simplfying gives

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

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

Easier and simpler way

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

$$\hookrightarrow \ln(\xi_t) - \in \xi_0 = \left\{/mu - \frac{1}{2}\sigma^2\right\}t + \sigma w_t$$

$$\hookrightarrow \xi_t = \xi_0 \exp\left(\left\{\mu - \frac{1}{2}\sigma^2\right\}t + \sigma w_t\right)$$

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

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