analyse

June 13, 2024

[1]:
```
import analyse

import matplotlib.pyplot as plt
import time
import numpy as np
import pandas as pd
import scipy.optimize

plt.style.use('classic')
```

[2]:
```
# Load data
tic = time.perf_counter()
first_frame = 0
frame_stride = 1
last_frame = None
time_step = 2e-15
steps_per_printout = 40
print(f'{first_frame = } {frame_stride = } {last_frame = } {steps_per_printout␣
 ↪= }')
spns = int(1e-9 / time_step / steps_per_printout / frame_stride)  # Steps per␣
 ↪nanosecond
print(f'Steps per nanosecond: {spns = }')
df = analyse.thermo_data_as_dataframe(filename='../../log-file/T380_L35.944/log.
 ↪lammps',
                                      time_step=time_step,
                                      first_frame=first_frame,
                                      stride_frame=frame_stride,
                                      last_frame=last_frame)
toc = time.perf_counter()
print(f'Wallclock time to load data: {toc-tic} s')
```

```
first_frame = 0 frame_stride = 1 last_frame = None steps_per_printout = 40
Steps per nanosecond: spns = 12500
Wallclock time to load data: 9.400851506000436 s
```

[3]:
```
df.head()
```

[3]:

```
           Time   Step       Temp        Press     PotEng     KinEng  \
0  0.000000e+00    0.0  344.93695 -26171.19600  5196.6258  4111.7379
1  8.000000e-14   40.0  384.74831  -1813.19590  5029.1247  4586.2996
2  1.600000e-13   80.0  386.35782   2081.59420  4969.0675  4605.4855
3  2.400000e-13  120.0  386.06626   -548.78717  4866.6535  4602.0099
4  3.200000e-13  160.0  376.68499   2197.93110  5051.6645  4490.1828

      E_vdwl     E_coul      E_mol     Volume  Density    c_virial
0 -647.60531  2486.3671  6072.3676  46438.611  1.02942 -30218.6240
1 -393.51470  2504.6959  5631.3149  46438.611  1.02942  -6327.7625
2 -359.18030  2485.0399  5558.2705  46438.611  1.02942  -2451.8581
3 -478.21544  2501.6095  5557.8171  46438.611  1.02942  -5078.8183
4 -390.06892  2511.7764  5645.6552  46438.611  1.02942  -2222.0219
```

[4]:

```
join_trajectories = True
if join_trajectories:
    df_2nd = analyse.thermo_data_as_dataframe(filename='../../log-file/T380_L35.
 ↪944/log_2nd.lammps',
                                             time_step=time_step,
                                             first_frame=first_frame,
                                             stride_frame=frame_stride,
                                             last_frame=last_frame)
    df_2nd['Time'] = df_2nd.Time + df.Time.max()
    df_2nd.head()
    df = pd.concat([df, df_2nd], axis=0)
df.head()
```

[4]:


```
           Time   Step       Temp        Press     PotEng     KinEng  \
0  0.000000e+00    0.0  344.93695 -26171.19600  5196.6258  4111.7379
1  8.000000e-14   40.0  384.74831  -1813.19590  5029.1247  4586.2996
2  1.600000e-13   80.0  386.35782   2081.59420  4969.0675  4605.4855
3  2.400000e-13  120.0  386.06626   -548.78717  4866.6535  4602.0099
4  3.200000e-13  160.0  376.68499   2197.93110  5051.6645  4490.1828

      E_vdwl     E_coul      E_mol     Volume  Density    c_virial
0 -647.60531  2486.3671  6072.3676  46438.611  1.02942 -30218.6240
1 -393.51470  2504.6959  5631.3149  46438.611  1.02942  -6327.7625
2 -359.18030  2485.0399  5558.2705  46438.611  1.02942  -2451.8581
3 -478.21544  2501.6095  5557.8171  46438.611  1.02942  -5078.8183
4 -390.06892  2511.7764  5645.6552  46438.611  1.02942  -2222.0219
```


[5]:

```
df['E_inter'] = df.PotEng - df.E_mol
```

[6]:

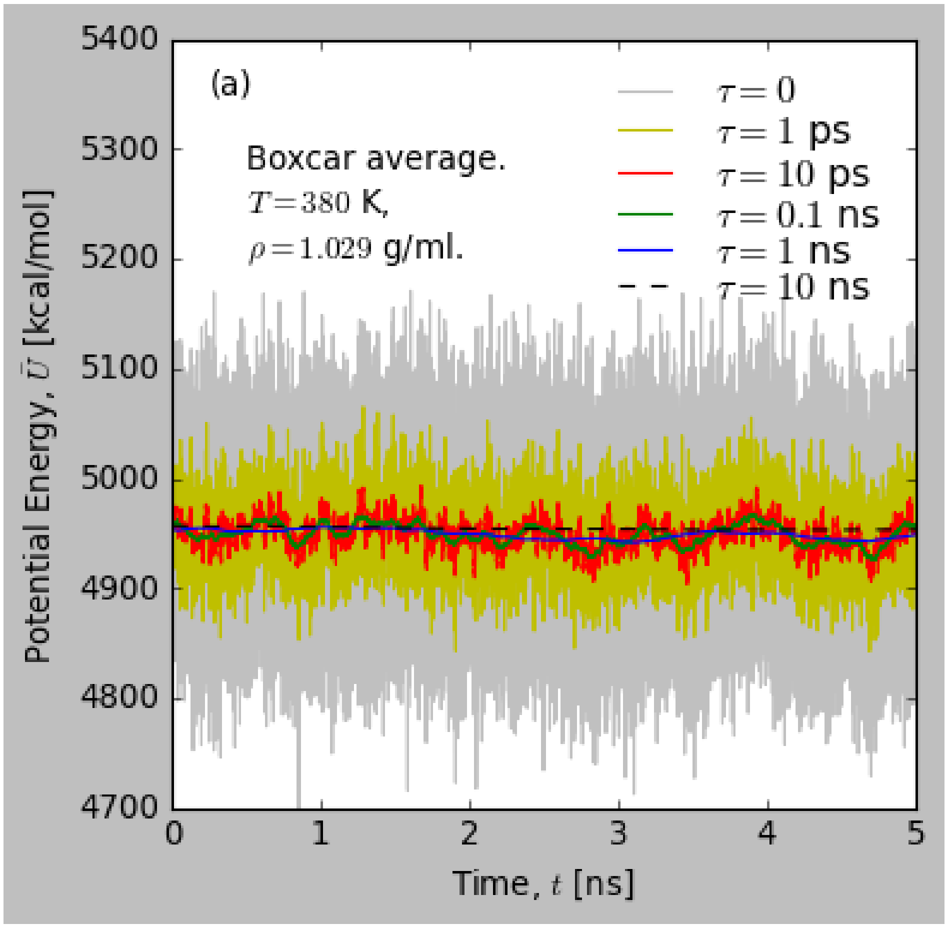
```
print(f'Trajectory of {df.Time.max()/1e-9} ns')
```

```
Trajectory of 468.435456 ns
```

