PHYS 414 Problem Set 1: Brownian Motion

Problem 1

In class we derived a Fokker-Planck equation for the velocity distribution $\mathcal{P}(v_x, t)$ starting from the assumption of small random changes in velocity at each time step:

$$v_x(t + \delta t) = v_x(t) + \frac{f_x(t)}{M}\delta t \tag{1}$$

where $f_x(t)$ is chosen from a distribution $W(f_x; v_x)$. Einstein's original approach to Brownian motion had a different starting point, focusing on position differences at each time step:

$$x(t + \Delta t) = x(t) + \xi(t) \tag{2}$$

where $\xi(t)$ is a random displacement chosen from some distribution $W(\xi)$. Underlying this approach is the assumption that each successive random displacement is independent, i.e. $\xi(t) = x(t + \Delta t) - x(t)$ and $\xi(t + \Delta t) = x(t + 2\Delta t) - x(t + \Delta t)$ are uncorrelated. We know that this can only be true if the corresponding velocities at $x(t)$ and $x(t + \Delta t)$ are uncorrelated. Einstein's theory did not explicitly treat velocities, but we know from the results in class that $\langle v_x(t + \Delta t)v_x(t)\rangle = (k_B T/M)\exp(-\gamma\Delta t/M)$. Hence Einstein's approach is a good approximation assuming $\Delta t \gg M/\gamma$. It will describe dynamics at coarser time scales than the Fokker-Planck equation from lecture.

a) Derive a Fokker-Planck equation for the position distribution $\mathcal{P}(x, t)$ using Einstein's approach. Follow the same reasoning as shown in class, but with $W(\xi)$ instead of $W(f_x; v_x)$. For the first and second moments $\langle\xi\rangle$ and $\langle\xi^2\rangle$ of the distribution $W(\xi)$, use the class results for $\langle(x(t + \Delta t) - x(t))\rangle$ and $\langle(x(t + \Delta t) - x(t))^2\rangle$, taking the limit $\Delta t \gg M/\gamma$. In the end you should derive the following dynamical equation:

$$\frac{\partial\mathcal{P}}{\partial t}(x, t) = D\frac{\partial^2}{\partial x^2}\mathcal{P}(x, t) \tag{3}$$

where $D = k_B T/\gamma$. This is the Fokker-Planck equation for the position of a Brownian particle in the absence of a potential (otherwise known as the diffusion equation).

b) Solve Eq. (3) for the distribution $\mathcal{P}(x, t; x_0)$ with initial condition $\mathcal{P}(x, 0; x_0) = \delta(x - x_0)$. *Hint:* Assume $\mathcal{P}(x, t; x_0)$ is a Gaussian with arbitrary time-dependent mean and variance, and determine what those two quantities have to be in order for Eq. (3) to be satisfied.

c) Using your solution from part b, calculate the mean squared displacement (MSD) $\Delta x^2_{\text{rms}}(t) = \langle(x(t) - x(0))^2\rangle$. You can define a rough measure of "mean velocity" over the time interval between 0 and t as: $\bar{v}(t) = \Delta x_{\text{rms}}(t)/t$. In the limit $t \to 0$, compare the result of Einstein's theory for $\bar{v}(t)$ to the result from the theory presented in class. Show that Einstein's result gives nonsense as $t \to 0$, while the class theory (which is applicable to smaller time scales) gives the expected Maxwell-Boltzmann value. This underscores the fact that Einstein's approach should only be used when $t \gg M/\gamma$.

Problem 2

In 2010 Mark Raizen and collaborators pulled off something Einstein thought essentially impossible: measuring the instantaneous velocity distribution of a Brownian particle [T. Li et al., Science **328**, 1673 (2010); pdf available on the course website]. To do so, one needs to be able to probe time scales smaller than the velocity correlation time M/γ, where M is the mass of the particle and γ the friction coefficient of the surrounding medium. Air is ideal for such measurements, because it has small γ compared to fluids, but Brownian particles tend to fall under the influence of gravity.

To overcome this obstacle, the researchers took advantage of an optical tweezer [Fig. 1] which uses counter-propagating laser beams focused on one point to form a trap for a silica bead (in this case with a $R = 1.5$ μm radius). Light is refracted through the bead, and the momentum change associated with the bending of the rays induces a small force on the bead. The net result is a three-dimensional harmonic potential with a minimum at the laser focus. If the center of the bead is away from the focus, it feels an attractive force, i.e. $F_{\text{trap}} = -k_{\text{trap}}x$ for displacements along the x direction. The spring constant k_{trap} can be tuned by changing the laser intensity. This setup prevents the bead from moving too far away from the focus, and the deflection of the two beams caused by bead movements (monitored by a detector) allows extremely precise measurements of the bead position $x(t)$ as a function of time. The goal of this problem is to work out a dynamical theory of a Brownian particle in a harmonic potential which is valid at time scales both smaller and larger than M/γ. You will derive expressions for two of the quantities directly measured in the experiment: the mean squared displacement $\langle (x(t) - x(0))^2 \rangle$ and the velocity autocorrelation function $\langle v_x(t)v_x(0)\rangle$ [Fig. 2].

