

Spring Semester (2016)

School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

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Homework #16: Dissipative Dynamics of Particles and Fields*(extra-credit problem set)*

Due: August 30, 2016

Note: References from which some of the following problems have been taken/adopted are available upon request.

- 1: 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

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

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

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

where ω is a real frequency variable, and that $\gamma(\omega) = \lim_{\epsilon \rightarrow 0} \gamma(\omega + i\epsilon) = \gamma'(\omega) + i\gamma''(\omega)$, 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

$$C_{\zeta\zeta}(\omega) = 2k_B T m \gamma'(\omega) \quad (3)$$

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

$$C_{vv}(\omega) = \frac{2k_B T}{m} \frac{\gamma'(\omega)}{|-i\omega + \gamma(\omega)|^2} \quad (4)$$

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

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

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

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

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

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

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where $\sigma^2 = (m/m^*)\gamma\tau_v = 9\rho/(2\rho_0 + \rho)$. This implies that $F(\tau) \rightarrow \sigma\tau^{-3/2}/(2\sqrt{\pi})$ as $\tau \rightarrow \infty$. 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

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

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, $\sigma \rightarrow 0$, $m^* \rightarrow m$, and $F(t) \rightarrow e^{-\gamma|t|}$, and one recovers the result for Brownian motion without memory, i.e., $C_{vv}(t) \rightarrow (k_B T/m)e^{-\gamma|t|}$. Explain why?

2: Random pinning of a flat interface. The Hamiltonian of an elastic d -dimensional interface such as a domain wall in a ferromagnet is given by

$$\mathcal{H} = \int d\mathbf{x} \left[\frac{\sigma}{2} (\nabla h)^2 + V(\mathbf{x}, h) - f_{\text{ext}} h(\mathbf{x}) \right], \tag{10}$$

in which $h(\mathbf{x}, t)$ is the height of the interface with respect to its flat d -dimensional plane (see Fig. 1 for a schematic one-dimensional illustration), σ is the elastic constant and $V(\mathbf{x}, z)$ is the potential energy due to fixed (quenched), randomly positioned pinning sites that tend to ‘stop’ the interface and f_{ext} is the external driving force trying to release the interface from the pinning sites. The random potential is characterized by its mean and two-point correlation function

$$\overline{V(\mathbf{x}, z)} = 0, \quad \overline{V(\mathbf{x}, z)V(\mathbf{x}', z')} = \delta^d(\mathbf{x} - \mathbf{x}')R(z - z'). \tag{11}$$

The equation of motion of such an interface, assuming its inertia is negligible, is

$$\mu^{-1} \frac{\partial h}{\partial t} = \sigma \nabla^2 h + f(\mathbf{x}, h) + f_{\text{ext}}, \tag{12}$$

where μ is the mobility of the interface and $f(\mathbf{x}, z) = -\partial V(\mathbf{x}, z)/\partial z$ is the force due to the pinning sites. The variance of this force follows as

$$\overline{f(\mathbf{x}, z)f(\mathbf{x}', z')} = \delta^d(\mathbf{x} - \mathbf{x}')\Delta(z - z'). \tag{13}$$

(i) Express $\Delta(z)$ in terms of $R(z)$.

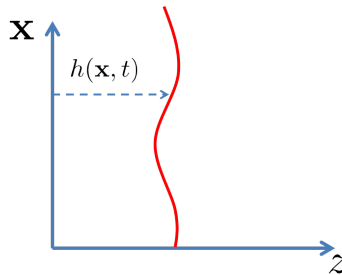


Figure 1. (See Problem 2)

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(ii) Assume that the interface is flat $h(\mathbf{x}, t) = h_0(t)$ and that it is pinned, meaning $\partial h/\partial t = 0$. We would like to argue that this situation is not possible for any non-zero value of f_{ext} . By making use of the above assumptions, approximate what is left in the equation of motion by integrating over a scale L and show that the contribution from the pinning force scales as $-|\Delta(0)|^{1/2}L^{d/2}$, while the contribution from the external driving force scales as $f_{\text{ext}}L^d$. Show that one must have $f_{\text{ext}} \rightarrow 0$ in order to satisfy the resultant equation at large length scales $L \rightarrow \infty$.