[7]:
```
from scipy.ndimage import uniform_filter1d
```

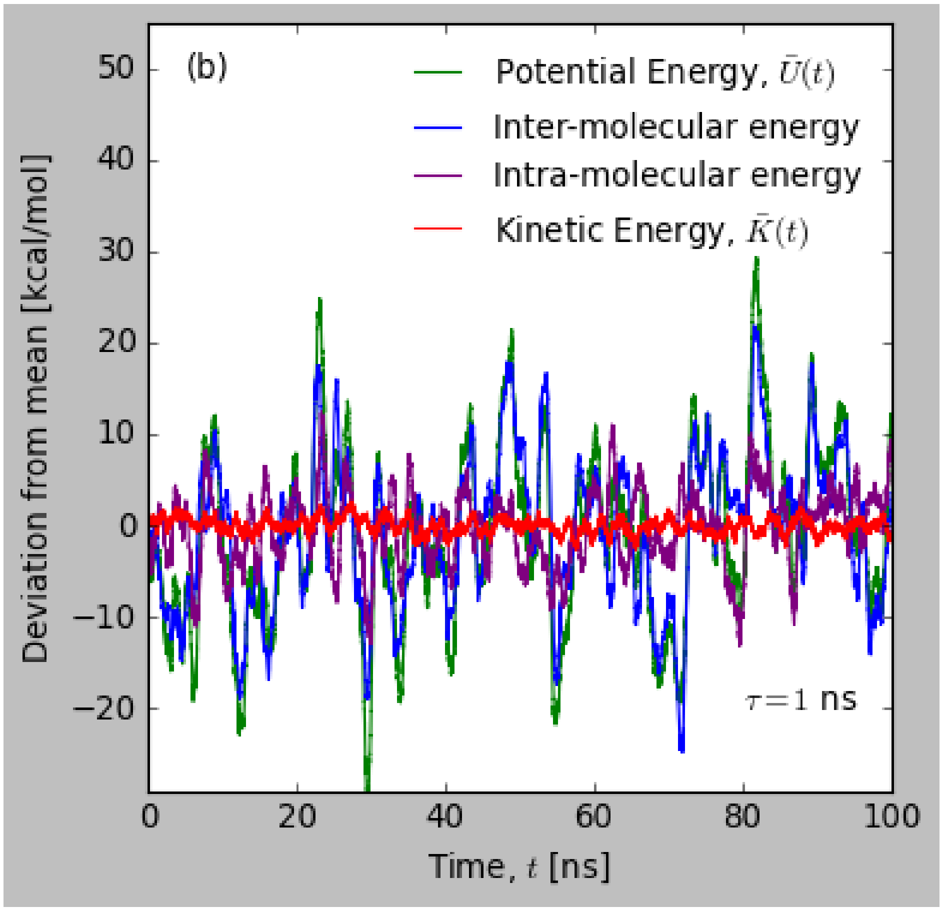
[8]:
```
u_mean = uniform_filter1d(df.PotEng, int(spns))
```

[9]:
```
t = df.Time*1e9-21
plt.figure(figsize=(5, 5))
plt.plot(t, df.PotEng, '-', color='silver', label=r'$\tau=0$')
plt.plot(t, uniform_filter1d(df.PotEng, int(spns/1000)), 'y-', label=r'$\tau=1$␣
↪ps')
plt.plot(t, uniform_filter1d(df.PotEng, int(spns/100)), 'r-', label=r'$\tau=10$␣
↪ps')
plt.plot(t, uniform_filter1d(df.PotEng, int(spns/10)), 'g-', label=r'$\tau=0.1$␣
↪ns')
plt.plot(t, uniform_filter1d(df.PotEng, int(spns)), 'b-', label=r'$\tau=1$ ns')
plt.plot(t, uniform_filter1d(df.PotEng, int(spns)*10), 'k--', label=r'$\tau=10$␣
↪ns')
plt.legend(frameon=False, labelspacing=0.01)
plt.xlabel(r'Time, $t$ [ns]')
plt.ylabel(r'Potential Energy, $\bar U$ [kcal/mol]')
plt.text(0.5, 5200, 'Boxcar average.\n' + r'$T = 380$ K,' + '\n' + r'$\rho=1.
↪029$ g/ml.')
# Put (a) in the upper left corner
plt.text(0.05, 0.93, '(a)', transform=plt.gca().transAxes)
plt.xlim(0, 5)
plt.ylim(4700, 5400)
plt.savefig('boxcar.pdf', bbox_inches='tight')
plt.savefig('boxcar.png', bbox_inches='tight')
```



[10]:
```
t = df.Time*1e9-21
plt.figure(figsize=(5, 5))
plt.plot(t, uniform_filter1d(df.PotEng, int(spns))-df.PotEng.mean(), 'g-',␣
 ↪label=r'Potential Energy, $\bar U(t)$')
plt.plot(t, uniform_filter1d(df.E_inter, int(spns))-df.E_inter.mean(), 'b-',␣
 ↪label=r'Inter-molecular energy')
plt.plot(t, uniform_filter1d(df.E_mol, int(spns))-df.E_mol.mean(), '-',␣
 ↪color='purple', label=r'Intra-molecular energy')
plt.plot(t, uniform_filter1d(df.KinEng, int(spns))-df.KinEng.mean(), 'r-',␣
 ↪label=r'Kinetic Energy, $\bar K(t)$')
plt.xlabel(r'Time, $t$ [ns]')
plt.ylabel(r'Deviation from mean [kcal/mol]')
#plt.text(0.5, 5250, 'Boxcar average.\n' + r'$T = 380$ K,' + '\n' + r'$\rho=1.
 ↪030$ g/ml.')
plt.text(80, -20, r'$\tau=1$ ns')
plt.text(0.05, 0.93, '(b)', transform=plt.gca().transAxes)
plt.xlim(0, 100)
plt.ylim(-29, 55)
```

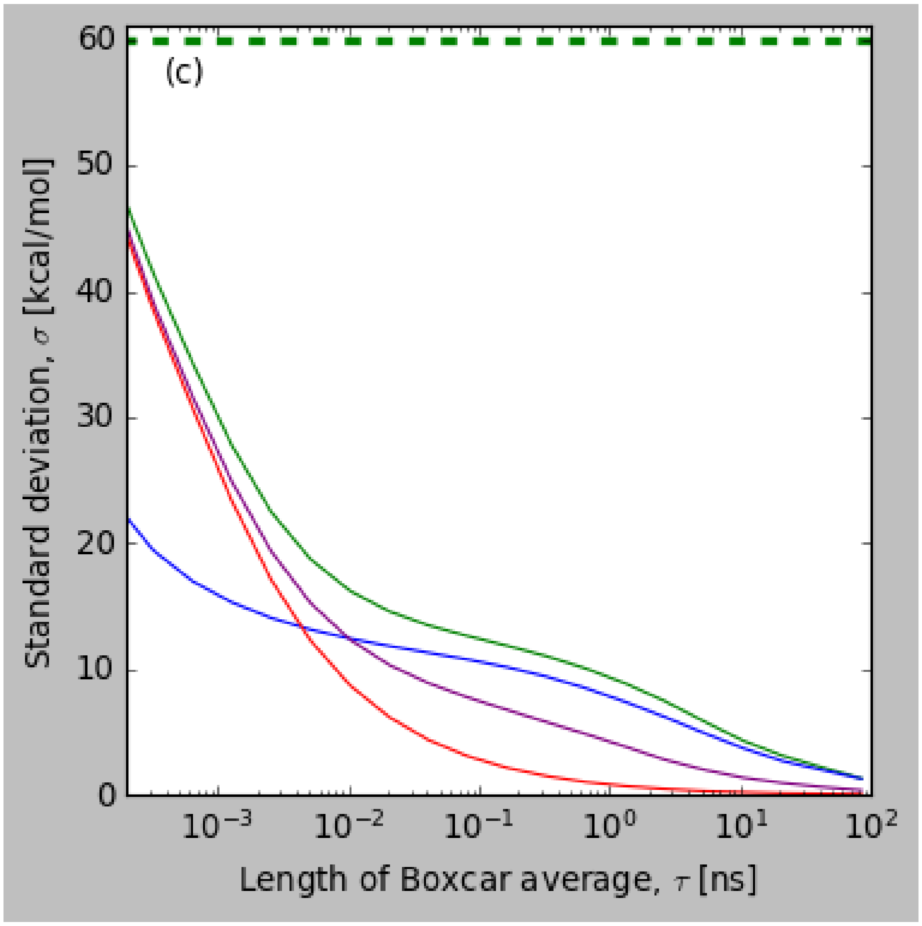
```
plt.legend(frameon=False, loc='upper right', fontsize=12)
plt.savefig('boxcar_energy.pdf', bbox_inches='tight')
plt.savefig('boxcar_energy.png', bbox_inches='tight')
```



