009x_51

March 18, 2017

Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 3: data analysis
-Distribution and time correlation-

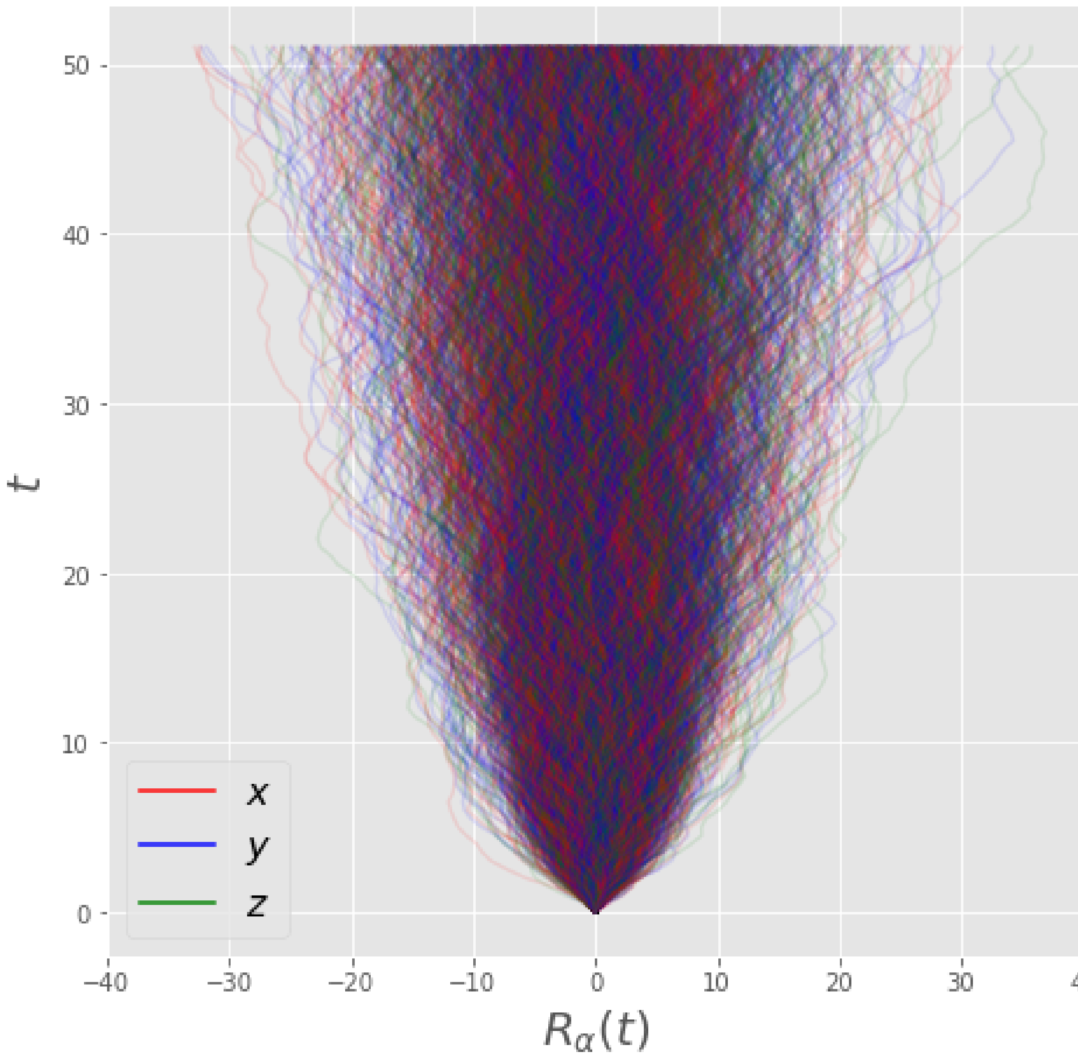
1 Generate trajectories

```
In [1]: % matplotlib inline
        import numpy as np
        import matplotlib.pyplot as plt
        import matplotlib as mpl
        plt.style.use('ggplot')
        dim  = 3    # system dimension (x,y,z)
        nump = 1000 # 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 initia
        V = np.zeros([nump,dim]) # array to store current velocities and set initia
        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 steps
        time = np.zeros([nums]) # an array to store time at all steps
        for i in range(nums): # repeat the following operations from i=0 to nums-1
            W = std*np.random.randn(nump,dim) # generate an array of random forces
            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 Rs
            Vs[i]=V # accumulate particle velocitys at each step in an array Vs
            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 Analysis 1

