A15282W1

Honour School of Mathematical and Theoretical Physics Part C
Master of Science in Mathematical and Theoretical Physics

NONEQUILIBRIUM STATISTICAL PHYSICS

Trinity Term 2018

THURSDAY, 31ST MAY 2018, 2:30pm to 4:00pm

You should submit answers to 2 of the 3 questions.

You must start a new booklet for each question which you attempt. Indicate on the front sheet the numbers of the questions attempted. A booklet with the front sheet completed must be handed in even if no question has been attempted.

The numbers in the margin indicate the weight that the Examiners anticipate assigning to each part of the question.

Do not turn this page until you are told that you may do so

1. Consider the Newton equation for a particle with mass m and hydrodynamic drag coefficient ζ, in a harmonic trap with spring constant k

$$m\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = -\zeta\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} - k\mathbf{r} + \mathbf{f}(t) \quad , \tag{1}$$

where $\mathbf{f}(t)$ is the random force from the environment that is in thermal equilibrium at temperature T.

(a) [4 marks] Multiply Eq. (1) by $\mathbf{r}$ and re-arrange the terms to obtain a differential equation that includes $\mathbf{r}^2$ and $\dot{\mathbf{r}}^2$.

(b) [6 marks] Perform an averaging over the resulting equation, following the original method used by Paul Langevin in his 1908 paper. Discuss the assumptions used in the calculation and how they can be justified. Derive a differential equation for the Mean-Squared Displacement (MSD), i.e. $\langle \mathbf{r}^2 \rangle$.

(c) [2 marks] What are the relevant time scales in the system and what regimes do they correspond to?

(d) [6 marks] Solve the resulting equation and derive a compact expression for the time dependence of $\langle \mathbf{r}^2 \rangle$.

(e) [4 marks] Discuss the different asymptotic regimes and the time scales at which the crossovers occur.

(f) [3 marks] Sketch the MSD versus time.

2. A stochastic Brownian dynamics is described by the Langevin equations

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{v}\left(\mathbf{r}(t)\right) + \mathbf{u}(t) \quad , \tag{2}$$

where the components of $\mathbf{u}(t)$ are Gaussian white noise variables with correlations

$$\langle u_i(t)\rangle = 0 \quad , \quad \langle u_i(t)u_j(t')\rangle = 2D\,\delta_{ij}\delta(t-t') \quad ,$$

and $\mathbf{v}(\mathbf{r})$ represents an arbitrary drift velocity.

(a) [3 marks] Discuss how the Markov property of (2) can be used in constructing a path-integral representation for the conditional probability $\mathcal{P}(\mathbf{x},t|\mathbf{x}_0,t_0)$ of finding the system at position $\mathbf{x}$ at time t, knowing that it has started from position $\mathbf{x}_0$ at time t_0.

(b) [3 marks] Show that a key building block in the constructed path-integral will be

$$\mathcal{P}(\mathbf{y},t'+\Delta t|\mathbf{y}',t') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{y}')+W} \quad ,$$

where

$$W = \ln\left\langle e^{-ik_i\Delta r_i}\right\rangle \simeq -ik_i\left\langle \Delta r_i\right\rangle - \frac{1}{2}k_ik_j\left[\left\langle \Delta r_i\Delta r_j\right\rangle - \left\langle \Delta r_i\right\rangle\left\langle \Delta r_j\right\rangle\right] \quad ,$$

and Δr_i represents the time integral of (2) over a finite time interval Δt.

(c) [2 marks] Show that

$$\left\langle \Delta r_i\right\rangle \simeq v_i(\mathbf{r}(t'))\Delta t + O(\Delta t^{3/2}) \quad .$$

(d) [7 marks] Show that

$$\left\langle \Delta r_i\Delta r_j\right\rangle - \left\langle \Delta r_i\right\rangle\left\langle \Delta r_j\right\rangle = \mathcal{M}_{ij}(2D\Delta t) + O(\Delta t^{5/2}) \quad ,$$

where

$$\mathcal{M}_{ij} = \delta_{ij} + \Theta(0)\,\Delta t\,(\partial_j v_i + \partial_i v_j) \quad ,$$

involves the Heaviside function at the origin $\Theta(0)$, which is ambiguous.

