Inertial_Vs_Overdamped_Notebook

May 15, 2023

1 Open TA: Inertial vs overdamped:

In this exercise, you will study the transition between an inertial and overdamped motion of a Brownian particle numerically. We assume a Brownian particle moving in a (1D) liquid without additional external forces, which is described by the Klein-Kramers Langevin equation: 1.
$dX = V dt$
2.
$dV = -\gamma V dt + \sqrt{2D} dW$

1.1 Question a):

Why can you assume that: $\gamma \sim D$? What determines the proportionality factor? - The Fluctuation-Dissipation theorem states that: $\gamma = \frac{M}{k_B T} D$, i.e., $\gamma \sim D$. As the theorem suggests, the proportionality factor is determined by the particle's mass, M, and the temperature of the system, T.

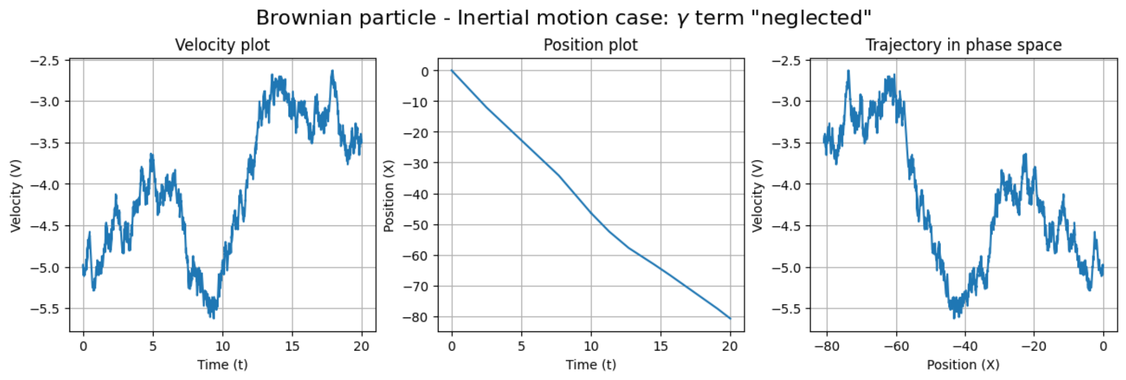
1.2 Question b):

Numerically compute the trajectory for a single Brownian particle that starts at the origin with finite velocity v_0. Find suitable parameters for v_0, γ, D (assuming $D \sim \gamma$) so that by changing γ, you can demonstrate the transition between inertial and overdamped motion.

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
plt.style.use('fast')
```

1.2.1 Inertial case

[ ]:
```
x0     = 0;    v0   = -5.  # Initial position and velocity
Gamma  = 0.00005; D = 0.1  # Model parameters
tMax   = 20; tSteps = 10_000; dt = tMax/tSteps

TrajsX = []; TrajsV = []
M      = 1                 # Number of trajectories

# Euler-Maruyama loop
for m in range(M):
    xVec   = [x0]
    vVec   = [v0]
    dW      = np.random.normal(0., np.sqrt(dt), size = tSteps) # Wiener process:␣
  ↪Mean = 0; Std_Dev = Sqrt(Var) = Sqrt(dt).
    for i in range(tSteps):
        xVec.append(xVec[i] + vVec[i] * dt)
        vVec.append(vVec[i] - Gamma * vVec[i] * dt + np.sqrt(2*D) * dW[i])
    TrajsX.append(xVec)
    TrajsV.append(vVec)

# Plotting results
fig, axs = plt.subplots(1, 3, layout='constrained', figsize=(12, 4))
fig.suptitle(r'Brownian particle - Inertial motion case: $\gamma$ term␣
  ↪"neglected"', fontsize = 16)
for i in range(M):
    axs[0].plot(np.linspace(0., tMax, tSteps + 1), TrajsV[i])
axs[0].set_xlabel("Time (t)")
axs[0].set_ylabel("Velocity (V)")
axs[0].set_title(r"Velocity plot")
axs[0].grid(True)

for i in range(M):
    axs[1].plot(np.linspace(0., tMax, tSteps + 1), TrajsX[i])
axs[1].set_xlabel("Time (t)")
axs[1].set_ylabel("Position (X)")
axs[1].set_title(r"Position plot")
axs[1].grid(True)