[11]:
```
plt.figure(figsize=(5, 5))

def plot_curve(data, **kwarks):
    sigmas = []
    taus = []
    size = 1
    while size < len(data)/10:
        size=size*2
        taus.append(size/spns)
        sigmas.append(uniform_filter1d(data, size).std())
    plt.plot(taus, sigmas, '-', **kwarks)
    zero_level = data.std()
    #plt.plot([1e-4, 1e0], [zero_level]*2, '--', **kwarks)
    print(zero_level)
```

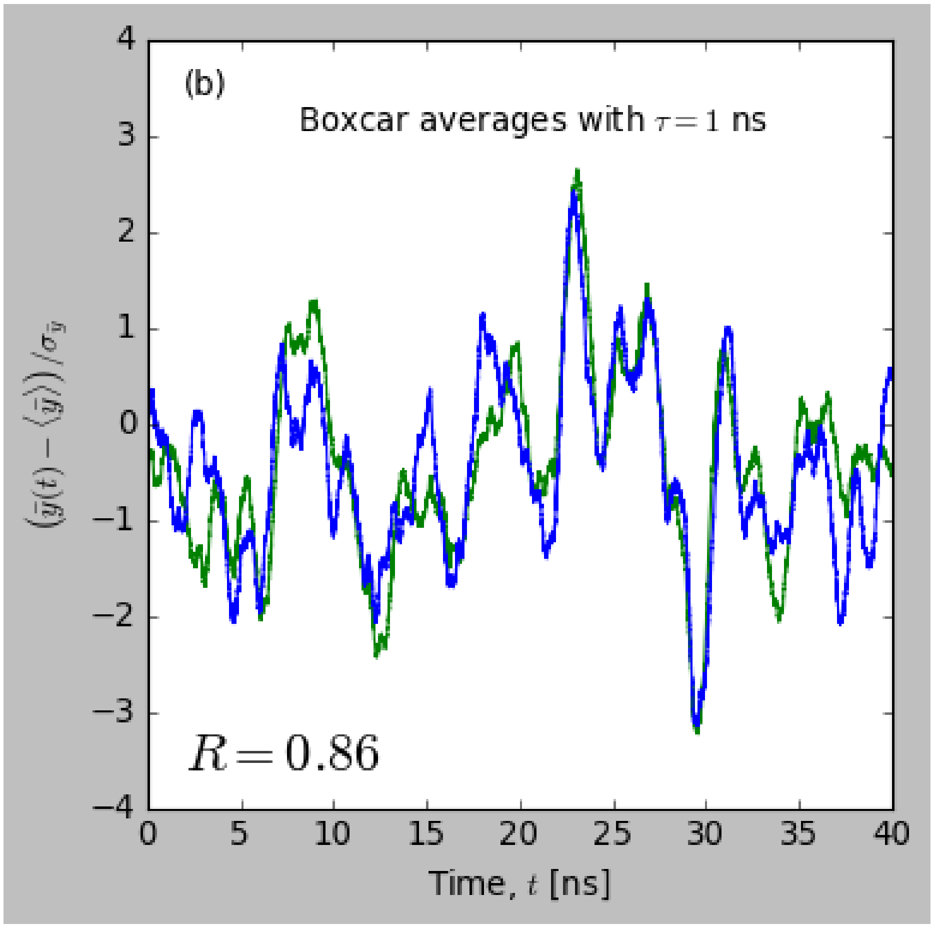
```
plot_curve(df.PotEng, color='g', label=r'Potential Energy, $\bar U(t)$')
plot_curve(df.E_inter, color='b', label=r'Inter-molecular energy')
plot_curve(df.E_mol, color='purple', label=r'Intra-molecular energy')
plot_curve(df.KinEng, color='r', label=r'Kinetic Energy, $\bar K(t)$')

zero_level = df.PotEng.std()
plt.plot([1e-4, 1e2], [zero_level]*2, 'g--', lw=3)
plt.ylabel(r'Standard deviation, $\sigma$ [kcal/mol]')
plt.xlabel(r'Length of Boxcar average, $\tau$ [ns]')
plt.xscale('log')
plt.ylim(0, 61)
plt.xlim(2e-4,1e2)
#plt.legend(frameon=False, loc='upper right', fontsize=12)
plt.text(0.05, 0.93, '(c)', transform=plt.gca().transAxes)
#plt.text(5e-1, 25, 'Ortho-terphenyl:\n' + r'$T = 380$ K,' + '\n' + r'$\rho=1.
 ↪029$ g/ml.')
plt.savefig('boxcar_standard_deviation.pdf', bbox_inches='tight')
plt.savefig('boxcar_standard_deviation.png', bbox_inches='tight')
```

```
59.980637982893676
28.145155888219342
59.089076131093776
58.511670449264315
```



