

Non-equilibrium physics WS 18/19 – Exercise Sheet 13:

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1 Discussion:

- i) What is a Markov process? Under which assumptions can Brownian motion be described as a Markov process? What is the Fokker-Planck equation for a stochastic process?

2 In-class problems:

2.1 Spectral analysis of Brownian motion

We consider the process of Brownian motion of a particle in one dimension, described by the stochastic differential equation

$$M \frac{dv}{dt} = -M\gamma v(t) + F_L(t), \quad (1)$$

where $F_L(t)$ is the stochastic Langevin Force with $\langle F_L(t) \rangle = 0$. We will assume that the stochastic process is stationary, i.e. $\langle F_L(t)F_L(t') \rangle = \kappa(t-t')$, and that the Brownian particle is in equilibrium with the thermal bath at all times.

- i) Show that the spectral density of the velocity of the Brownian particle is given by

$$S_v(\omega) = \frac{1}{M^2} \frac{1}{|\gamma - i\omega|^2} S_{F_L}(\omega)$$

where $S_{F_L}(\omega)$ is the spectral density of the stochastic force.

- ii) Calculate the un-equal time correlation function $\langle v(t)v(t+\Delta t) \rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{(2\pi)} S_v(\omega) e^{i\omega\Delta t}$ for a white noise spectrum $S_{F_L}(\omega) = 2D_v M^2$ and for a non-white noise spectrum $S_{F_L}(\omega) = 2D_v M^2 \frac{a^2}{\omega^2 + a^2}$ for $a \neq \gamma$. (Hints: Contour integration; Distinguish between the cases $\Delta t > 0$ and $\Delta t < 0$)

3 Homework problems:

3.1 Brownian motion in the viscous limit

Consider the process of Brownian motion in the viscous limit, described by the stochastic differential equation

$$M\gamma \frac{dx}{dt} = F_L(t) \quad (2)$$

where $F_L(t)$ is a stochastic force with vanishing expectation value $\langle F_L(t) \rangle = 0$ and auto-correlation function $\langle F_L(t)F_L(t') \rangle = 2DM^2\gamma^2\delta(t-t')$.

- i) Derive the associated Fokker-Planck equation

$$\frac{\partial}{\partial t} f(t, x) = D \frac{\partial^2}{\partial x^2} f(t, x), \quad (3)$$

for the probability distribution $f(t, x) = p_1(t, x)$

- ii) Calculate the probability distribution $f(t, x)$ for the case that the initial position of the Brownian particle is known exactly, i.e. $f(t=0, x) = \delta(x - x_0)$.

3.2 Caldera-Leggett model

We consider a system of a heavy particle of mass M with position X and momentum P interacting with a set of N light particles with masses m_n described by their positions and momenta x_n, p_n . In the absence of external forces acting on the heavy-particle, the dynamics of the system is governed by the Caldera-Leggett Hamiltonian

$$H_{C-L} = \frac{P^2}{2M} + \sum_{n=1}^N \frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 \left(x_n - \frac{c_n}{m_n \omega_n^2} X \right)^2 \quad (4)$$

where the light particles are modeled by an ensemble of harmonic oscillators with frequencies ω_n , and couplings $\frac{c_n}{m_n \omega_n^2}$ to the heavy particle.

- i) Derive Hamilton's equations of motion for the positions and momenta X, P of the heavy particle and for the position and momenta x_n, p_n of the light particles.
- ii) Show that the general solution for the equations of motion for the light particles can be formally expressed as

$$x_n(t) = x_n(t_0) \cos(\omega_n(t - t_0)) + \frac{p_n(t_0)}{m_n \omega_n} \sin(\omega_n(t - t_0)) + c_n \int_{t_0}^t dt' \frac{\sin(\omega_n(t - t'))}{m_n \omega_n} X(t') \quad (5)$$

We will now specialize on the case where the initial position of the heavy particle is fixed at $X(t_0) = 0$

- iii) Show that in this case the solution for the position of the light particles $x_n(t)$ can be expressed as

$$x_n(t) - \frac{c_n}{m_n \omega_n^2} X(t) = x_n(t_0) \cos(\omega_n(t - t_0)) + \frac{p_n(t_0)}{m_n \omega_n} \sin(\omega_n(t - t_0)) - c_n \int_{t_0}^t dt' \frac{\cos(\omega_n(t - t'))}{m_n \omega_n^2} \frac{P(t')}{M} \quad (6)$$

(Hint: Integration by parts)

- iv) Based on your results in (i) and (iii) show that the equations of motion for the momentum P of the heavy particle can be expressed in the form

$$\frac{d}{dt} P(t) = - \int_{t_0}^t dt' \gamma(t - t') P(t') + F(t), \quad (7)$$

and determine the functions $\gamma(t)$ and $F(t)$. (Check: $\gamma(t) = \frac{1}{M} \sum_{n=1}^N \frac{c_n^2}{m_n \omega_n^2} \cos(\omega_n t)$ and $F(t) = \sum_{n=1}^N c_n \left[x_n(t_0) \cos(\omega_n(t - t_0)) + \frac{p_n(t_0)}{m_n \omega_n} \sin(\omega_n(t - t_0)) \right]$)

So far we have considered the Hamiltonian dynamics of an individual microscopic realizations of the system. However, if we consider the bath of oscillators to be in thermal equilibrium we still have to perform an averaging over the initial conditions $x_n(t_0)$, $p_n(t_0)$ according to the thermal N -body phase-space distribution with

$$\langle x_n(t_0) \rangle_{eq} = 0, \quad \langle p_n(t_0) \rangle_{eq} = 0, \quad (8)$$

and

$$\langle x_n(t_0)x_{n'}(t_0) \rangle_{eq} = \frac{k_B T}{m_n \omega_n^2} \delta_{nn'}, \quad \langle x_n(t_0)p_{n'}(t_0) \rangle_{eq} = 0, \quad \langle p_n(t_0)p_{n'}(t_0) \rangle_{eq} = m_n k_B T \delta_{nn'}, \quad (9)$$

- v) Calculate the thermal expectation values of the average force $\langle F(t) \rangle$ and its auto-correlation function $\langle F(t)F(t + \Delta t) \rangle$.