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Advanced Statistical Physics II – Problem Sheet 12

Problem 1 – **Many-Particle Non-Equilibrium System**

In the lecture, we discussed a class of non-equilibrium systems whose dynamics can be modelled by the following multi-dimensional Langevin equation

$$\dot{z}_k(t) = -A_{km} z_m(t) + \Phi_{km} F_m(t), \quad \langle F_m(t) F_n(t') \rangle = 2\delta_{mn}\delta(t-t') \quad . \tag{1}$$

Note, that we make use of the Einstein summation convention for double indices. The corresponding Fokker-Planck equation reads

$$\dot{P}(\vec{z},t) = \left[\nabla_k A_{km} z_m + \nabla_k \nabla_m C_{km}\right] P(\vec{z},t), \quad C_{ij} := \Phi_{ik}\Phi_{jk} \quad . \tag{2}$$

a) (5P) Use a Gaussian ansatz $P_0(\vec{z}) = \mathcal{N}^{-1} \exp(-z_i E^{-1}_{ij} z_j/2)$, for the stationary solution. Here $E_{ij} = \langle z_i z_j \rangle$ denotes the entries of the symmetric covariance matrix. Derive the Lyapunov equation discussed in the lecture:

$$A_{ik}E_{kj} + A_{jk}E_{ki} = 2C_{ij} \tag{3}$$

b) (5P) As a concrete example, we will discuss a simple system of an overdamped particle in harmonic confinement of strength M. Furthermore, it is harmonically coupled to a second particle:

$$H(x,y) = \frac{M}{2}\, x^2 + \frac{K}{2}(x-y)^2 \tag{4}$$

Both particles are subject to friction $\gamma_{x,y}$ and noise of strength $b_{x,y}$. This leads to

$$z(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}, \quad A = \begin{pmatrix} (K+M)/\gamma_x & -K/\gamma_x \\ -K/\gamma_y & K/\gamma_y \end{pmatrix}, \quad \Phi = \begin{pmatrix} b_x/\gamma_x & 0 \\ 0 & b_y/\gamma_y \end{pmatrix}, \tag{5}$$

In equilibrium, friction and noise strength are related via $b_x^2/\gamma_x = b_y^2/\gamma_y = k_B T$. Formally, we can understand departure from equilibrium by introducing different temperatures for each particle $k_B T_x = b_x^2/\gamma_x$ and $k_B T_y = b_y^2/\gamma_y$. Find the entries of the covariance matrix

$$E = \begin{pmatrix} \langle x^2 \rangle & \langle xy \rangle \\ \langle xy \rangle & \langle y^2 \rangle \end{pmatrix} \tag{6}$$

by solving the Lyapunov equation (3). Express the resulting covariances in terms of the dimension-less parameter

$$\alpha := \frac{T_y - T_x}{T_x} = \frac{\gamma_x}{b_x^2} \cdot \frac{b_y^2}{\gamma_y} - 1 \tag{7}$$

which quantifies departure from equilibrium, and in terms of T_x. Check that in equilibrium ($\alpha = 0$) the equipartition theorem for the variables x and $x-y$ is obeyed.

c) (3P) Consider a hypothetical experiment in which only the position x can be observed. Thus the position y of the other particle is a hidden degree of freedom. An example would be a colloid in a laser trap whose position is tracked. In equilibrium, the position of the trapped particle obeys a Boltzmann distribution

$$P_{\text{eq}}(x) \propto e^{-Mx^2/2k_B T} \tag{8}$$

i.e. the variance is given by $\langle x^2 \rangle = k_B T/M$. How does the variance/width of the observed distribution change for $T_x > T_y$ and $T_x < T_y$?

Problem 2 – **Run and Tumble Particle**

Consider the following dynamics of a free, overdamped particle in d dimensions:

$$\dot{\vec{x}}(t) = \vec{u}(t) + \gamma^{-1}\vec{F}_R(t), \qquad \langle \vec{F}_R(t)\vec{F}_R(t')\rangle = 2dk_BT\gamma\delta(t-t') \tag{9}$$

Here, γ denotes the friction coefficient and $\vec{F}_R(t)$ is the random force, which accounts for thermal fluctuations. The particle propels itself forward at constant velocity $|\vec{u}(t)| = v_0$. (For $v_0 = 0$ (and thus $\vec{u}(t) = \vec{0}$), this corresponds to standard Brownian motion.) The particle goes in the same direction for an average time τ and then chooses a new direction completely at random - independent of the previous orientation and thermal noise. Assuming the time for going in one direction is exponentially distributed, the autocorrelation of $\vec{u}(t)$ is given by

$$\langle \vec{u}(t)\vec{u}(t')\rangle = v_0^2 e^{-|t-t'|/\tau} \tag{10}$$

This model has been proposed for the dynamics of bacterial motility. Fig. 1 shows a simulated trajectory of such a run and tumble particle.

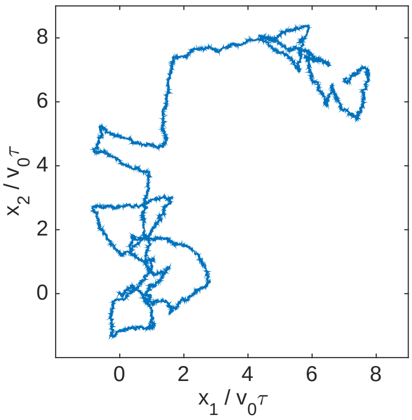

Figure 1: Trajectory of a run and tumble particle in two dimensions.

a) (4P) Calculate the mean-square displacement $\Delta x^2(t) = \langle (x(t) - x(0))^2\rangle$. Note that you need to average over both $\vec{F}_R(t)$ and $\vec{u}(t)$. *Hint:* It is helpful to first calculate the velocity autocorrelation function $\langle \dot{\vec{x}}(t)\dot{\vec{x}}(t')\rangle$ and then obtain the mean-square displacement via integration.

b) (3P) For both short and long times t, the dynamics is diffusive. Calculate the diffusion constants for short and long times:

$$D_{\text{short}} = \lim_{t\to 0} \frac{\Delta x^2(t)}{2t}, \qquad D = \lim_{t\to\infty} \frac{\Delta x^2(t)}{2t} \tag{11}$$

Interpret the result. How does the active self propulsion affect the diffusion constant?