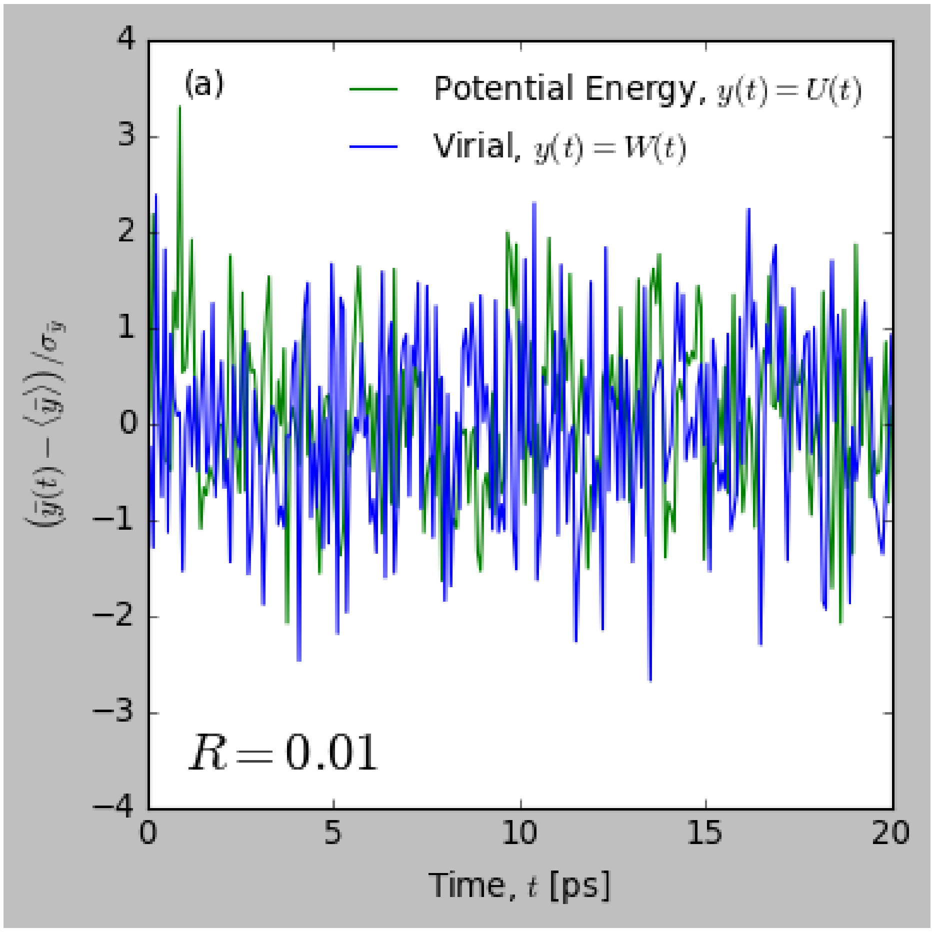
[50]:
```
t = df.Time*1e9-21
plt.figure(figsize=(5, 5))
y = uniform_filter1d(df.PotEng, int(spns))-df.PotEng.mean()
plt.plot(t, y/np.std(y), 'g-', label=r'Potential Energy, $\bar y(t) = \bar U(t;␣
↪\tau)$')
y = uniform_filter1d(df.c_virial, int(spns))-df.c_virial.mean()
plt.plot(t, y/np.std(y), 'b-', label=r'Virial, $\bar y(t) = \bar W(t; \tau)$')
plt.xlabel(r'Time, $t$ [ns]')
plt.ylabel(r'$\left(\bar y(t)-\langle \bar y\rangle\right)/\sigma_{\bar y}$')
#plt.text(0.5, 5250, 'Boxcar average.\n' + r'$T = 380$ K,' + '\n' + r'$\rho=1.
↪030$ g/ml.')
plt.text(0.2, 0.88, r'Boxcar averages with $\tau=1$ ns', transform=plt.gca().
↪transAxes, fontsize=12)
plt.text(0.05, 0.93, '(b)', transform=plt.gca().transAxes)
plt.text(0.05, 0.05, f'$R = 0.86$', transform=plt.gca().transAxes, ha='left',␣
↪fontsize=20)
plt.xlim(0, 40)
#plt.ylim(-29, 55)
```

```
#plt.legend(frameon=False, loc='upper right', fontsize=12)
plt.savefig('boxcar_virial_energy.pdf', bbox_inches='tight')
plt.savefig('boxcar_virial_energy.png', bbox_inches='tight')
```



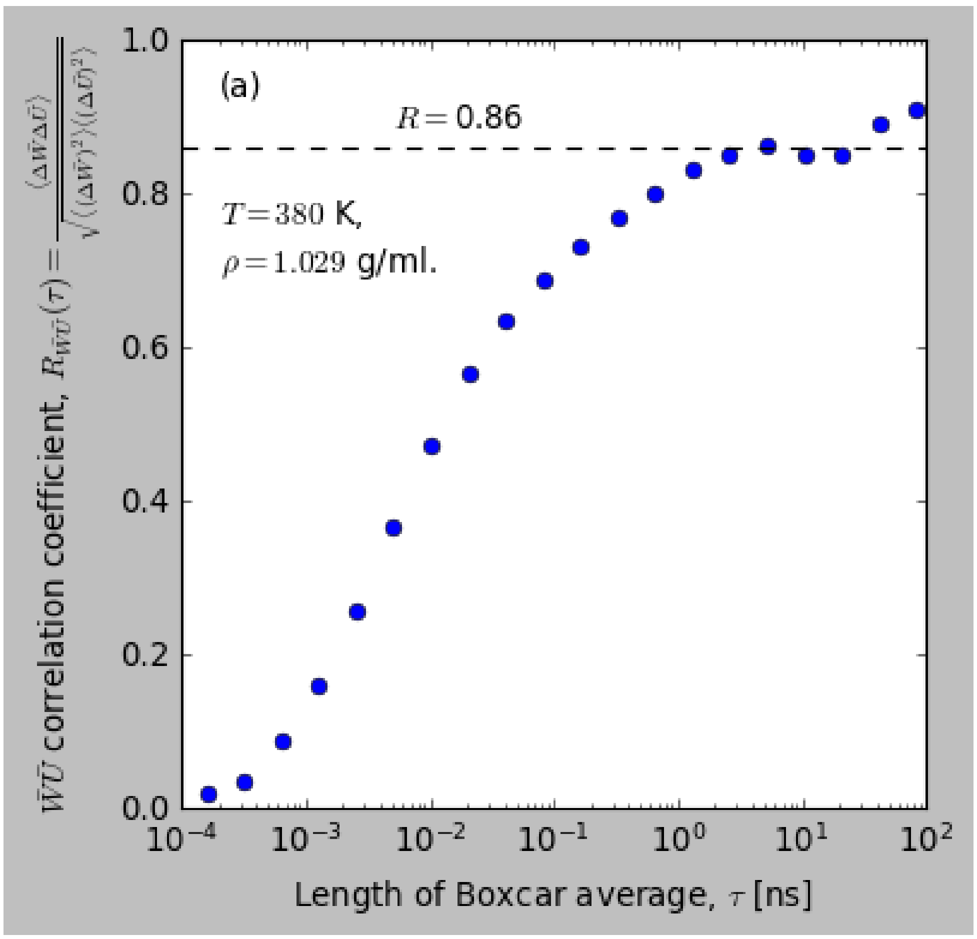
[45]:
```
t = df.Time*1e9-21
plt.figure(figsize=(5, 5))
y = df.PotEng-df.PotEng.mean()
plt.plot(t*1e3, y/np.std(y), 'g-', label=r'Potential Energy, $y(t) = U(t)$')
y = df.c_virial-df.c_virial.mean()
plt.plot(t*1e3, y/np.std(y), 'b-', label=r'Virial, $y(t) = W(t)$')
plt.xlabel(r'Time, $t$ [ps]')
plt.ylabel(r'$\left(\bar y(t)-\langle \bar y\rangle\right)/\sigma_{\bar y}$')
#plt.text(0.5, 5250, 'Boxcar average.\n' + r'$T = 380$ K,' + '\n' + r'$\rho=1.
↪030$ g/ml.')
#plt.text(0.1, 0.1, r'$\tau=0$ ns', transform=plt.gca().transAxes)
corrcoef = np.corrcoef(df.PotEng, df.c_virial)[0,1]
plt.text(0.05, 0.05, f'$R = {corrcoef:.2f}$', transform=plt.gca().transAxes,␣
↪ha='left', fontsize=20)
```

```
plt.text(0.05, 0.93, '(a)', transform=plt.gca().transAxes)
plt.xlim(0, 20)
plt.ylim(-4, 4)
plt.legend(frameon=False, loc='upper right', fontsize=12)
plt.savefig('boxcar_virial_energy_fast.pdf', bbox_inches='tight')
plt.savefig('boxcar_virial_energy_fast.png', bbox_inches='tight')
```