2.1 Position R vs. time t for all particles

```
In [2]: # particle positions vs time
        fig, ax = plt.subplots(figsize=(7.5,7.5))
        ax.set_xlabel(r"$R_{\alpha}(t)$", fontsize=20)
        ax.set_ylabel(r"$t$", fontsize=20)
        ax.set_xlim(-40,40)
        ts = 10 # only draw every 10 points to make it faster
        for n in range(nump):
            lx, = ax.plot(Rs[::ts,n,0],time[::ts],'r', alpha=0.1)
            ly, = ax.plot(Rs[::ts,n,1],time[::ts],'b', alpha=0.1)
            lz, = ax.plot(Rs[::ts,n,2],time[::ts],'g', alpha=0.1)
        # add plot legend for last x,y,z lines and remove alpha from legend lines
        leg = ax.legend([lx,ly,lz], [r"$x$",r"$y$",r"$z$"],loc=0, fontsize=16)
        for l in leg.get_lines():
            l.set_alpha(1)
        plt.show()
```



2.2 Distribution of the particle position (theoretical results)

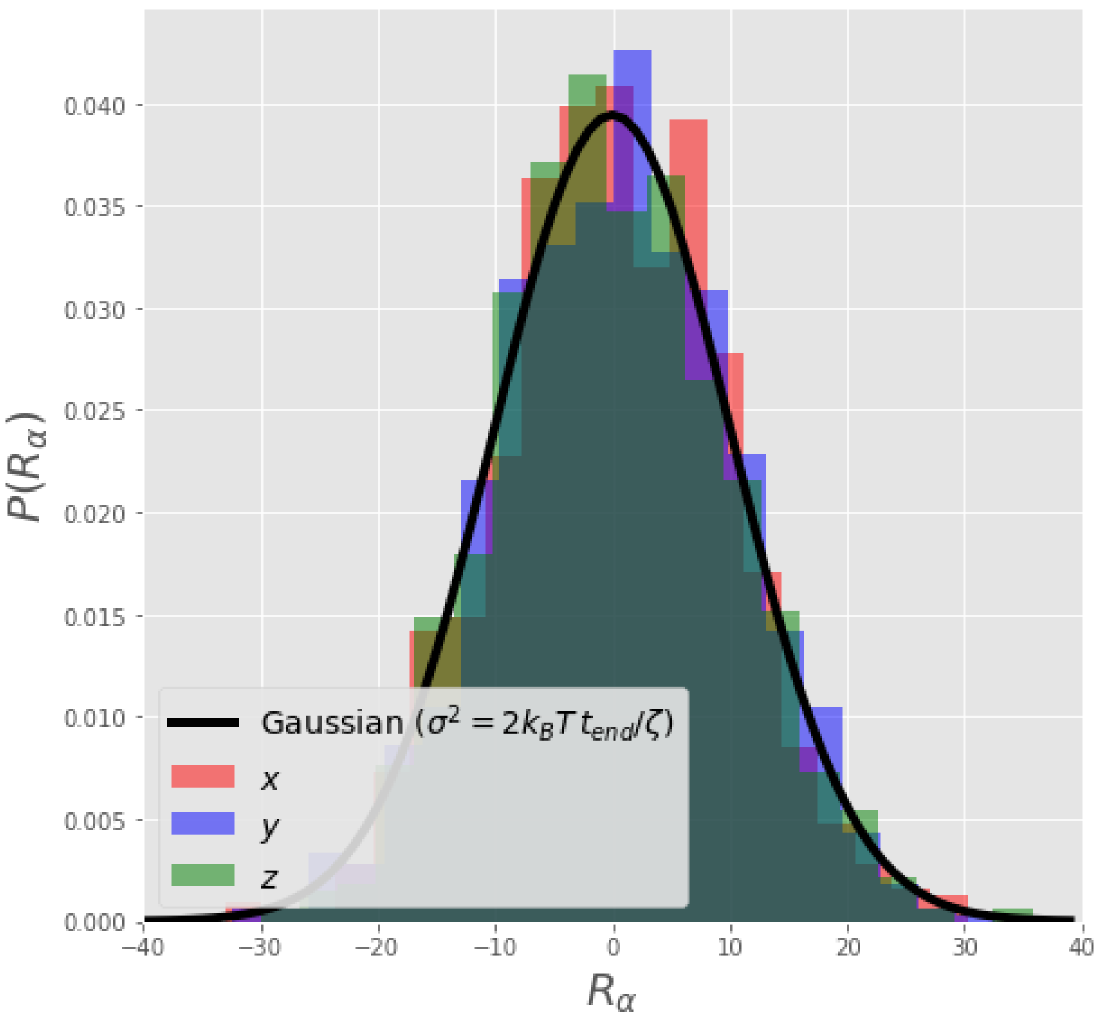
- Calculate the distribution functions for R_α ($\alpha = x, y, z$) at $t = t_{\text{end}}(= \texttt{nums} \times \Delta t)$, and compare them with the following theoretical result (see the supplemental note for the derivation).

