Course on "Advanced Statistical Physics"
Spring Semester (2016)
School of Nano Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
Lecturer: Ali Naji (School of Physics, IPM)
Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #11: Dissipative Dynamics of Particles (***extra-credit problem set***)
Due: August 30, 2016

Note: *References from which the following problems have been taken are available upon request.*

1: *Brownian rotor.* Consider a Brownian rotor with moment of inertia I constrained to rotate through angle θ about the z axis. The Langevin equations of motion for the rotor are $Id\omega/dt = -\Gamma\omega + \xi(t)$ and $d\theta/dt = \omega$, where ω is the angular velocity of the rotor, F is the friction coefficient, and $\xi(t)$ is a Gaussian white noise torque. The torque is delta-correlated, $\langle\xi(t)\xi(t')\rangle = D\delta(t-t')$, where G is the noise strength.

(i) For the case of large friction coefficient, Γ, write the Fokker-Planck equation for the probability density, $P(\theta, t)$, to find the Brownian rotor in the interval $(\theta, \theta + d\theta)$ at time t.

(ii) Solve the Fokker-Planck equation assuming that at time $t = 0$ the rotor is at $\theta = \theta_0$.

(iii) Compute the probability current at time t.

2: *Brownian dynamics with memory and long-time tails.* In the most common treatment of Brownian dynamics of a particle in a viscous fluid, one assumes that the friction force at any given time is given simply by a constant friction coefficient, γ, times the velocity, $v(t)$, at the same time (note that, for the sake of simplicity, we consider a one-dimensional motion in what follows; the generalization to higher dimensions is straightforward). In general, the dissipative force acting on a Brownian particle at time t can depend on the particle velocity at earlier times and, hence, given time translational invariance, the friction coefficient can be assumed to depend on the time difference, $t - t'$. In the presence of an external force $F(t)$, the velocity Langevin equation can thus be expressed in terms of a memory kernel $\tilde{\gamma}(t - t')$ as

$$\frac{\partial v}{\partial t} = -\int_{-\infty}^{+\infty} \tilde{\gamma}(t-t')v(t')dt' + \frac{1}{m}F(t) + \frac{1}{m}\zeta(t), \tag{1}$$

where causality implies that the memory kernel be non-zero only for $t > t'$ and may thus be written as $\tilde{\gamma}(t-t') = 2\theta(t-t')\tilde{\gamma}'(t-t')$, where $\theta(\cdot)$ is the Heaviside step function.

(i) Show that the Laplace transform as a function of complex frequency z follows as

$$\gamma(z) = \int_0^\infty dt\, e^{izt}\, \tilde{\gamma}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi i}\frac{\gamma'(\omega)}{\omega - z}, \tag{2}$$

where ω is a real frequency variable, and that $\gamma(\omega) = \lim_{\epsilon\to 0}\gamma(\omega + i\epsilon) = \gamma'(\omega) + i\gamma''(\omega)$, where the imaginary part $\gamma''(\omega)$ is related to the real part $\gamma'(\omega)$ by a Kramers-Kronig relation. Show also that $\gamma^*(\omega) = \gamma(-\omega)$.

(ii) Calculate the mobility $\mu(\omega)$ relating the velocity to the external force via $v(\omega) = \mu(\omega)F(\omega)$ in terms of $\gamma(\omega)$. What is the complex electrical conductivity of a system with a density n, of non-interacting Brownian particles, each carrying a charge e?

(iii) Show that noise correlations must satisfy

$$C_{\zeta\zeta}(\omega) = 2k_BTm\gamma'(\omega) \tag{3}$$

to produce thermal equilibrium. Then show that the velocity correlation function is

$$C_{vv}(\omega) = \frac{2k_BT}{m}\frac{\gamma'(\omega)}{|-i\omega + \gamma(\omega)|^2} \tag{4}$$

Hint: Note that $\gamma(\omega)$ is analytic in the upper half plane to obtain this result.

(iv) If a particle of radius a and density ρ_0 moves with a time-dependent velocity in a fluid of density ρ and shear viscosity η, it will excite viscous shear waves in the fluid with frequency $\omega_v = -i\eta q^2/\rho$, where q is the wave number. This leads to a singular memory function

$$\gamma(\omega) = -2i\omega\rho/\rho_0 + \gamma(\sqrt{-i\omega\tau_v} + 1), \tag{5}$$

where $\tau_v = \rho a^2/\eta$ is the viscous relaxation time (the time for a shear wave to diffuse across a particle radius). Show that

$$C_{vv}(t) = \frac{k_B T}{m^*} F(\tau), \tag{6}$$

where $m^* = m[1 + \rho/(2\rho_0)]$, $\tau = (m/m^*)\gamma t$, and

$$F(\tau) = \frac{\sigma}{\pi} \tau^{-3/2} \int_0^\infty \frac{e^{-u^2} u^2 du}{(\tau^{-1} u - 1)^2 + \sigma^2 \tau^{-1} u^2}, \tag{7}$$

where $\sigma^2 = (m/m^*)\gamma\tau_v = 9\rho/(2\rho_0 + \rho)$. This implies that $F(\tau) \to \sigma\tau^{-3/2}/(2\sqrt{\pi})$ as $\tau \to \infty$. Such algebraic rather than exponential fall-off of correlation functions at long times is often referred to as a *long-time tail*. Use the above expression for $C_{vv}(t)$ and the definition

$$D(t) = \int_0^t d\tau \, C_{vv}(\tau) \tag{8}$$

to show that

$$D(t) \simeq D[1 - (\tau_v/t)^{1/2}] \qquad t \to \infty, \tag{9}$$

where $D = k_B T/m\gamma$ is the diffusion constant. Thus, the Einstein relation is satisfied even though the approach to this result at long time is algebraic rather than exponential. Note that when the density of the Brownian particle is much greater than the fluid density, $\sigma \to 0$, $m^* \to m$, and $F(t) \to e^{-\gamma|t|}$, and one recovers the result for Brownian motion without memory, i.e., $C_{vv}(t) \to (k_B T/m) e^{-\gamma|t|}$. Explain why?