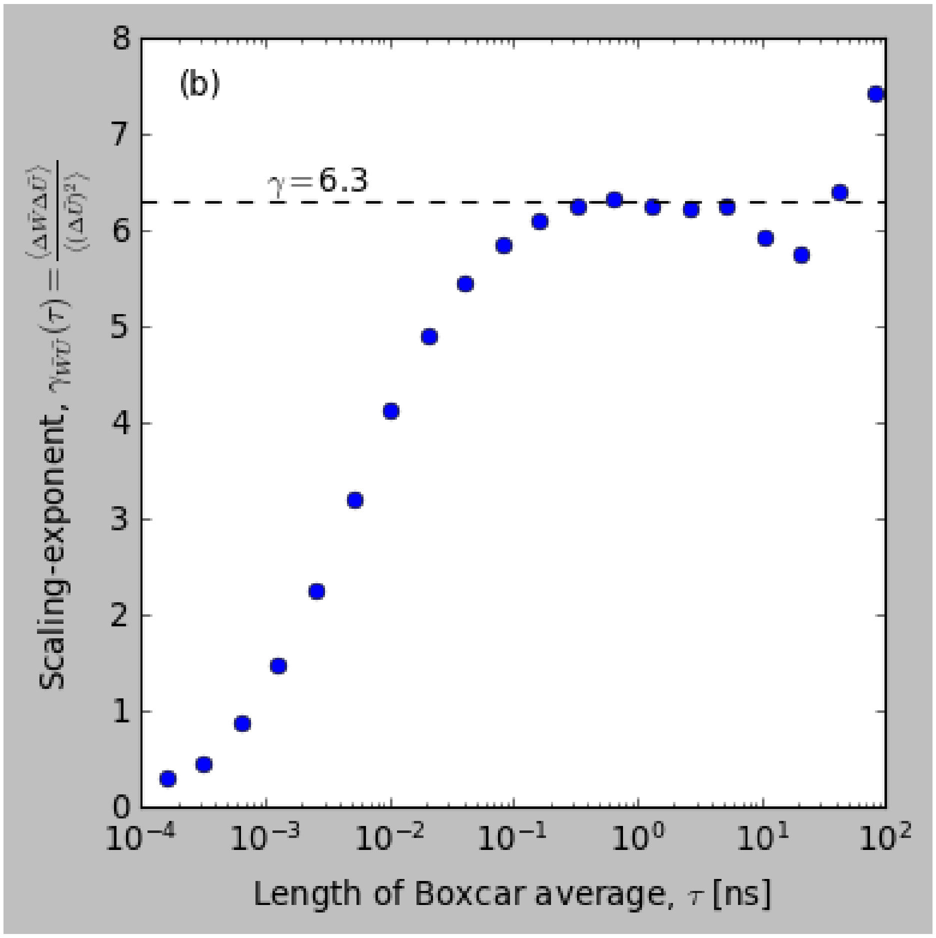
[12]:
```
plt.figure(figsize=(5, 5))
Rs = []
taus = []
size = 1
while size < len(df.PotEng)/10:
    size=size*2
    taus.append(size/spns)
    A = uniform_filter1d(df.PotEng, size)
    B = uniform_filter1d(df.c_virial, size)
    R = np.corrcoef(A, B)
    Rs.append(R[0, 1])
```

```
plt.plot(taus, Rs, 'bo')
R_long_time = 0.86
plt.plot([1e-4, 100], [R_long_time]*2, 'k--')
plt.text(5e-3, 0.9, r'$R=$' f'{R_long_time}', va='center')
plt.xscale('log')
plt.xlabel(r'Length of Boxcar average, $\tau$ [ns]')
plt.ylabel(r'$\bar W$$\bar U$ correlation coefficient, $R_{\bar W\bar␣
↪U}(\tau)=\frac{\langle \Delta \bar W\Delta \bar U\rangle}{\sqrt{\langle␣
↪(\Delta \bar W)^2\rangle\langle (\Delta \bar U)^2\rangle}}$')
plt.text(0.05, 0.93, '(a)', transform=plt.gca().transAxes)
plt.text(2e-4, 0.7,'$T = 380$ K,' + '\n' + r'$\rho=1.029$ g/ml.')
plt.ylim(0, 1)
plt.xlim(1e-4, 1e2)
plt.savefig('boxcar_correlation_coefficient.pdf', bbox_inches='tight')
plt.savefig('boxcar_correlation_coefficient.png', bbox_inches='tight')
```



[13]:
```
plt.figure(figsize=(5, 5))
gammas = []
```

```
taus = []
size = 1
while size < len(df.PotEng)/10:
    size=size*2
    taus.append(size/spns)
    A = uniform_filter1d(df.PotEng, size)
    B = uniform_filter1d(df.c_virial, size)
    cov = np.cov(A, B)
    gammas.append(cov[0, 1]/A.var())
plt.plot(taus, gammas, 'bo')
gamma_long_time = 6.3
plt.plot([1e-4, 100], [gamma_long_time]*2, 'k--')
plt.text(1e-3, gamma_long_time+0.2, r'$\gamma=$' f'{gamma_long_time}',␣
 ↪va='center')
plt.text(0.05, 0.93, '(b)', transform=plt.gca().transAxes)
plt.xscale('log')
plt.xlabel(r'Length of Boxcar average, $\tau$ [ns]')
plt.ylabel(r'Scaling-exponent, $\gamma_{\bar W\bar␣
 ↪U}(\tau)=\frac{\langle\Delta\bar W\Delta\bar U\rangle}{\langle(\Delta\bar␣
 ↪U)^2\rangle}$')
#plt.text(2e-1, 0.7, r'ortho-terphenyl,' + '\n' + '$T = 380$ K,' + '\n' +␣
 ↪r'$\rho=1.030$ g/ml.')
#plt.ylim(0, 1)
plt.xlim(1e-4, 1e2)
plt.savefig('boxcar_scaling_exponent.pdf', bbox_inches='tight')
plt.savefig('boxcar_scaling_exponent.png', bbox_inches='tight')
```



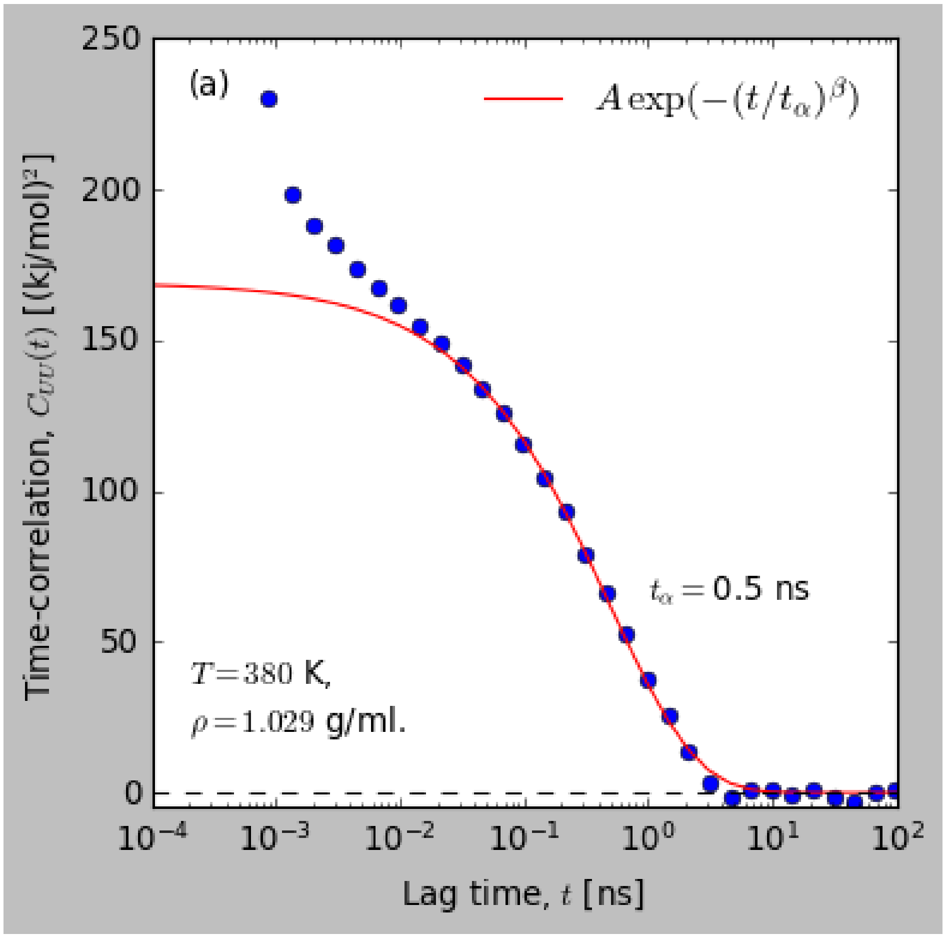
[14]:
```
C_UU = analyse.time_correlation(df.PotEng)
C_WW = analyse.time_correlation(df.c_virial)
C_WU = analyse.time_correlation(df.c_virial, df.PotEng)
```

