CHEM/CHPH/PHYS 703: Introduction to Nonequilibrium Statistical Physics

PROBLEM SET # 3, due ~~at the start of class, Tuesday, March 24,~~ 5pm, Tue, 3/31/2020

**Problem 1**

For a one-dimensional harmonic oscillator described by the Hamiltonian

$$H(q,p) = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \tag{1}$$

the points along a given energy shell $E$ can be labelled by the oscillator phase $\theta$, which evolves at a fixed rate $\dot{\theta} = \omega$. On this energy shell, an observable $A(q,p)$ can be expressed as $A(\theta)$. Such observables are elements of a Hilbert space, on which operators $U_t$ and $\mathcal{L}$ are defined as follows:

$$\left(U_t A\right)(\theta) = A(\theta + \omega t) \quad , \quad U_t A = e^{i\mathcal{L}t} A \tag{2}$$

(a) Show that $(\mathcal{L}A)(\theta) = -i\omega A'(\theta)$, where $A' = \partial A/\partial\theta$.

(b) Let $\{\phi_n(\theta)\}$ denote the set of eigenstates of the self-adjoint operator $\mathcal{L}$, and let $\{\lambda_n\}$ be the corresponding eigenvalues. Solve for these eigenstates and eigenvalues, normalizing the eigenstates so that they form an orthonormal basis on the Hilbert space.

(c) Since the oscillator momentum $p$ is an observable, it can be expanded as follows:

$$p(\theta) = \sum_n \alpha_n \phi_n(\theta) \tag{3}$$

Solve for the coefficients $\{\alpha_n\}$ in this expansion, and show that the expression $U_t p = e^{i\mathcal{L}t} p$ combines with Eq. 3 to give the expected result

$$\left(U_t p\right)(\theta) = p(\theta + \omega t) \tag{4}$$

(d) An ensemble of trajectories evolving on the energy shell is described by a probability distribution

$$f(\theta, t) = f_0(\theta - \omega t) \tag{5}$$

where $f_0(\theta)$ is the distribution at $t = 0$. Writing $f_0(\theta) = \sum_n \beta_n \phi_n(\theta)$, show that

$$f(\theta, t) = e^{-i\mathcal{L}t} f_0(\theta) \tag{6}$$

**Problem 2**

In this problem you will derive the master equation (Eq. 15) for the Ornstein-Uhlenbeck (OU) process. Recall that the OU stochastic equation of motion is

$$\dot{x} = -\alpha x + \tilde{v}(t) \tag{7}$$

where $\alpha > 0$,$\langle \tilde{v}(t) \rangle = 0$ and $\langle \tilde{v}(s)\tilde{v}(s+t) \rangle = 2D\delta(t)$. If a trajectory starts at a point $x_0$ at time $t$, then for a short time $\delta t$ it remains very close to $x_0$, hence

$$\dot{x} \approx -\alpha x_0 + \tilde{v}(t) \tag{8}$$

We can then use the kernel for a particle with drift + diffusion, i.e. $\dot{x} = v + \tilde{v}(t)$, to write

$$K(x, t+\delta t | x_0, t) \approx \mathcal{N} \exp\left[ -\frac{(x - x_0 + \alpha x_0 \delta t)^2}{4D\delta t} \right] \tag{9}$$

where $\mathcal{N} = 1/\sqrt{4\pi D \delta t}$. For a general, smooth probability distribution given by $f(x, t)$ at time $t$, we can use this kernel to write the distribution a short time later:

$$f(x, t+\delta t) = \int dx_0 f(x_0, t)\, K(x, t+\delta t | x_0, t) \tag{10}$$

(a) Defining $\epsilon \equiv x - x_0$, use Eq. 9 to rewrite the right side of Eq. 10 as follows

$$\frac{1}{1-\alpha\delta t} \int d\epsilon\, f(x-\epsilon, t) \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[ -\frac{(\epsilon + \beta x \delta t)^2}{2\sigma^2} \right] \tag{11}$$

and solve for $\sigma^2$ and $\beta$ in terms of $\alpha$, $D$ and $\delta t$.

(b) For short $\delta t$, the Gaussian in Eq. 11 is sharply peaked. Hence, although the integration is from $-\infty$ to $+\infty$, only the region near $\epsilon = 0$ contributes to the integral. We thus expand

$$f(x-\epsilon, t) \approx f(x, t) - \epsilon f'(x, t) + \frac{1}{2}\epsilon^2 f''(x, t) \tag{12}$$

Substituting this expansion into Eq. 11, show that you get

$$f(x, t+\delta t) = \frac{1}{1-\alpha\delta t} \left[ I_0 f(x, t) + I_1 f'(x, t) + I_2 f''(x, t) \right] \tag{13}$$

and solve for $I_0$, $I_1$ and $I_2$ in terms of $x$, $\alpha$, $\beta$, $D$ and $\delta t$.

(c) Rewriting Eq. 13 keeping only terms up to order $\delta t$, you should obtain

$$f(x, t+\delta t) = f(x, t) + \delta t\, [\cdots] \tag{14}$$

Solve for $[\cdots]$ and show that Eq. 14 leads to the master equation

$$\frac{\partial f}{\partial t} = \alpha \frac{\partial}{\partial x}(xf) + D\frac{\partial^2 f}{\partial x^2} \tag{15}$$

**Problem 3**

A particle performs a one-dimensional random walk by taking steps of length $d$, either to the right ($+d$) or to the left ($-d$). The interval of time between consecutive steps is $\epsilon$. Over a time scale that is much longer than $\epsilon$, and a length scale much longer than $d$, the behavior of this particle is diffusive. In both parts of this problem, $0 < p < 1$ and $p + q = 1$.

(a) Suppose the steps are uncorrelated with one another, and let $p$ and $q$ denote the probability to take a step to the right and to the left, respectively. Write down the Fokker-Planck equation describing the diffusive motion of this particle.

(b) Now suppose the steps are correlated. At each step, with probability $p$ the particle moves in the same direction as the previous step, and with probability $q$ the particle moves in the opposite direction. Again, write down the corresponding Fokker-Planck equation.

As a consistency check, verify that your results for (a) and (b) are identical when $p = q = 1/2$.

**Problem 4**

A Brownian particle with charge $q$ in an oscillatory electric field evolves according to

$$\dot{p} = -\gamma \frac{p}{m} + qE_0 \cos(\omega t) + \xi(t) \qquad , \qquad \langle \xi(t)\xi(t') \rangle = 2D_p \delta(t - t') \tag{16}$$

(a) Obtain equations of motion for all of the cumulants of the momentum, $\kappa_n(t)$.

(b) Show that in the long-time limit, the momentum distribution is a Gaussian with a fixed variance $\sigma^2$, and a time-dependent mean, $\langle p \rangle_t = \psi \cos(\omega t - \phi)$, and solve for $\sigma^2$, $\psi$ and $\phi$.

(c) The particle absorbs energy from the oscillating field at a rate given by the formula *power* = *force* $\times$ *velocity*, and this energy is in turn dissipated into the surrounding thermal environment. What is the average rate of energy dissipation?

(d) Confirm that when $\omega \ll \gamma/m$, your results for parts (b) and (c) agree with what you would predict from a much simpler analysis.