for i in range(M):
    axs[2].plot(TrajsX[i], TrajsV[i])
axs[2].set_xlabel("Position (X)")
axs[2].set_ylabel("Velocity (V)")
axs[2].set_title(r"Trajectory in phase space")
axs[2].grid(True)
```

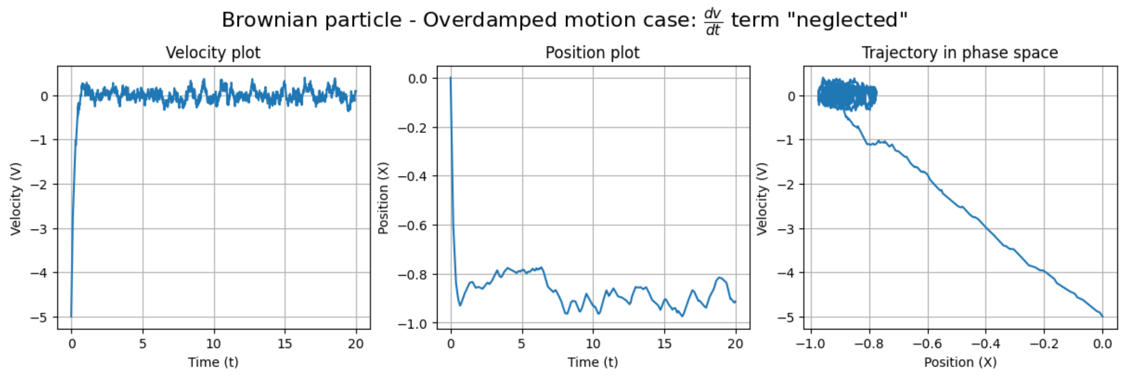


Inertial case: Here, we can *almost* neglect the damping term! We can see that the velocity plot shows very evident signs of diffusive motion (even more evident if we plot more trajectories - change `M` value). The damping here is barely visible! The position plot, on the other hand, appears to be close to a straight line, which implies *almost* constant velocity, as a consequence of an almost negligeble damping term (consistent with the velocity plot). As far as the trajectory in phase-space is concerned, not much useful information can be extracted from it… However, I note that we can no longer see the same "cloud" as in the **overdamped case**. Also, the overall behaviour is clearly distinct: we can also no longer see the same diagonal line as before (c.f. **Overdamped case** section, below).

1.2.2 Overdamped case

[ ]:
```
x0     = 0; v0     = -5.  # Initial position and velocity
Gamma  = 5; D      = 0.1  # Model parameters
tMax   = 20; tSteps = 10_000; dt = tMax/tSteps

TrajsX = []; TrajsV = []
M      = 1                # Number of trajectories

# Euler-Maruyama loop
for m in range(M):
    xVec   = [x0]
    vVec   = [v0]
    dW     = np.random.normal(0., np.sqrt(dt), size = tSteps) # Wiener process:␣
 ↪Mean = 0; Std_Dev = Sqrt(Var) = Sqrt(dt).
    for i in range(tSteps):
        xVec.append(xVec[i] + vVec[i] * dt)
        vVec.append(vVec[i] - Gamma * vVec[i] * dt + np.sqrt(2*D) * dW[i])
    TrajsX.append(xVec)
    TrajsV.append(vVec)

# Plotting results
fig, axs = plt.subplots(1, 3, layout='constrained', figsize=(12, 4))
fig.suptitle(r'Brownian particle - Overdamped motion case: $\frac{dv}{dt}$ term␣
 ↪"neglected"', fontsize = 16)
for i in range(M):
    axs[0].plot(np.linspace(0., tMax, tSteps + 1), TrajsV[i])
axs[0].set_xlabel("Time (t)")
axs[0].set_ylabel("Velocity (V)")
axs[0].set_title(r"Velocity plot")
axs[0].grid(True)

for i in range(M):
    axs[1].plot(np.linspace(0., tMax, tSteps + 1), TrajsX[i])
axs[1].set_xlabel("Time (t)")
axs[1].set_ylabel("Position (X)")
axs[1].set_title(r"Position plot")
axs[1].grid(True)
```