$$P(R_\alpha) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(R_\alpha - \langle R_\alpha \rangle)^2}{2\sigma^2}\right] \qquad (\alpha = x, y, z) \tag{G1}$$

$$\langle R_\alpha \rangle = 0, \qquad \sigma^2 = \frac{2k_B T t_{\text{end}}}{\zeta} \tag{G2, G3}$$

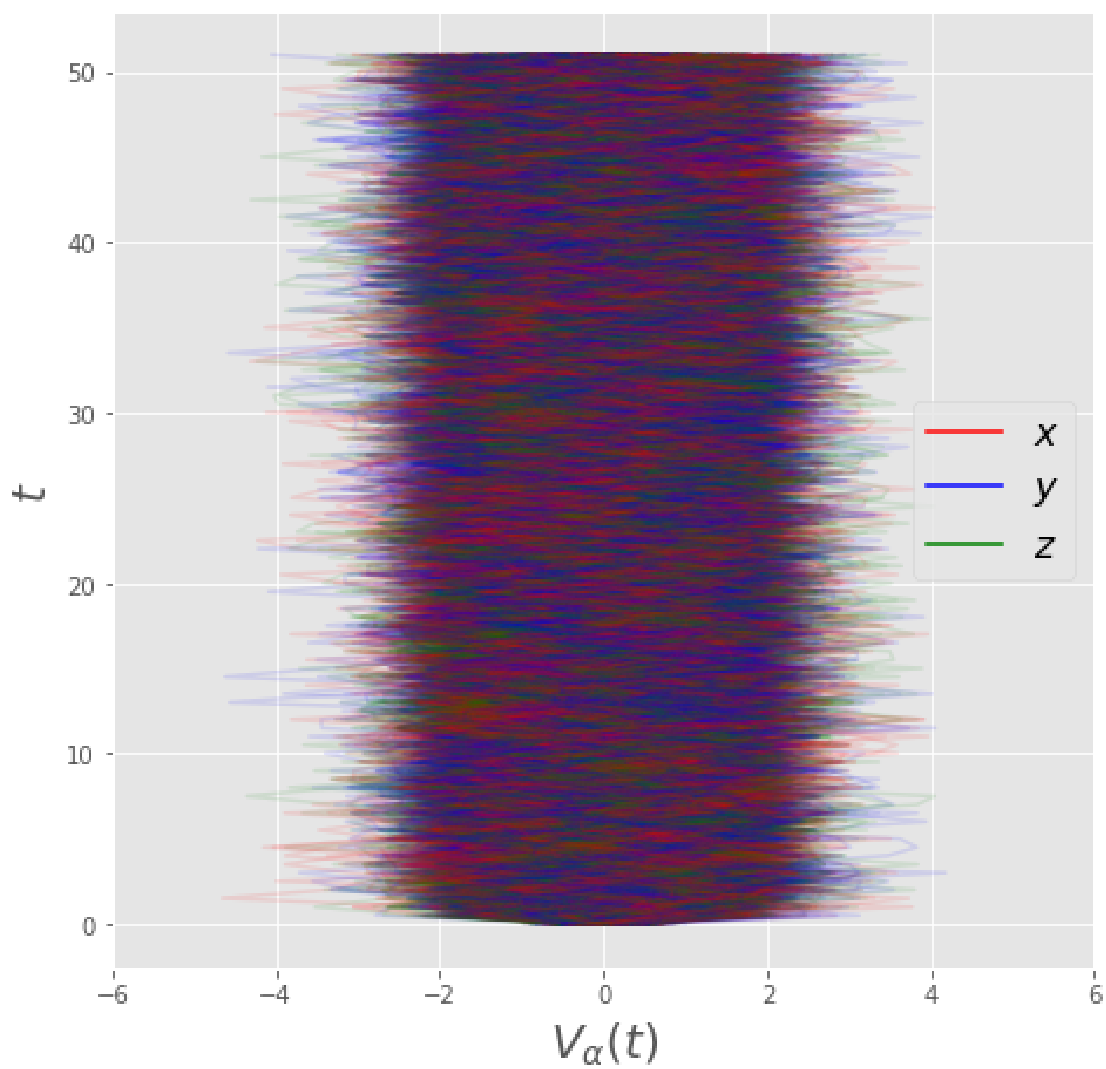
```
In [3]: # positional distribution of particles at the end of the simulation
        fig, ax = plt.subplots(figsize=(7.5,7.5))
```

```
ax.set_xlabel(r"$R_{\alpha}}(t=t_\mathrm{end})$", fontsize=20)
ax.set_ylabel(r"$P(R_{\alpha})$", fontsize=20)
# plot simulation histograms
ax.hist(Rs[-1,:,0], bins=20,normed=True,color='r',alpha=0.5,lw=0,label=r"$x
ax.hist(Rs[-1,:,1], bins=20,normed=True,color='b',alpha=0.5,lw=0,label=r"$y
ax.hist(Rs[-1,:,2], bins=20,normed=True,color='g',alpha=0.5,lw=0,label=r"$z
# plot theoretical gaussian distribution
sig2=2*kBT/zeta*dt*nums
ave=0.0
x = np.arange(-40,40,1)