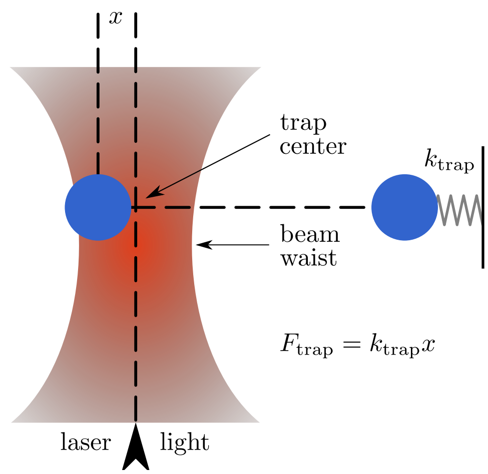

Figure 1: Optical tweezer

a) Start with the same argument used in class to derive the Fokker-Planck equation for the velocity distribution $\mathcal{P}(v_x, t)$ in the absence of a harmonic potential. When the force due to the trap, $F_{\text{trap}} = -k_{\text{trap}}x$ is added to the problem, convince yourself that the distribution $W(f_x; v_x)$ for observing an incremental net force f_x between t and $t + \delta t$ has to be replaced by $W(f_x; x, v_x)$. In other words, W now depends not only on the instantaneous velocity v_x at time t, but also on the particle position x. The position evolves in time as $x(t + \delta t) = x(t) + v_x(t)\delta t$. Similarly $\mathcal{P}(v_x, t)$ should be replaced by $\mathcal{P}(x, v_x, t)$: the probability density to observe the particle at x with velocity v_x at time t. Using an analogous approximation to the one in lecture, derive a Fokker-Planck equation for $\mathcal{P}$. This equation should take the form:

$$\frac{\partial \mathcal{P}}{\partial t} = \sum_{ij} \left[B_{ij} \frac{\partial}{\partial q_i}(q_j \mathcal{P}) + A_{ij} \frac{\partial^2 \mathcal{P}}{\partial q_i \partial q_j} \right], \tag{4}$$

where $\mathbf{q} = (x, v_x)$, and A, B are 2×2 matrices. From the derivation you should be able to determine the components of B in terms of the physical constants in the problem. For convenience,

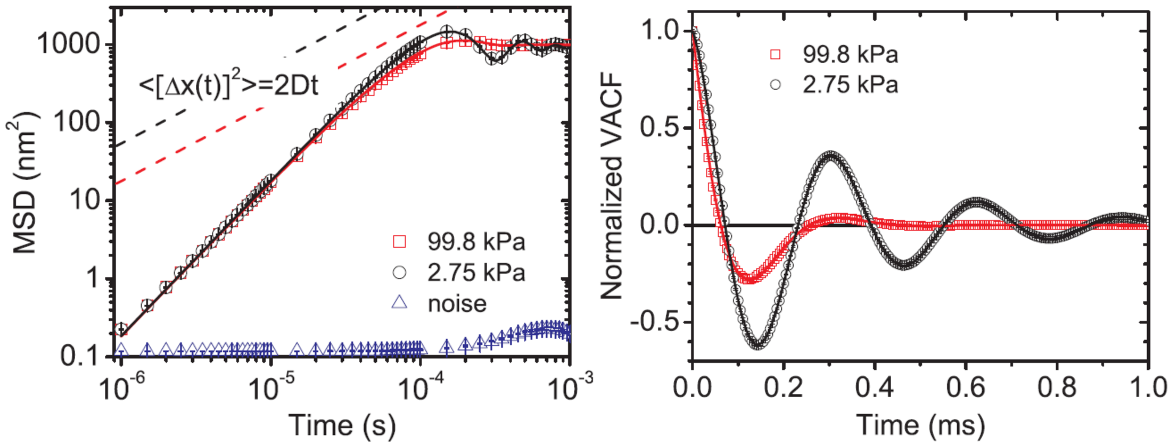

Figure 2: Experimental results from T. Li et al., Science **328**, 1673 (2010). Left: the mean squared displacement (MSD) $\langle (x(t)-x(0))^2\rangle$ for a Brownian particle in air at two different pressures, 99.8 kPa (red symbols) and 2.75 kPa (black symbols). For comparison the dashed lines show the long-time diffusive regime (MSD $= 2Dt$) which would be achieved for a free Brownian particle in the absence of a trap as $t \to \infty$. In contrast, the short time behavior of the experimental MSD is ballistic (MSD $\propto t^2$). Right: the corresponding normalized velocity autocorrelation function (VACF) $\langle v_x(t)v_x(0)\rangle/\langle v_x^2(0)\rangle$, where $\langle v_x^2(0)\rangle = k_BT/M$, in agreement with the Maxwell-Boltzmann distribution from the kinetic theory of gases.