```python
for i in range(M):
    axs[2].plot(TrajsX[i], TrajsV[i])
axs[2].set_xlabel("Position (X)")
axs[2].set_ylabel("Velocity (V)")
axs[2].set_title(r"Trajectory in phase space")
axs[2].grid(True)
```



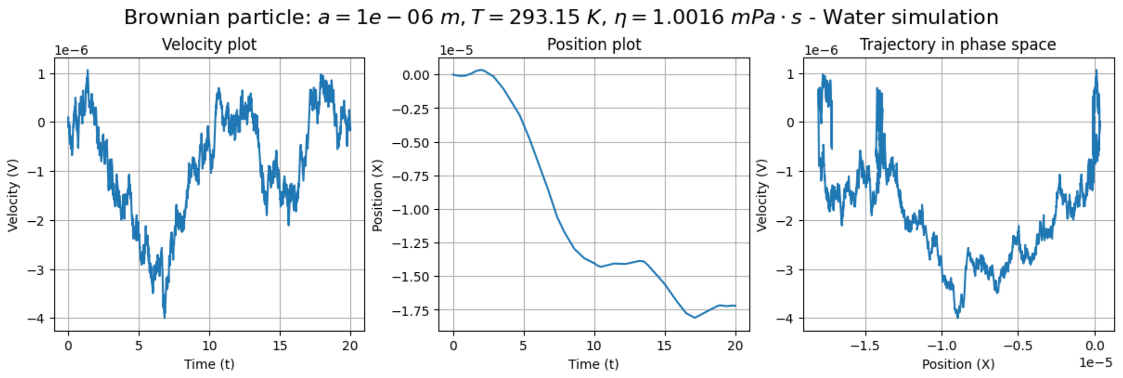
Overdamped case: Velocity plot is rather self-explanatory. We have some initial velocity, which is damped until it reaches zero. This reflects in the position graph, in which we can see that we initially move in the negative x direction, as a consequence of a negative v_0. At some point, $v = 0$, such that x would remain constant, if not for the diffusion term! Note that in this case, $D_x = \frac{D}{\gamma^2}$, which is small since γ is large! Hence, we don't see much diffusion, in x, after the initial velocity has been completely damped, i.e., for (roughly) $t > 5$. In phase-space, we can see the damping (diagonal line), followed by some diffusive motion ("cloud" around $v = 0$).

1.3 Question c)

Stokes formula states that $\gamma = 6\pi\eta a$, i.e., $\gamma \sim a$. This means that larger particles (i.e., with a larger radius, a) are, effectively, more affected by this damping term. Additionally, the more viscous the fluid is, the stronger the damping is, which seems logical/intuitive enough. In the code that follows, I attempt to model a brownian particle in water, for which $\eta = 1.0016 \times 10^{-3} Pa \cdot s$ (Taken from Wikipedia).

```python
[ ]: x0      = 0;  v0     = 0.0                     # Initial position and velocity
     tMax    = 20; tSteps = 10_000; dt = tMax/tSteps
     TrajsX  = []; TrajsV = []
     M       = 1                                     # Number of trajectories

     # Physical parameters
     eta     = 1.0016e-3                             # Viscosity of water
     a       = 1e-6                                  # Particle's radius
     H2O_Rho = 997                                   # Density of water (SI: Kg/m^3)
```

```python
Mass     = (4/3)*np.pi*(a**3)*(5e-2*H2O_Rho)  # Particle is considered to be 0.
 ↪05 times as dense as water!
Gamma    = 6*np.pi*eta*a                      # Damping coefficient
T        = 293.15                             # Room temperature: ~300K
kB       = 1.380649e-23                       # Boltzmann constant (SI units)
D        = kB*T*Gamma/Mass                    # Diffusion constant: From the␣
 ↪Fluctuation-Dissipation theorem.

# Euler-Maruyama loop
for m in range(M):
    xVec    = [x0]
    vVec    = [v0]
    dW      = np.random.normal(0., np.sqrt(dt), size = tSteps) # Wiener process:␣
 ↪Mean = 0; Std_Dev = Sqrt(Var) = Sqrt(dt).
    for i in range(tSteps):
        xVec.append(xVec[i] + vVec[i] * dt)
        vVec.append(vVec[i] - Gamma * vVec[i] * dt + np.sqrt(2*D) * dW[i])
    TrajsX.append(xVec)
    TrajsV.append(vVec)

# Plotting results
fig, axs = plt.subplots(1, 3, layout='constrained', figsize=(12, 4))
fig.suptitle(rf'Brownian particle: $a = {a}$ $m, T = {T}$ $K$, $\eta =␣
 ↪{eta*1e3}$ $mPa \cdot s$ - Water simulation', fontsize = 16)
for i in range(M):
    axs[0].plot(np.linspace(0., tMax, tSteps + 1), TrajsV[i])
axs[0].set_xlabel("Time (t)")
axs[0].set_ylabel("Velocity (V)")
axs[0].set_title(r"Velocity plot")
axs[0].grid(True)

for i in range(M):
    axs[1].plot(np.linspace(0., tMax, tSteps + 1), TrajsX[i])
axs[1].set_xlabel("Time (t)")
axs[1].set_ylabel("Position (X)")
axs[1].set_title(r"Position plot")
axs[1].grid(True)

for i in range(M):
    axs[2].plot(TrajsX[i], TrajsV[i])
axs[2].set_xlabel("Position (X)")
axs[2].set_ylabel("Velocity (V)")
axs[2].set_title(r"Trajectory in phase space")
axs[2].grid(True)
```



Conditions: - Radius: $a = 1\ \mu m$; - Viscosity of water: $\eta = 1.0016 \times 10^{-3} Pa \cdot s$; - Room temperature: $T = 293.15\ K$.

Under these conditions, we can have displacements of the order of 10 μm! I also tried with $a = 1$ nm, which yielded displacements of the order of cm! To see this, just change the value of a. It probably isn't useful to go further than that, since we cannot really fabricate (meaningful) things much smaller than that.