y = np.exp(-(x-ave)**2/2/sig2)/np.sqrt(2*np.pi*sig2)
ax.plot(x,y,lw=4,color='k',label=r"Gaussian $(\sigma^2=2k_BT\,t_{end}/\zeta
ax.legend(fontsize=14,loc=3, framealpha=0.9)
ax.set_xlim(-40,40)
plt.show()
```



2.3 Velocity V vs. time t for all particles

```
In [4]: # particle velocities vs time
        fig, ax = plt.subplots(figsize=(7.5,7.5))
        ax.set_xlabel(r"$V_{\alpha}(t)$", fontsize=20)
        ax.set_ylabel(r"$t$", fontsize=20)
        ts = 10 # only draw every 10 points to make it faster
        for n in range(nump):
            lx, = ax.plot(Vs[::ts,n,0],time[::ts],'r', alpha=0.1)
            ly, = ax.plot(Vs[::ts,n,1],time[::ts],'b', alpha=0.1)
            lz, = ax.plot(Vs[::ts,n,2],time[::ts],'g', alpha=0.1)
        ax.set_xlim(-6, 6)
        # add plot legend for last x,y,z lines and remove alpha from legend lines
        leg = ax.legend([lx,ly,lz], [r"$x$",r"$y$",r"$z$"],loc=0, fontsize=16)
