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

PROBLEM SET # 4, due at 5pm, Tuesday, April 21, 2020

Problem 1

Consider a Brownian particle with charge q in an oscillatory electric field:

$$\dot{p} = -\gamma \frac{p}{m} + qE_0 \cos(\omega t) + \xi(t) \qquad , \qquad \langle \xi(t)\xi(t')\rangle = 2D_p \delta(t-t') \ , \ \gamma = \beta D_P \tag{1}$$

where the particle begins in equilibrium at $t = 0$.

(a) Use linear response theory to solve for the average momentum, $\langle p \rangle_t$, for $t > 0$.

(b) For $t \gg m/\gamma$, compare your answer with that of Problem Set #3, Problem 4b.

Problem 2

An overdamped Brownian particle in a harmonic well with stiffness k is described by the Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{k}{\gamma}\frac{\partial}{\partial x}(xf) + D\frac{\partial^2 f}{\partial x^2} \equiv \mathcal{L}f \qquad , \qquad \frac{1}{\gamma} = \beta D \tag{2}$$

The eigenvalues of $\mathcal{L}$ are real and can be ordered as follows: $0 = \lambda_0 > \lambda_1 > \lambda_2 > \cdots$ Use the operator formalism discussed on March 12 (the notes have been posted to the course website) to solve the following problems.

(a) Determine λ_1 and λ_2, and solve for first three eigenstates of both $\mathcal{L}$ and $\mathcal{L}^\dagger$, corresponding to the eigenvalues λ_0, λ_1 and λ_2.

(b) Use these results to compute the autocorrelation function $C_x(t) = \langle x_0 x_t \rangle$. Compare with the result for $C_x(t)$ provided in the notes on the Ornstein-Uhlenbeck process, obtained directly from the kernel $K(x,t|x_0,0)$.

(c) For an observable $A(x)$, we can introduce a formalism similar to the Heisenberg picture in quantum mechanics: we use the equations $A(x,0) = A(x)$ and $\partial A/\partial t = \mathcal{L}^\dagger A$ to define a time-dependent function $A(x,t)$. For the overdamped oscillator (Eq. 2), use this formalism to determine $A(x,t)$ when $A(x) = x$, and when $A(x) = x^2$.

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Problem 3

The following rate matrix describes random transitions among three states:

$$\mathcal{R} = \frac{1}{6}\begin{pmatrix} -5 & 4 & 1 \\ 2 & -4 & 2 \\ 3 & 0 & -3 \end{pmatrix} \tag{3}$$

(a) After solving for the eigenvalues and eigenvectors, express $\mathcal{R}$ in Jordan normal form, then use this result to obtain an explicit expression for the matrix $\exp(\mathcal{R}t)$.

(b) Let $A = (a_1, a_2, a_3)^T = (1, 1, -2)^T$ denote an observable: when the system is in state n, the value of A is given by a_n. As the system makes transitions, the value of A changes with time. Compute the autocorrelation function $C_A(t) = \langle A_0 A_t \rangle - \langle A \rangle^2$ in the steady state.