Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 2: computer simulation

2. Simple Python code to simulate Brownian motion

2.1. Equations to be solved

Difference equations

$$\mathbf{R}_{i+1} = \mathbf{R}_i + \mathbf{V}_i \Delta t \tag{F5}$$

$$\mathbf{V}_{i+1} = \left(1 - \frac{\zeta}{m}\Delta t\right)\mathbf{V}_i + \frac{1}{m}\Delta\mathbf{W}_i \tag{F9}$$

Random force

$$\langle \Delta\mathbf{W}_i \rangle = \mathbf{0} \tag{F10}$$

$$\langle \Delta\mathbf{W}_i \Delta\mathbf{W}_j \rangle = 2k_B T\zeta\Delta t\mathbf{I}\delta_{ij} \tag{F11}$$

Initial condition

$$\mathbf{R}_0 = 0, \quad \mathbf{V}_0 = 0 \tag{F12}$$

2.2. A simple simulation code

Import libraries

In [1]:
```
% matplotlib nbagg
import numpy as np # import numpy library as np
import matplotlib.pyplot as plt # import pyplot library as plt
from mpl_toolkits.mplot3d import Axes3D # import Axes3D from `mpl_toolki
plt.style.use('ggplot') # use "ggplot" style for graphs
```

Define parameters and initialize variables

In [2]:
```
dim  = 3 # system dimension (x,y,z)
nump = 100 # number of independent Brownian particles to simulate
nums = 1024 # number of simulation steps
dt   = 0.05 # set time increment, \Delta t
zeta = 1.0 # set friction constant, \zeta
m    = 1.0 # set particle mass, m
kBT  = 1.0 # set temperatute, k_B T
std  = np.sqrt(2*kBT*zeta*dt) # calculate std for \Delta W via Eq.(F11)
np.random.seed(0) # initialize random number generator with a seed=0
R = np.zeros([nump,dim]) # array to store current positions and set init
V = np.zeros([nump,dim]) # array to store current velocities and set ini
W = np.zeros([nump,dim]) # array to store current random forcces
Rs = np.zeros([nums,nump,dim]) # array to store positions at all steps
Vs = np.zeros([nums,nump,dim]) # array to store velocities at all steps
Ws = np.zeros([nums,nump,dim]) # array to store random forces at all ste
time = np.zeros([nums]) # an array to store time at all steps
```

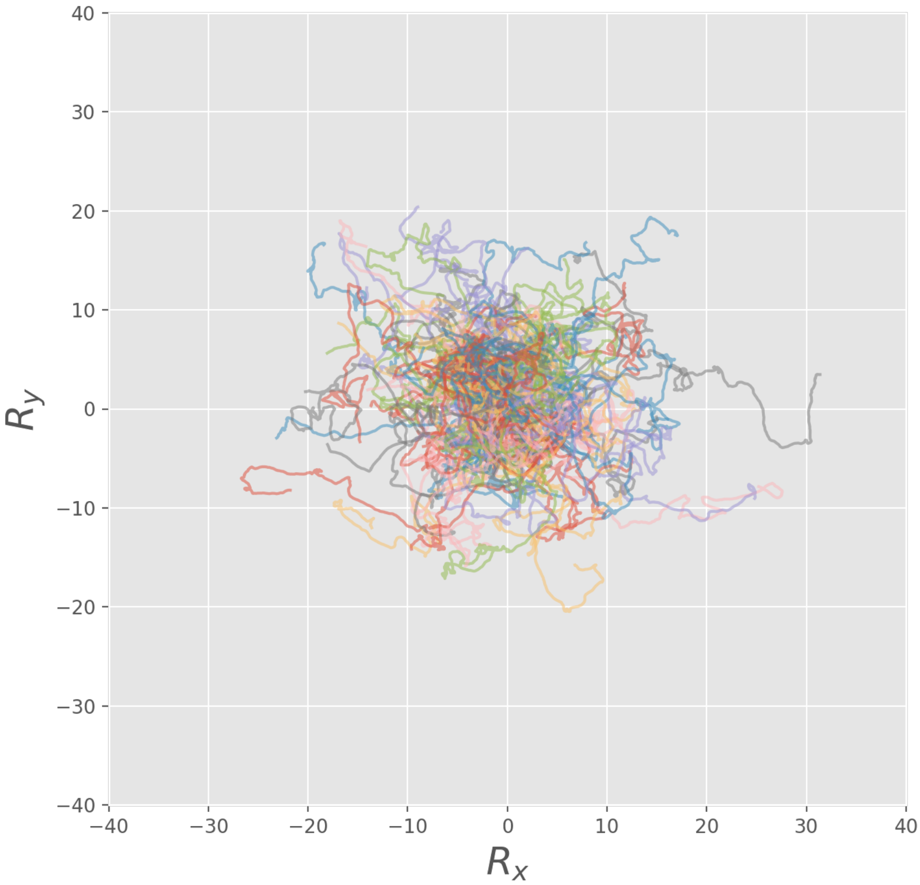
Perform simulation

In [3]:
```
for i in range(nums): # repeat the following operations from i=0 to nums
    W = std*np.random.randn(nump,dim) # generate an array of random forc
    V = V*(1-zeta/m*dt)+W/m # update velocity via Eq.(F9)
    R = R + V*dt # update position via Eq.(F5)
    Rs[i,:,:]=R # accumulate particle positions at each step in an array
    Vs[i,:,:]=V # accumulate particle velocitys at each step in an array
    Ws[i,:,:]=W # accumulate random forces at each step in an array Ws
    time[i]=i*dt # store time in each step in an array time
```

2.3. Plot trajectories of particles on a 2D plane

- Plot the temporal particle positions $R_x(t), R_y(t), R_z(t)$ in the x-y plane.

In [4]:
```
box=80. # set draw area as box^2
fig, ax = plt.subplots(figsize=(7.5,7.5)) # set fig with its size 7.5 x
ax.set_xlabel(r"$R_x$", fontsize=20) # set x-label
ax.set_ylabel(r"$R_y$", fontsize=20) # set y-label
plt.xlim(-box/2,box/2) # set x-range
plt.ylim(-box/2,box/2) # set y-range
for n in range(nump): # repeat from n=0 to nump-1
    ax.plot(Rs[:,n,0],Rs[:,n,1],alpha=0.5) # plot trajectiries of all pa
plt.show() # draw plots
```



2.4. Plot trajectories of particles in 3D space

- Plot the temporal particle positions $R_x(t), R_y(t), R_z(t)$ in 3D space.

In [5]:
```
box=80. # set draw area as box^3
fig = plt.figure(figsize=(10,10)) # set fig with its size 10 x 10 inch
ax = fig.add_subplot(111,projection='3d') # creates an additional axis t
ax.set_xlim(-box/2,box/2) # set x-range
ax.set_ylim(-box/2,box/2) # set y-range
ax.set_zlim(-box/2,box/2) # set z-range
ax.set_xlabel(r"x",fontsize=20) # set x-label
ax.set_ylabel(r"y",fontsize=20) # set y-label
ax.set_zlabel(r"z",fontsize=20) # set z-label
ax.view_init(elev=12,azim=120) # set view point
for n in range(nump): # repeat from n=0 to nump-1
    ax.plot(Rs[:,n,0],Rs[:,n,1],Rs[:,n,2],alpha=0.5) # plot trajectiries
plt.show() # draw plots
```