Nonequilibrium Statistical Mechanics

HW #1, Spring 2019

due : April 2, 2019

Note that you SHOULD show the details of your work.

1. (a) Show that if N independent random variables $X_i (i = 1, 2, \ldots, N)$ follow the Lorentzian distribution:

$$P(x) = \frac{1}{\pi}\frac{\gamma}{(x-a)^2 + \gamma^2} \quad \text{for } -\infty < x < \infty,$$

$Y = \sum_{i=1}^{N} X_i$ has also the Lorentian distribution. Why does the central limit theorem break down?
(b) Consider the Langevin equation for a Brownian particle, namely,

$$\frac{dv}{dt} = -\gamma v(t) + f(t)/m,$$

where the random process $f(t)$ is assumed to be Gaussian. Prove that the moments of $u = v - v_0 e^{-\gamma t}$ are given by

$$\langle u^{2n} \rangle = 1 \cdot 3 \cdot 5 \cdots (2n-1) \langle u^2 \rangle^n, \quad \langle u^{2n+1} \rangle = 0.$$

(c) The characteristic function of multivariate Gaussian distribution has the form

$$G(k_1, k_2, \ldots, k_n) = e^{i \sum_i k_i \mu_i - \frac{1}{2} \sum_{i,j} k_i k_j \sigma_{ij}}.$$

By explicit calculation, find the probability distribution and show that $\langle X_i X_j \rangle_c = \sigma_{ij}$. Also show that all higher moments can be expressed in terms of products of first two moments and that all cumulants higher than second order vanish.
(d) Show that if $X(t)$ is a Gaussian process, any linear transformation of it

$$Y(t) = \int_a^b c(t, t') X(t') dt'$$

is also Gaussian.

2. Consider a Brownian particle of mass m as a harmonic oscillator and then the equations of motions are

$$\frac{dx}{dt} = \frac{p}{m}$$
$$\frac{dp}{dt} = -m\omega_0^2 x - \frac{\zeta}{m} p(t) + f(t),$$

where the fluctuating random force is assumed to be delta-correlated, $\langle f(t) f(t') \rangle = 2\zeta k_B T \delta(t - t')$.
(a) Suppose that the momentum in the infinite past vanishes and $p(t)$ can be integrated as considering $x(t)$ as known. Then show that

$$\langle f_x(t) f_x(t') \rangle = \langle x^2 \rangle_{eq} \gamma(|t - t'|)$$

where the memory function and new fluctuating force for $x(t)$ are given as

$$\gamma(t) = \omega_0^2 e^{-\zeta|t|/m}, \quad f_x(t) = \frac{1}{m} \int_{-\infty}^{t} dt' \, e^{-\zeta(t-t')/m} f(t')$$

(b) Now consider that the noise strength as well as $x(t)$ are unknown, and let x_0 and v_0 be the initial positions and velocity, respectively, of the Brownian particle. Assume that it is initially in equilibrium with a thermal bath, the average kinetic energy and potential energy are given by $k_B T/2$ according to the equipartition theorem. x_0 and v_0 are also assumed to be statistically independent so $\langle x_0 v_0 \rangle = 0$. After obtaining explicit expression for the velocity at time t in terms of x_0 and v_0, determine the noise strength Q to ensure that the process be stationary when $\langle f(t) f(t') \rangle = Q\delta(t - t')$. Also evaluate the velocity correlation function, $\langle v(t) v(t') \rangle$ and the its spectral density, $S_v(\omega)$. What are the peak positions and width of the spectral density?

3. Consider the Caldeira-Leggett model where a particle of mass m, position x, and conjugate momentum p, under an external potential $U(x)$ is coupled with a bath of N independent harmonic oscillator of mass m_j, position x_j and momenta p_j. Then the Hamiltonian of the system reads as

$$H = \frac{p^2}{2m} + U(x) + \frac{1}{2}\sum_{j=1}^{N}\left[\frac{p_j^2}{2m_j} + m_j\omega_j^2\left(x_j - \frac{c_j}{m_j\omega_j^2}x\right)^2\right].$$

Show that there is no correlation between different modes and the generalized fluctuation-dissipation theorem can be obtained as

$$\langle f(t)f(t')\rangle_0 = mk_BT\gamma(t-t')$$

where the memory kernel is given as $\gamma(t) = (1/m)\sum_j c_j/(m_j\omega_j^2)\cos\omega_j t$. Note that $\langle\ldots\rangle_0$ denotes ensemble average over initial equilibrium distribution.