[15]:
```
points_per_decade = 6
t_log = analyse.run_avg_log(df.Time, points_per_decade)
C_UU_log = analyse.run_avg_log(C_UU, points_per_decade)
C_WW_log = analyse.run_avg_log(C_WW, points_per_decade)
C_WU_log = analyse.run_avg_log(C_WU, points_per_decade)
```

[16]:
```
# Plot energy-energy correlation function

# Fit stretch exponential to the long-time tail of C_UU
max_y_value = 150
def stretched_exponential(t, A, beta, t_alpha):
    return A*np.exp(-(t/t_alpha)**beta)
# Find long tail data
long_tail = C_UU_log < max_y_value
```

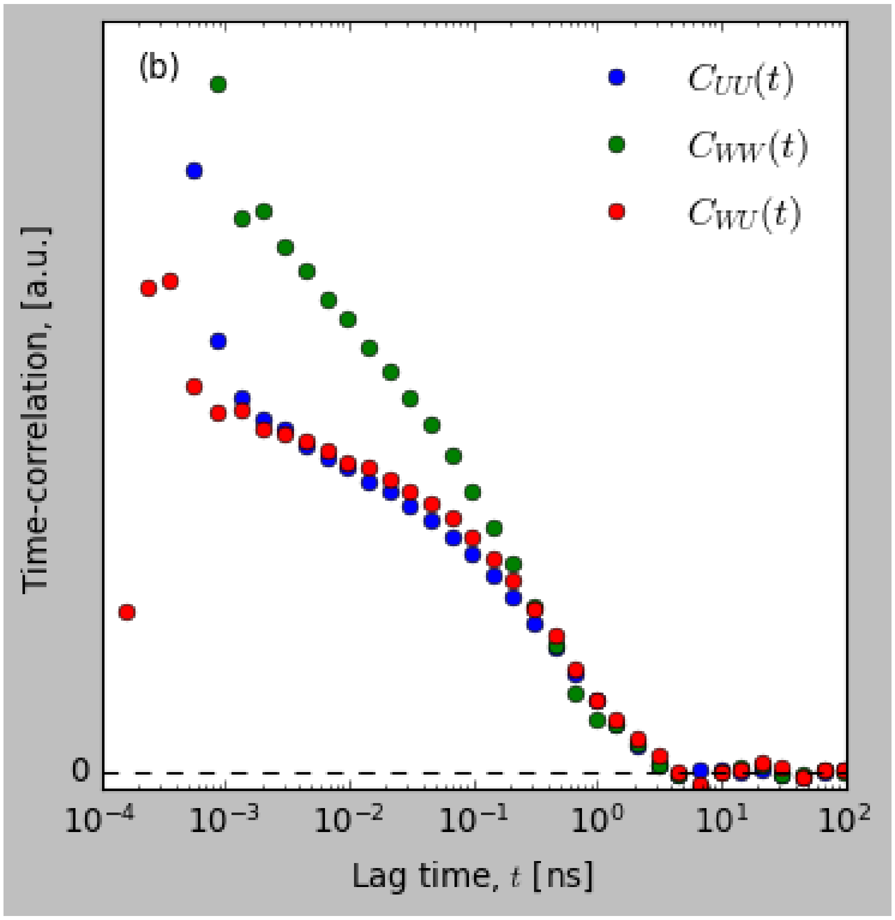
```
pguess = [150, 0.8, 0.8]
popt, pcov = scipy.optimize.curve_fit(stretched_exponential,␣
 ↪t_log[long_tail]*1e9, C_UU_log[long_tail], p0=pguess)
print(popt)
A, beta, t_alpha = popt


# Plot energy-energy correlation function
plt.figure(figsize=(5, 5))
plt.plot(t_log*1e9, C_UU_log, 'bo')
#plt.plot(t_log*1e9, stretched_exponential(t_log*1e9, *pguess), 'r--',␣
 ↪label='guess')
plt.plot(t_log*1e9, stretched_exponential(t_log*1e9, *popt), 'r-',␣
 ↪label=r'$A\,\exp(-(t/t_\alpha)^\beta)$')
plt.xscale('log')
plt.text(t_alpha*2, A/2.5, r'$t_\alpha = $' f'{t_alpha:.1g} ns', va='center')
plt.plot([1e-4, 100], [0]*2, 'k--')
plt.ylim(-5, 250)
plt.xlim(1e-4, 100)
plt.ylabel(r'Time-correlation, $C_{UU}(t)$ [(kj/mol)$^2$]')
plt.xlabel(r'Lag time, $t$ [ns]')
plt.text(0.05, 0.1,'$T = 380$ K,' + '\n' + r'$\rho=1.029$ g/ml.', transform=plt.
 ↪gca().transAxes)
plt.text(0.05, 0.93, '(a)', transform=plt.gca().transAxes)
plt.legend(frameon=False, loc='upper right', numpoints=1)
plt.savefig('CUU_time_correlation.pdf', bbox_inches='tight')
plt.savefig('CUU_time_correlation.png', bbox_inches='tight')
plt.show()
```

```
[169.13726871   0.62187108   0.49308171]
```



[17]:

```
plt.figure(figsize=(5, 5))
plt.plot(t_log*1e9, C_UU_log/100, 'bo', label=r'$C_{UU}(t)$')
plt.plot(t_log*1e9, C_WW_log/5000, 'go', label=r'$C_{WW}(t)$')
plt.plot(t_log*1e9, C_WU_log/600, 'ro', label=r'$C_{WU}(t)$')
plt.plot([1e-4, 100], [0]*2, 'k--')
plt.xscale('log')
plt.ylim(-0.1, 4)
plt.xlim(1e-4, 100)
plt.yticks([0])
plt.text(0.05, 0.93, '(b)', transform=plt.gca().transAxes)

plt.ylabel(r'Time-correlation, [a.u.]')
plt.xlabel(r'Lag time, $t$ [ns]')
plt.legend(frameon=False, loc='upper right', numpoints=1)
plt.savefig('all_time_correlation.pdf', bbox_inches='tight')
plt.savefig('all_time_correlation.png', bbox_inches='tight')
plt.show()
```