        for l in leg.get_lines():
            l.set_alpha(1)
        plt.show()
```



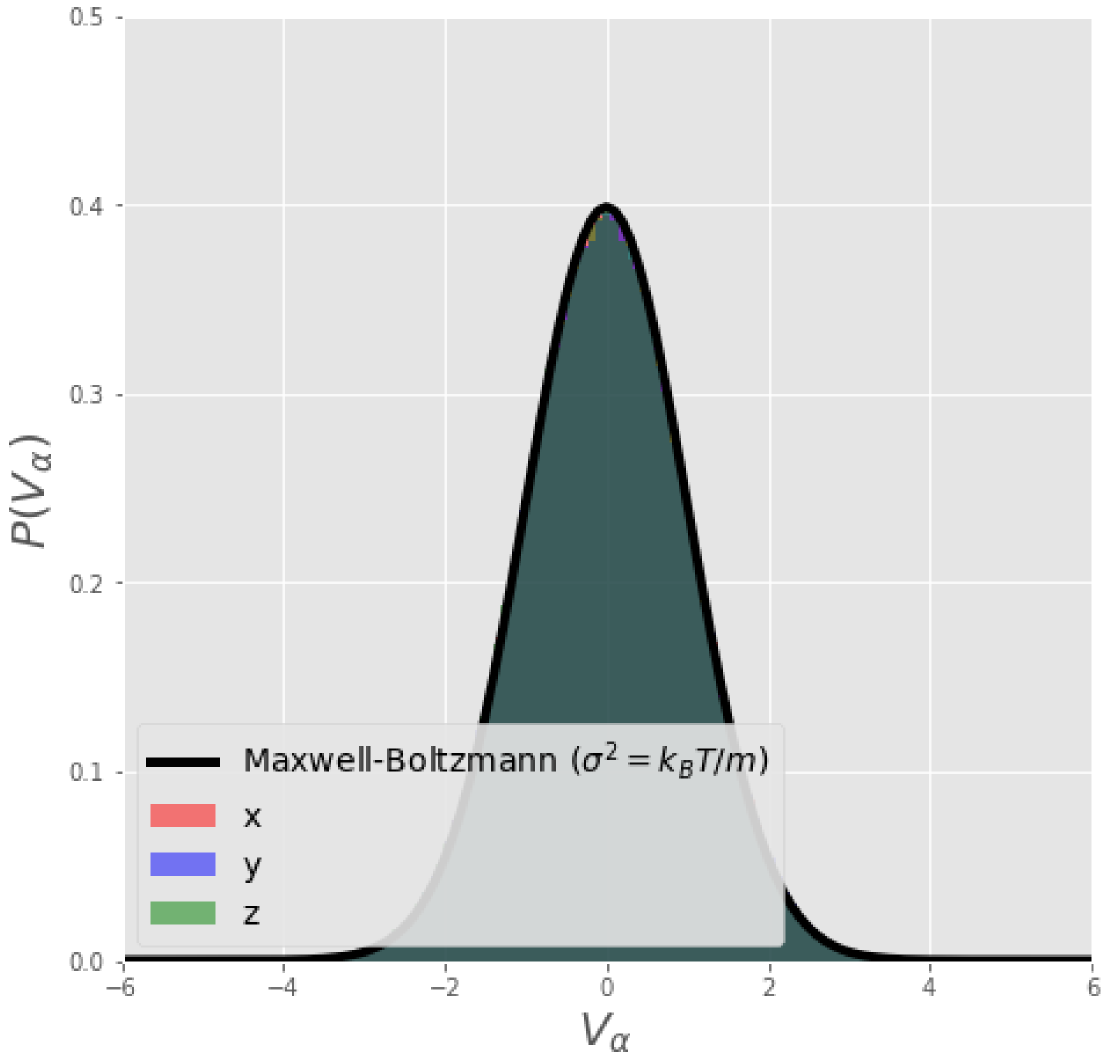
2.4 Distribution of the particle velocity (c.f. Maxwell-Boltzmann distribution)

- Calculate the distribution functions for V_α ($\alpha = x, y, z$) for $t_{\text{end}}/2 \le t \le t_{\text{end}}$, and compare them with the theoretical Maxwell-Boltzmann distribution function given below

$$P(V_\alpha) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(V_\alpha - \langle V_\alpha \rangle)^2}{2\sigma^2}\right] \quad (\alpha = x, y, z) \tag{G4}$$

$$\langle V_\alpha \rangle = 0, \quad \sigma^2 = \frac{2k_BT}{m} \tag{G5, G6}$$

In [5]:
```
# velocity distribution of particles at the end of the simulation
fig, ax = plt.subplots(figsize=(7.5,7.5))