3: Fokker-Planck equation for stochastic field dynamics. Consider the Langevin equation describing the dissipative dynamics of a scalar field, $\varphi(\mathbf{x}, t)$, in d -dimension,

$$\frac{\partial \varphi}{\partial t} = v(\varphi(\mathbf{x}, t)) + \eta(\mathbf{x}, t), \quad (14)$$

where $v(\varphi(\mathbf{x}, t))$ is the local deterministic ‘velocity’ of the field and $\eta(\mathbf{x}, t)$ is a Gaussian white ‘noise’ with no spatial correlations, characterized by its mean and two-point correlation function

$$\langle \eta(\mathbf{x}, t) \rangle = 0, \quad \langle \eta(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = 2D \delta^d(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (15)$$

(i) Show that the probability distribution function, $\mathcal{P}([\varphi], t)$, for the field having a configuration $\varphi(\mathbf{x})$ at time t is governed by the Fokker-Planck equation

$$\frac{\partial \mathcal{P}([\varphi], t)}{\partial t} = \int d\mathbf{x} \frac{\delta}{\delta \varphi(\mathbf{x})} \left[D \frac{\delta \mathcal{P}([\varphi], t)}{\delta \varphi(\mathbf{x})} - v(\varphi(\mathbf{x})) \mathcal{P}([\varphi], t) \right]. \quad (16)$$

(ii) Derive a more general form of the above Fokker-Planck equation by assuming that the noise exhibits spatial correlations with the two-point correlation function

$$\langle \eta(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = 2D(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (17)$$

The uncorrelated case in part (i) is recovered by setting $D(\mathbf{x} - \mathbf{x}') \rightarrow D \delta^d(\mathbf{x} - \mathbf{x}')$.

(iii) Consider a system whose equilibrium state is described by a free energy functional $\mathcal{F}[\varphi]$. The dissipative dynamics of *near-equilibrium* fluctuations in this system can be described by Eq. (14) if the deterministic velocity is set equal to the generalized force times a mobility coefficient, μ , as

$$v(\varphi(\mathbf{x})) = -\mu \frac{\delta \mathcal{F}[\varphi]}{\delta \varphi(\mathbf{x})}. \quad (18)$$

Prove that the stationary ($t \rightarrow \infty$) solution of the Fokker-Planck equation, if it exists, is given by the Boltzmann probability weight, provided that Einstein’s relation, $D = \mu k_B T$, is satisfied.

(iv) Generalize the Langevin equation (14) to describe the near-equilibrium dynamics of the scalar field, $\varphi(\mathbf{x}, t)$, subject to a noise term with finite spatial correlations as shown in Eq. (17). To this end, first generalize the form of the deterministic velocity, Eq. (18), by taking a spatially varying mobility kernel $\mu(\mathbf{x} - \mathbf{x}')$, which is to be determined by requiring Boltzmann equilibrium in the stationary limit, $t \rightarrow \infty$. This latter task can be achieved by deriving the corresponding Fokker-Planck equation for the time evolution of the probability distribution function in the presence of spatial noise correlations and, thereby, establishing a generalized Einstein’s relation that guarantees approach to equilibrium in the stationary limit.

4: Stationary distribution for Kardar-Parisi-Zhang equation. The Kardar-Parisi-Zhang (KPZ) equation for the stochastic dynamics of a scalar field $\varphi(\mathbf{x}, t)$,

$$\frac{\partial \varphi}{\partial t} = \nu \nabla^2 \varphi + \frac{\lambda}{2} (\nabla \varphi)^2 + \eta(\mathbf{x}, t) \quad \nu, \lambda > 0, \quad (19)$$

describes a large class of dissipative dynamical processes occurring *far from equilibrium*. This means that the long-time dynamics in such cases does not converge to an equilibrium state described by a free energy functional

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(or Hamiltonian) and, thus, in general, the stationary probability distribution function of the field under KPZ evolution is not known.

(i) Write down the Fokker-Planck equation corresponding to KPZ equation following the steps described in Problem 3.

(ii) Show that, in one spatial dimension ($d = 1$), the following distribution function is a stationary solution for the Fokker-Planck equation obtained in part (i), i.e.,

$$\mathcal{P}_{\text{st}}[\varphi] = C \exp \left[-\frac{\nu}{2D} \int dx (\partial_x \varphi)^2 \right]. \quad (20)$$

(iii) Show explicitly that the result in part (ii) cannot be generalized to higher spatial dimensions.