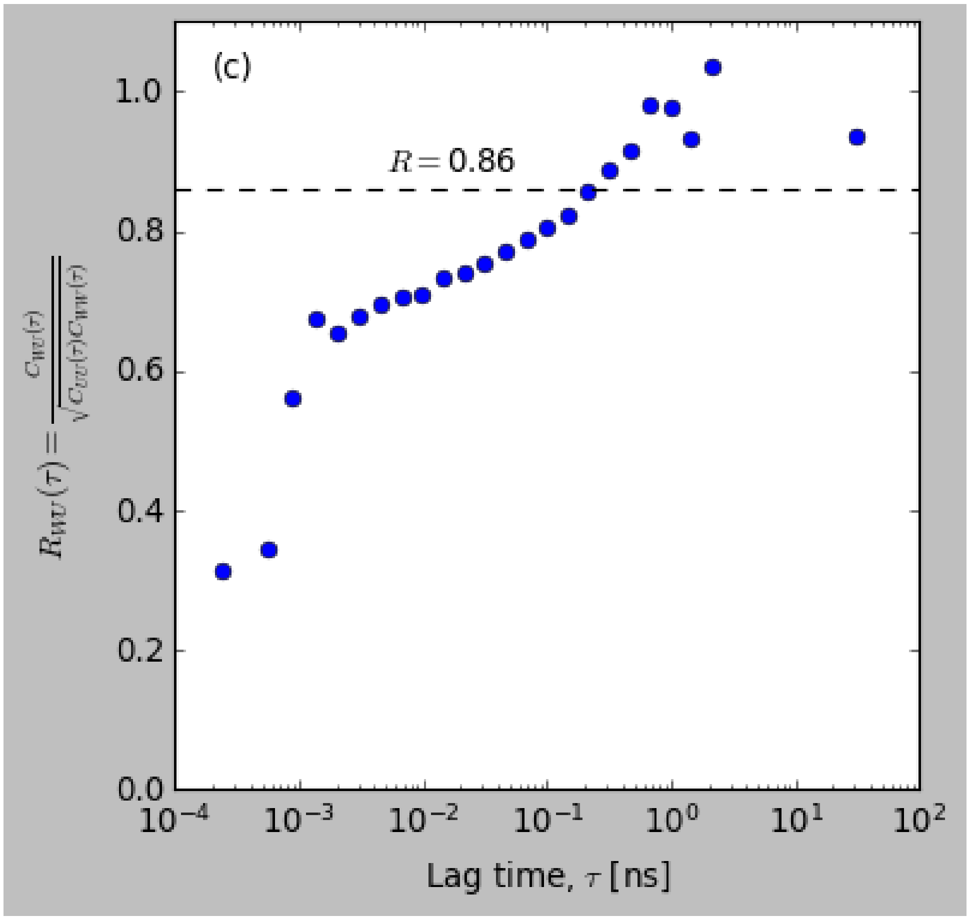


[18]:

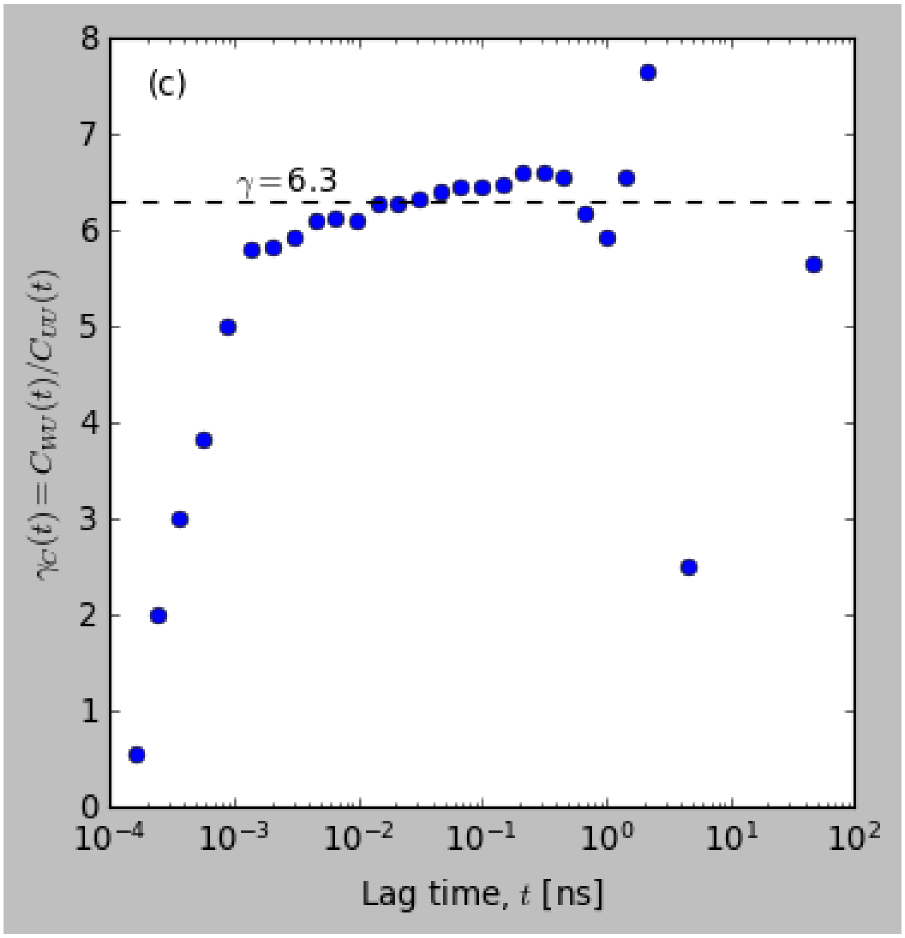
```
# Time-dependent correlation coefficient
plt.figure(figsize=(5, 5))
plt.plot(t_log*1e9, C_WU_log/np.sqrt(C_UU_log*C_WW_log), 'bo',␣
 ↪label=r'$R_{WU}(\tau)$')
plt.plot([1e-4, 100], [R_long_time]*2, 'k--')
plt.text(5e-3, 0.9, r'$R=$' f'{R_long_time}', va='center')
plt.text(0.05, 0.93, '(c)', transform=plt.gca().transAxes)

plt.xscale('log')
plt.ylim(0, 1.1)
plt.xlim(1e-4, 100)
plt.
 ↪ylabel(r'$R_{WU}(\tau)=\frac{C_{WU}(\tau)}{\sqrt{C_{UU}(\tau)C_{WW}(\tau)}}$')
plt.xlabel(r'Lag time, $\tau$ [ns]')
plt.show()
```

```
/tmp/ipykernel_9783/929768490.py:3: RuntimeWarning: invalid value encountered in
sqrt
  plt.plot(t_log*1e9, C_WU_log/np.sqrt(C_UU_log*C_WW_log), 'bo',
```

```
label=r'$R_{WU}(\tau)$')
```



[19]:
```
# Time-dependent scaling exponent
plt.figure(figsize=(5, 5))
plt.plot(t_log*1e9, C_WU_log/C_UU_log, 'bo', label=r'$\gamma_{WU}(\tau)$')
plt.plot([1e-4, 100], [gamma_long_time]*2, 'k--')
plt.text(1e-3, gamma_long_time+0.2, r'$\gamma = $' f'{gamma_long_time}',␣
↪va='center')
plt.xscale('log')
plt.text(0.05, 0.93, '(c)', transform=plt.gca().transAxes)
plt.ylim(0, 8)
plt.xlim(1e-4, 100)
plt.ylabel(r'$\gamma_{C}(t)=C_{WU}(t)/C_{UU}(t)$')
plt.xlabel(r'Lag time, $t$ [ns]')
plt.savefig('gamma_WU_time_correlation.pdf', bbox_inches='tight')
plt.savefig('gamma_WU_time_correlation.png', bbox_inches='tight')
plt.show()
```