# Compute histogram of velocities using the last half of the trajectory dat
# Note: flatten is required to transform the 2d array into a 1d array
ax.hist(Vs[nums//2:,:,0].flatten(),bins=100,normed=True,alpha=0.5,lw=0,colo
ax.hist(Vs[nums//2:,:,1].flatten(),bins=100,normed=True,alpha=0.5,lw=0,colo
ax.hist(Vs[nums//2:,:,2].flatten(),bins=100,normed=True,alpha=0.5,lw=0,colo
# Draw theoretical gaussian distribution
sig2=kBT/m
ave=0.0
x = np.arange(-10,10,0.1)
y = np.exp(-(x-ave)**2/2/sig2)/np.sqrt(2*np.pi*sig2)
ax.plot(x,y,lw=4,color='k',label=r"Maxwell-Boltzmann $(\sigma^2=k_BT/m)$")
ax.set_xlabel(r"$V_{\alpha}$",fontsize=20)
ax.set_ylabel(r"$P(V_{\alpha})$", fontsize=20)
ax.set_xlim(-6, 6)
ax.set_ylim(0, 0.5)
ax.legend(fontsize=14, loc=3,framealpha=0.9)
plt.show()
```



3 Analysis 2

3.1 Velocity auto-correlation function

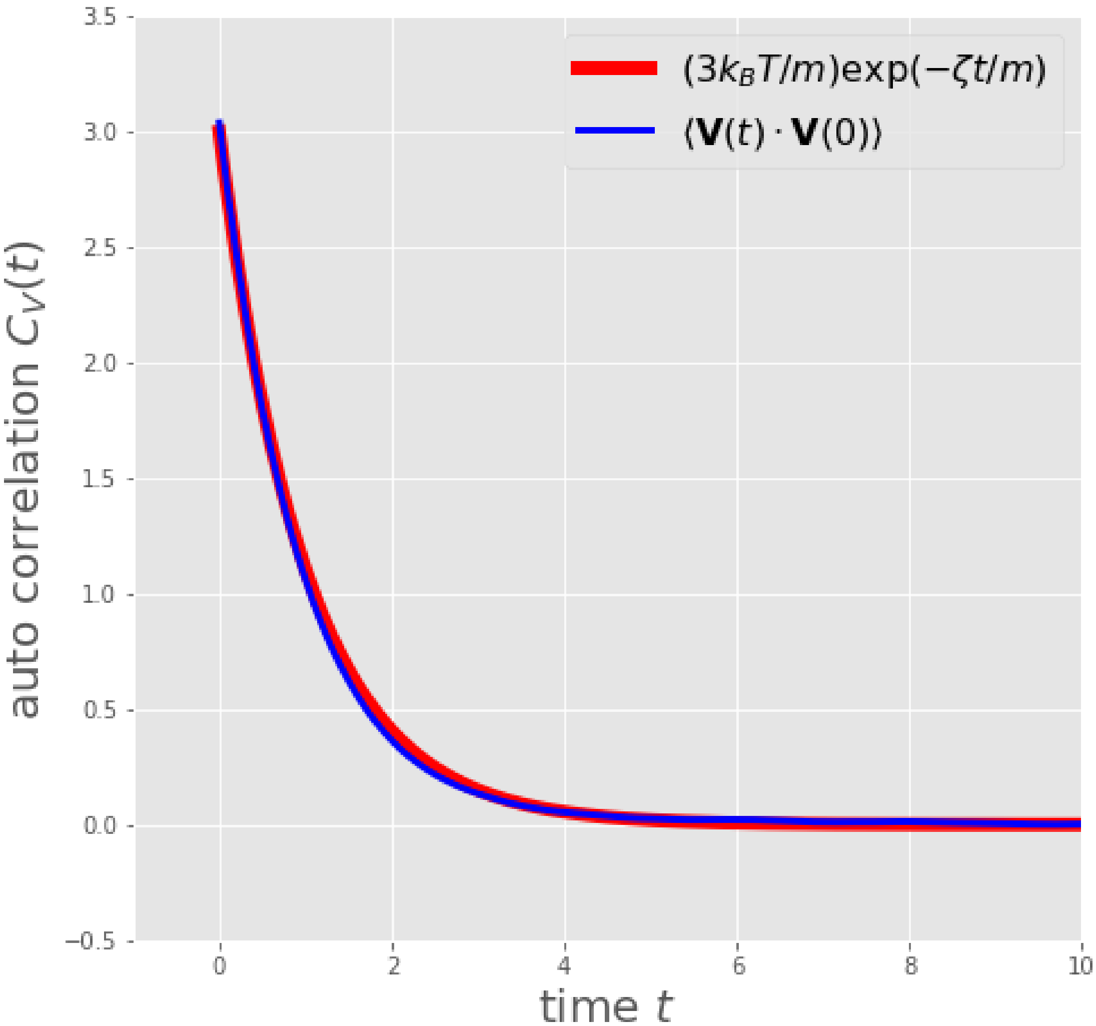
- Calculate the velocity auto-correlation function, and compare it with the following theoretical result (see the derivation for Eq.(26)).