you will find it useful to introduce variables $\Gamma \equiv \gamma/M$ and $\omega = \sqrt{k_{\text{trap}}/M}$, both of which have units of inverse time. The matrix A must be symmetric since the order of the partial derivatives in the second order term of the Taylor expansion does not matter. Thus assume it involves three unknown constants, A_{11}, $A_{12} = A_{21}$, and A_{22}. You will determine these in the next part.

b) Find the unknown constants in the matrix A by demanding that the joint equilibrium distribution $\mathcal{P}_{\text{eq}}(x, v_x)$ be a solution to Eq. (4) with the left side set to zero, $\partial\mathcal{P}/\partial t = 0$. The equilibrium distribution is given by the product of the Maxwell-Boltzmann distributions for position and velocity,

$$\mathcal{P}_{\text{eq}}(x, v_x) = \frac{M\omega}{2\pi k_BT}\exp\left(-\frac{Mv_x^2 + M\omega^2x^2}{2k_BT}\right). \tag{5}$$

Hint: Show that the above demand leads to a polynomial in x and v_x being equal to zero. Since the statement is true for all x and v_x, each coefficient of every power of x and v_x must separately equal zero.

You have now completely determined the multi-dimensional Fokker-Planck equation for the system. Your result is known as the *Kramers equation.*

c) Sanity check: when the trap strength $k_{\text{trap}} = 0$, or equivalently $\omega = 0$, can you recover the Fokker-Planck equation for the velocity distribution alone derived in class,

$$\frac{\partial\mathcal{P}}{\partial t}(v_x, t) = \Gamma\frac{\partial}{\partial v_x}(v_x\mathcal{P}(v_x, t)) + \frac{\Gamma k_BT}{M}\frac{\partial^2\mathcal{P}}{\partial v_x^2}(v_x, t). \tag{6}$$

To do so, integrate both sides of Eq. (4) over x, and note that $\mathcal{P}(v_x, t) = \int dx\, \mathcal{P}(x, v_x, t)$. You can assume that $\mathcal{P}(x, v_x, t)$ is well behaved at $x = \pm\infty$, i.e. it goes to zero rapidly, as must be true of a normalizable distribution.

d) Starting from some initial condition $\mathbf{q}(0) = \mathbf{q}_0 \equiv (x_0, v_0)$, Eq. (4) describes the subsequent evolution of the joint probability $\mathcal{P}(\mathbf{q}, t; \mathbf{q}_0)$. At any given time $t \geq 0$, denote the instantaneous average of $q_i(t)$ given the initial condition as $\langle q_i(t)\rangle_{\mathbf{q}_0} = \int d\mathbf{q}\, q_i \mathcal{P}(\mathbf{q}, t; \mathbf{q}_0)$. Show that this quantity obeys the differential equation,

$$\frac{d}{dt}\langle q_m(t)\rangle_{\mathbf{q}_0} = \sum_j C_{mj}\langle q_j(t)\rangle_{\mathbf{q}_0}, \tag{7}$$

and determine the components of the 2×2 matrix C. *Hint:* multiply both sides of Eq. (4) by q_m and integrate over both components of $\mathbf{q}$, simplifying the results through integration by parts.

e) Solve Eq. (7) for $\langle \mathbf{q}(t)\rangle_{\mathbf{q}_0}$. *Hint:* Though Eq. (7) is a vector equation, the form of the solution is exactly analogous to the one-dimensional equation $dq(t)/dt = Cq(t)$ where C is a scalar. You will need the formula for the matrix exponential of a 2×2 matrix. To spare you the tedious eigenvalue decomposition, here is the result:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad e^A = e^{(a+d)/2}\begin{pmatrix} \cosh(\Delta) + \frac{(a-d)}{2\Delta}\sinh\Delta & \frac{b}{\Delta}\sinh\Delta \\ \frac{c}{\Delta}\sinh\Delta & \cosh\Delta - \frac{(a-d)}{2\Delta}\sinh\Delta, \end{pmatrix} \tag{8}$$

where $\Delta = \frac{1}{2}\sqrt{(a-d)^2 + 4bc}$.

f) Using the result of part e, find the equilibrium averages $\langle x(t)x(0)\rangle$ and $\langle v_x(t)v_x(0)\rangle$, assuming $\mathbf{q}_0$ is distributed with the equilibrium probability $\mathcal{P}_{\text{eq}}(x_0, v_0)$ from Eq. (5). Calculate in addition the MSD $\langle (x(t) - x(0))^2\rangle$. If you did everything correctly, you can reproduce the results of Fig. 2 by plugging in $\omega = (50\,\mu\text{s})^{-1}$ and one of two values for Γ: at the pressure 99.8 kPa the value is $\Gamma = (49\,\mu\text{s})^{-1}$, while at 2.75 kPa we have $\Gamma = (147\,\mu\text{s})^{-1}$. Note that for $t = 0$, $\langle v_x^2(0)\rangle = k_B T/M$, exactly as predicted by the Maxwell-Boltzmann kinetic theory of gases. This is the instantaneous measurement dreamed of by Einstein.