Active Matter Physics

Prepare the solutions for the seminar on 2024.5.22

Exercise Sheet 4

4.1

The interaction of a spherical Brownian particle ($r = 100\,\mathrm{nm}$, $\rho_{\mathrm{part}} = 1.8\,\mathrm{g\,cm^{-3}}$) with the ambient water molecules ($\eta = 0.001\,\mathrm{N\,s\,m^{-2}}$ at $T = 300\,\mathrm{K}$) can be separated into two parts: At first, a force $\mathbf{f}_{\mathrm{rand}}(t)$ that fluctuates on a time scale of $\sim 10^{-14}\,\mathrm{s}$ results from the random collisions of the water molecules with the Brownian particle. Secondly, due to systematic collisions with the water molecules and the, hence, resulting particle velocity $\mathbf{v} = \mathbf{p}/M$ with $\mathbf{p}$ the particle's momentum and M the specific particle mass (corrected for the mass of displaced water, $\rho_{\mathrm{H_2O}} = 1.0\,\mathrm{g\,cm^{-3}}$), there is a friction force. For a Brownian particle obtaining a much larger volume than that of a single water molecule and a not too large particle velocity the friction force is directly proportional to this velocity.

- Calculate the momentum relaxation time constant $\tau = M/\gamma$, where γ is the Brownian particle's friction coefficient.
- State Newton's equation of motion for the Brownian particle in terms of the momentum $\mathbf{p}$ and formally integrate it with respect to t.
- Derive from the previous bullet point the ensemble averaged Newton's equation of motion of the Brownian particle and solve this equation for the ensemble averaged momentum $\langle \mathbf{p}(t) \rangle$.

Extra tasks:

- Calculate the ensemble average of the 3×3-matrix $\mathbf{x} \otimes \mathbf{x}$, where $(\cdot \otimes \cdot)$ is the dyadic product of the vector $\mathbf{x}$ with itself. This vector is defined as

  $$\mathbf{x} = \int_0^t \mathrm{d}t'\, \mathbf{f}_{\mathrm{rand}}(t') \exp\!\left(-\frac{\gamma}{M}(t - t') \right). \tag{1}$$

  Use for your calculations that the random force has the correlation function

  $$\langle \mathbf{f}_{\mathrm{rand}}(t) \otimes \mathbf{f}_{\mathrm{rand}}(t') \rangle = 2\gamma k_{\mathrm{B}} T \delta(t - t') \underline{\mathbf{I}}, \tag{2}$$

  where $\delta(\cdot)$ is the delta function and $\underline{\mathbf{I}}$ is the unit matrix. (Hint: You may use the approximation $\int_{-t}^{t} \mathrm{d}\tau\, \delta(\tau) \approx 1$ which holds for $t \gg 10^{-14}\,\mathrm{s}$.)

- Calculate the particle's diffusive length scale

  $$l_{\mathrm{D}} = \int_0^\infty |\langle \mathbf{v}(t) \rangle| \,\mathrm{d}t \tag{3}$$

  using the equipartition theorem for $|\mathbf{p}_0|$, i.e., employing that

  $$|\mathbf{p}_0| \approx \sqrt{\mathrm{Tr}(\lim_{t\to\infty} \langle \mathbf{p}(t) \otimes \mathbf{p}(t) \rangle)}, \tag{4}$$

  where $\mathrm{Tr}(\cdot)$ is the trace of a matrix. Compare l_{D} to the size of the Brownian particle.

- Calculate the time at which the mean squared displacement is equal to r^2.

4.2

Consider a Brownian particle of mass m which is constrained to move in one dimension in a harmonic potential $V(x) = kx^2/2$. Show that on average the equipartition theorem is fulfilled. Stick to the following steps:

- Write down the Langevin equation for this system. The moments of the underlying random force $\xi(t)$ are

$$\langle \xi(t_1) \rangle = 0 \tag{5}$$
$$\langle \xi(t_1)\xi(t_2) \rangle = 2\gamma k_{\mathrm{B}} T \delta(t_1 - t_2), \tag{6}$$

  where γ is the friction coefficient.

- Calculate the Fourier transform of the Langevin equation in the temporal variable (i.e., $t \to \omega$) and solve for $x(\omega)$.
- Calculate the spectral density $S_x(\omega) = |x(\omega)|^2$. Note that $|\xi(\omega)|^2 = S_\xi(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t \mathrm{e}^{i\omega t} \langle \xi(t)\xi(0) \rangle$.

Extra tasks:

- The corresponding time-dependent correlation function can be calculated via

$$C_x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{-i\omega t} S_x(\omega). \tag{7}$$

  (Hint: Applying the residue theorem simplifies the calculation of the integral enormously. Which half-plane do you have to choose? Keep in mind that $\omega = \hat{x} + i\hat{y}$ and $t, \hat{x} \in [0, \infty)$.)

- The equipartition theorem follows then from $C_x(t = 0) = \langle x_0^2 \rangle$.