$$\varphi_V(t) = \langle \mathbf{V}(t) \cdot \mathbf{V}(0) \rangle = \langle V_x(t)V_x(0) \rangle + \langle V_y(t)V_y(0) \rangle + \langle V_z(t)V_z(0) \rangle$$

$$= \frac{3k_BT}{m} \exp\left[-\frac{\zeta}{m}t\right] \tag{G7}$$

In [6]:

```
# compute self-correlation of vector v
def auto_correlate(v):
    # np.correlate computes C_{v}[k] = sum_n v[n+k] * v[n]
    corr = np.correlate(v,v,mode="full") # correlate returns even array [0:
    return corr[len(v)-1:]/len(v) # take positive values and normalize by n
corr = np.zeros([nums])
for n in range(nump):
    for d in range(dim):
        corr = corr + auto_correlate(Vs[:,n,d]) # correlation of d-componen
corr=corr/nump #average over all particles
fig, ax = plt.subplots(figsize=(7.5,7.5))
ax.plot(time,dim*kBT/m*np.exp(-zeta/m*time),'r',lw=6, label=r'$(3k_BT/m)\ex
ax.plot(time,corr,'b',lw=3,label=r'$\langle\mathbf{V}(t)\cdot \mathbf{V}(0)
ax.set_xlabel(r"time $t$", fontsize=20)
ax.set_ylabel(r"auto correlation $C_V(t)$", fontsize=20)
ax.set_xlim(-1,10)
ax.set_ylim(-0.5,3.5)
ax.legend(fontsize=16)
plt.show()
```



3.2 Power spectrum of particle velocity

- Calculate the power spectrum of the particle velocity, and compare it with the following theoretical result (see the derivation for Eq.(25))

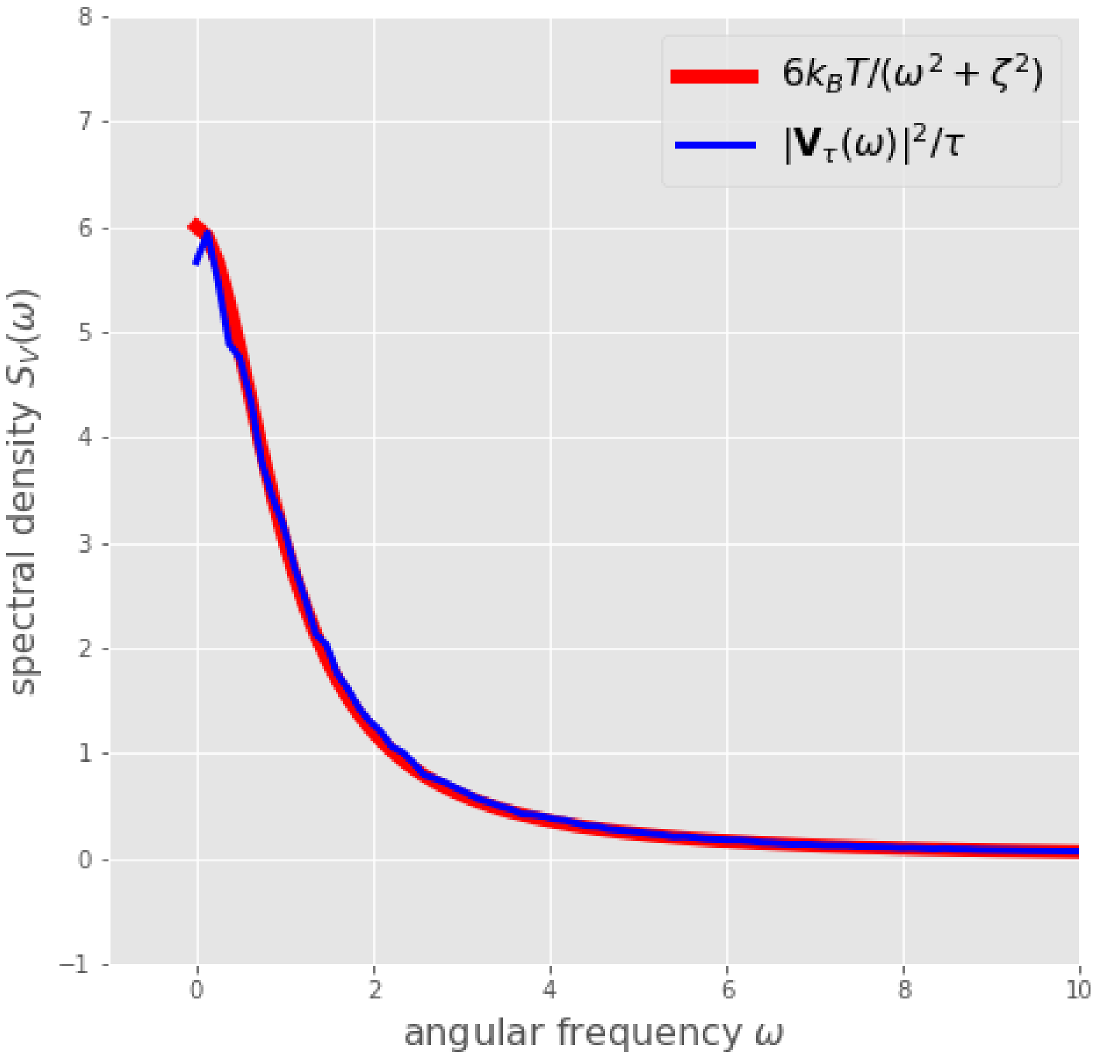
