GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Tutors:

Diego Tapias
diego.tapias@theorie.physik.uni-goettingen.de
Room A.04.112

Prof. Peter Sollich
peter.sollich@uni-goettingen.de
Room A.03.106, Tel: +49 551 39 28375

Jack Parley
jack.parley@theorie.physik.uni-goettingen.de
Room A.02.106

Advanced Statistical Physics
Wintersemester 2022/23

Problem sheet 3, handed out: Friday 11th November, 2022
due: **Sunday 20th November, 2022 (via email/ studip)**

1 Langevin equation with inertia and ballistic-diffusive crossover (26 pts.)

Consider a particle of mass m whose velocity v obeys the following Langevin equation

$$m\dot{v} = -\gamma v + \xi(t), \tag{1}$$

where γ is the friction coefficient and ξ a Gaussian fluctuating force with the properties

$$\langle \xi(t) \rangle = 0 \ \text{ and } \ \langle \xi(t)\xi(t') \rangle = 2D\gamma^2\delta(t-t'). \tag{2}$$

D is the diffusion constant and related to the temperature by the Einstein relation $D = T/\gamma$. The particle starts from position x_0 with velocity v_0 at time $t = 0$.

a) Verify that the solution of (1) is

$$v(t) = v_0\,\mathrm{e}^{-\gamma t/m} + \frac{1}{m}\int_0^t \mathrm{d}t'\,\mathrm{e}^{-\gamma(t-t')/m}\xi(t') \tag{3}$$

(3 pts.)

b) Calculate the velocity variance $\langle [\Delta v(t)]^2 \rangle$ where $\Delta v(t) = v(t) - \langle v(t) \rangle$. Discuss its short and long time limits. Compute the velocity autocorrelation function $\langle \Delta v(t)\Delta v(t') \rangle$ for large t and t' as a function of $\Delta t = t - t'$ and show that it decays with a time scale $\tau_v = m/\gamma$. (8 pts.)

c) Solve Eq. (1) for the position $x(t)$ of the particle and calculate its mean $\langle x(t) \rangle$. (7 pts.)

d) Calculate the mean-squared displacement $\left\langle [x(t) - x_0]^2 \right\rangle$ and discuss both its short and long time limit; you should find that these correspond to ballistic and diffusive dynamics. Discuss under what circumstances the mass m can be neglected, as done in the lecture (overdamped limit). (8 pts.)

2 Zwanzig-Mori projection (24 pts.)

We derived the Langevin equation in the lecture from an explicit elimination of irrelevant degrees of freedom (solvent molecules represented by harmonic oscillators). This elimination can be done quite generally, using the Zwanzig-Mori projection technique. This lets us choose a subset of relevant observables $A_i(t)$ and eliminate the remaining variables to obtain a reduced description.

a) Consider the simplest case of two dynamical variables $A(t) = (A_1(t), A_2(t))^{\mathrm{T}}$ whose time evolution is given by the linear equation

$$\frac{\partial A}{\partial t} = \mathcal{L}A(t). \tag{4}$$

where $\mathcal{L}$ is a matrix with fixed components l_{ij}.

Let us suppose that the relevant variable is $A_1(t)$. Show that this obeys

$$\frac{\partial A_1}{\partial t} = l_{11}A_1(t) + l_{12}\int_0^t \mathrm{d}t'\, \mathrm{e}^{l_{22}(t-t')} l_{21} A_1(t') + l_{12}\,\mathrm{e}^{l_{22}t} A_2(0). \tag{5}$$

Interpret the meaning of the three terms on the right hand side. Is this equation for $A_1(t)$ Markovian? (6 pts.)

b) This procedure can be formalized using projection operators which project the dynamics of the system onto the subset of relevant variables. We define the projection operator onto the relevant variable A_1 as a matrix $\mathcal{P}$ with components $p_{ij} = \delta_{i1}\delta_{j1}$. Rewrite equation (5) in terms of $\mathcal{L}$, $\mathcal{P}$ and its complement $\mathcal{Q} = 1 - \mathcal{P}$, which projects onto the irrelevant subspace. (4 pts.)

c) We now consider an arbitrary number of relevant variables $\{A_1, \cdots, A_m\}$ and seek to derive a Langevin equation starting from the Liouville equation

$$\frac{\partial A}{\partial t} = \mathcal{L}A(t). \tag{6}$$

The projection operator onto the relevant subspace

$$\mathbf{A} = \begin{pmatrix} A_1 \\ \vdots \\ A_m \end{pmatrix}$$

is given explicitly by its action on a generic observable B

$$\mathcal{P}B \equiv \left(B, A^{\mathrm{T}}\right)\left(A, A^{\mathrm{T}}\right)^{-1} A \tag{7}$$

where $\left(A, A^{\mathrm{T}}\right)$ is a matrix with components (A_i, A_j) defined by some inner product between observables; similarly $\left(B, A^{\mathrm{T}}\right)$ is a vector with components (B, A_i). As before define the orthogonal projector $\mathcal{Q} = 1 - \mathcal{P}$.

Starting from the evolution equation of $A(t)$ with initial condition A, split the Liouville operator into two parts $\mathcal{L} = \mathcal{PL} + \mathcal{QL}$ and use the Dyson operator identity

$$\mathrm{e}^{\mathcal{L}t} = \mathrm{e}^{\mathcal{QL}t} + \int_0^t \mathrm{d}t'\, \mathrm{e}^{\mathcal{L}(t-t')}\mathcal{PL}\,\mathrm{e}^{\mathcal{QL}t'} \tag{8}$$

to show that

$$\frac{\partial A(t)}{\partial t} = \Omega A(t) + \int_0^t \mathrm{d}t'\, K(t') A(t-t') + F(t), \tag{9}$$

where we have defined

- $\Omega \equiv \left(\mathcal{L}A, A^{\mathrm{T}}\right)\left(A, A^{\mathrm{T}}\right)^{-1}$,
- $K(t) \equiv \left(\mathcal{L}F(t), A^{\mathrm{T}}\right)\left(A, A^{\mathrm{T}}\right)^{-1}$
- and $F(t) \equiv \mathrm{e}^{\mathcal{QL}t}\mathcal{QL}A$.

(8 pts.)

Show also that

$$(F(t), A) = 0 \tag{10}$$

(2 pts.)

Discuss the origin and meaning of $F(t)$ and $K(t)$ in the result (9), using also the property (10). (4 pts.)