(e) [7 marks] Using the above results, show that

$$\mathcal{P}(\mathbf{y},t'+\Delta t|\mathbf{y}',t') = \frac{1}{(4\pi D\Delta t)^{3/2}} \times \exp\left\{-\frac{\Delta t}{4D}\left[\frac{(\mathbf{y}-\mathbf{y}')}{\Delta t} - \mathbf{v}(\mathbf{y}')\right]^2 - \Delta t\,\Theta(0)\left[\boldsymbol{\nabla}\cdot\mathbf{v}(\mathbf{y}')\right] + O(\Delta t^{3/2})\right\} \quad .$$

(f) [3 marks] Finally, take the continuum limit to show

$$\mathcal{P}(\mathbf{x},t|\mathbf{x}_0,t_0) = \mathcal{N}\int_{\mathbf{r}(t_0)=\mathbf{x}_0}^{\mathbf{r}(t)=\mathbf{x}} \mathcal{D}\mathbf{r}(\tau)\; e^{-\mathcal{S}} \quad ,$$

where $\mathcal{S}$ is an action. Find $\mathcal{S}$.

3. Rotational diffusion of a colloidal particle with rotational diffusion coefficient D_r can be described by the following path integral

$$Z = \int \mathcal{D}\hat{\mathbf{n}}(\tau)\; e^{-\frac{1}{4D_r}\int \mathrm{d}\tau\, \dot{\hat{\mathbf{n}}}^2} \quad . \tag{3}$$

for the dynamics of the unit vector $\hat{\mathbf{n}}$ in d dimensions, i.e. subject to the constraint $\hat{\mathbf{n}}^2 = 1$.

(a) [4 marks] Provide an argument (without explicit and detailed derivations) why we expect the following form for the auto-correlation function

$$\langle \hat{\mathbf{n}}(t) \cdot \hat{\mathbf{n}}(0) \rangle = e^{-(d-1)D_r t}. \tag{4}$$

(b) [4 marks] Equation (3) can be written as a constrained path integral in terms of $\mathbf{n}$

$$Z[\mathbf{j}] = \int \mathcal{D}\mathbf{n}(\tau)\; \delta\left\{\mathbf{n}(\tau)^2 - 1\right\}\; e^{-\int \mathrm{d}\tau \left[\frac{1}{4D_r}\, \dot{\mathbf{n}}^2 + \mathbf{j}(\tau)\cdot\mathbf{n}(\tau)\right]} \quad . \tag{5}$$

using a functional Dirac delta function, where we have added a source $\mathbf{j}$ to allow us to calculate correlation functions of $\mathbf{n}$ using functional differentiation. Explain how this technique works.

Use a Lagrange multiplier field to represent the delta function, and write down the resulting expression for the above path integral.

(c) [8 marks] An approximate description of Eq. (3) can be written as an unconstrained path integral

$$Z[\mathbf{j}]' = \int \mathcal{D}\mathbf{n}(\tau)\; e^{-\int \mathrm{d}\tau \left[\frac{1}{4D_r}\, \dot{\mathbf{n}}^2 + \frac{A}{2}\, \mathbf{n}^2 + \mathbf{j}(\tau)\cdot\mathbf{n}(\tau)\right]} \quad . \tag{6}$$

where the the additional "mass" term has a free parameter A. Show that the auto-correlation function calculated in this approximate description [from Eq. (6)] is given as

$$\langle \mathbf{n}(t) \cdot \mathbf{n}(0) \rangle = d\sqrt{\frac{D_r}{2A}}\; e^{-\sqrt{2D_r A}\, t} \quad .$$

(d) [4 marks] Use the freedom provided by the mass term to enforce the following average constraint:

$$\left\langle \mathbf{n}^2 \right\rangle = 1 \quad ,$$

and calculate the value of A.

(e) [5 marks] Show that within this description, the auto-correlation function for the director field is given as

$$\langle \mathbf{n}(t) \cdot \mathbf{n}(0) \rangle = e^{-dD_r t}.$$

Compare this with Eq. (4), and explain the reason behind the discrepancy.