$$S_V(\omega) = \lim_{\tau\to\infty} \frac{1}{\tau}|\mathbf{V}_\tau(\omega)|^2 = \frac{6k_BT}{m}\frac{\gamma_c}{\omega^2+\gamma_c^2} \tag{G8}$$

where $\gamma_c = \zeta/m$ is the decay constant in Eq.(G7) and

$$\mathbf{V}_\tau(\omega) = \int_0^\tau \mathrm{d}t\, \mathbf{V}(t)e^{i\omega t} \tag{G9}$$

```
In [7]: # return power spectrum for positive frequencies of even signal v
        from numpy import fft
```

```
def psd(v,dt):
    vw = fft.fft(v)*dt # V(w) with zero-frequency component at vw(0)
    return np.abs(vw[:nums//2])**2/(nums*dt) # S_V for w > 0 (Eq. (G9))
Sw   = np.zeros([nums//2])
for n in range(nump):
    for d in range(dim):
        Sw = Sw + psd(Vs[:,n,d],dt) # power spectrum of d-component of velo
Sw = Sw/nump
fig, ax = plt.subplots(figsize=(7.5,7.5))
gamma = zeta/m
omega = fft.fftfreq(nums,d=dt)[:nums//2]*2.0*np.pi
ax.plot(omega,(6.0*kBT/m)*gamma/(omega**2 + gamma**2),'r',lw=6,label=r'$6k_
ax.plot(omega,Sw,'b',lw=3,label=r'$|\mathbf{V}_\tau(\omega)|^2 / \tau$')
ax.set_xlabel(r"angular frequency $\omega$", fontsize=16)
ax.set_ylabel(r"spectral density $S_V(\omega)$", fontsize=16)
ax.legend(fontsize=16)
plt.xlim(-1, 10)
plt.ylim(-1, 8)
plt.show()
```



$6k_BT/(\omega^2+\zeta^2)$
$|\mathbf{V}_\tau(\omega)|^2/\tau$
spectral density $S_V(\omega)$
angular frequency ω
8
7
6
5
4
3
2
1
0
−1
0
2
4
6
8
10