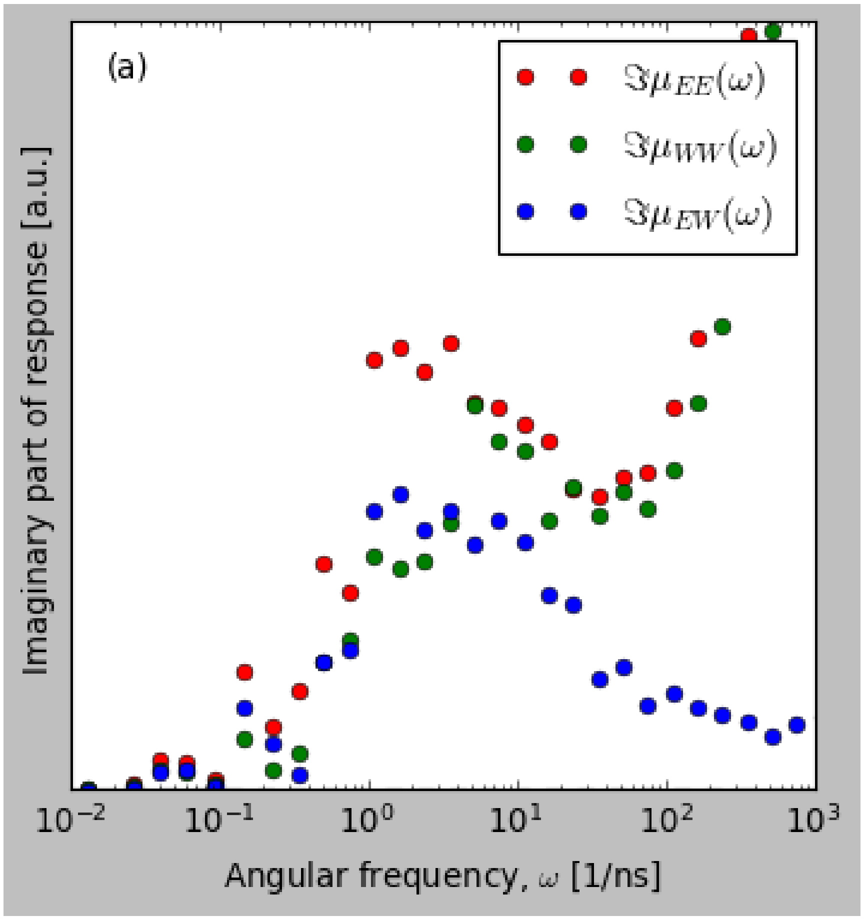


[20]:
```
dt = float(df.reset_index().Time[1] - df.reset_index().Time[0])*1e9  # Time␣
↪step in ns
omega, mu_EE = analyse.frequency_dependent_response(df.PotEng, df.PotEng, dt=dt)
_, mu_WW = analyse.frequency_dependent_response(df.c_virial, df.c_virial, dt=dt)
_, mu_EW = analyse.frequency_dependent_response(df.PotEng, df.c_virial, dt=dt)
```

[21]:
```
points_per_decade = 6
omega_log = analyse.run_avg_log(omega, points_per_decade)
mu_EE_log = analyse.run_avg_log(mu_EE, points_per_decade)
mu_WW_log = analyse.run_avg_log(mu_WW, points_per_decade)
mu_EW_log = analyse.run_avg_log(mu_EW, points_per_decade)
```

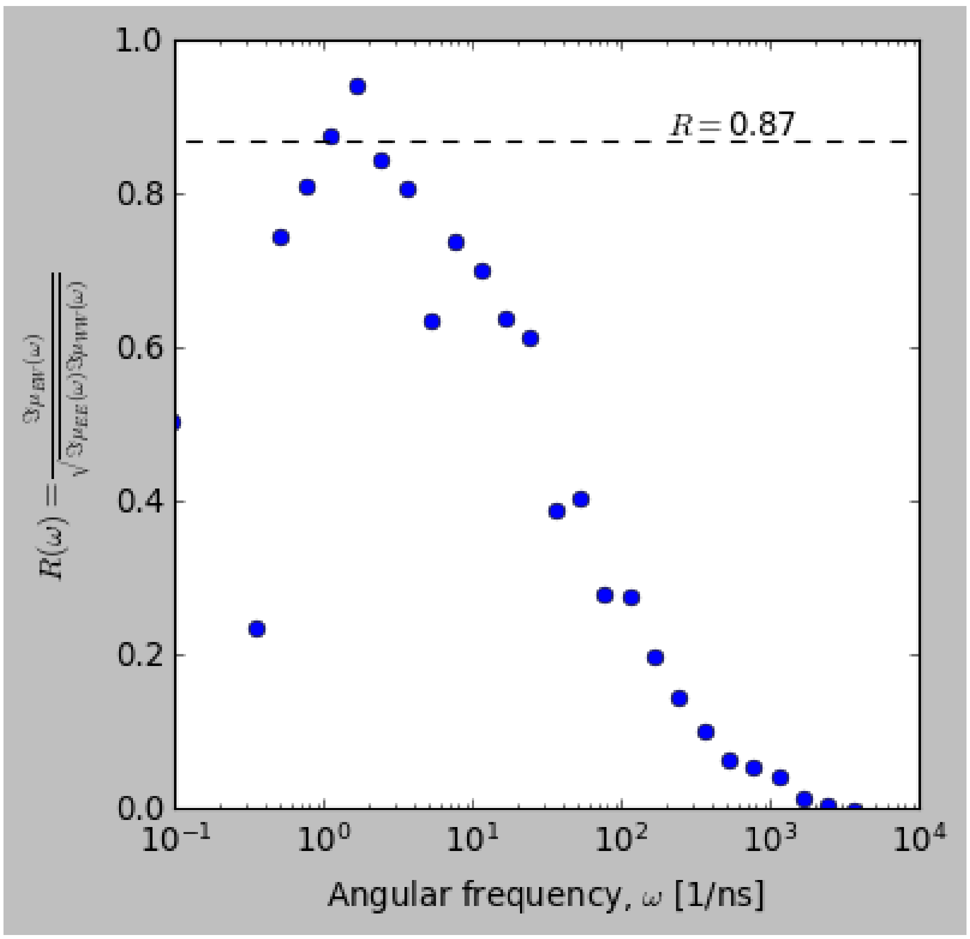
[22]:
```
# Plot frequency-dependent response
plt.figure(figsize=(5, 5))
plt.plot(omega_log, np.imag(mu_EE_log)/100, 'ro',␣
↪label=r'$\Im\mu_{EE}(\omega)$')
plt.plot(omega_log, np.imag(mu_WW_log)/10000, 'go',␣
↪label=r'$\Im\mu_{WW}(\omega)$')
```

```
plt.plot(omega_log, np.imag(mu_EW_log)/1000, 'bo',␣
    ↪label=r'$\Im\mu_{EW}(\omega)$')
plt.plot([0, 1e13], [0, 0], 'k--')
plt.xlim(1e-2,1e3)
plt.ylim(0, 1)
plt.yticks([])
plt.text(0.05, 0.93, '(a)', transform=plt.gca().transAxes)
plt.xscale('log')
plt.xlabel(r'Angular frequency, $\omega$ [1/ns]')
plt.ylabel(r'Imaginary part of response [a.u.]')
plt.legend()
plt.savefig('all_response.pdf', bbox_inches='tight')
plt.savefig('all_response.png', bbox_inches='tight')
plt.show()
```



[23]:
```
# Plot frequency-dependent correlation coefficient
plt.figure(figsize=(5, 5))
plt.plot(omega_log, np.imag(mu_EW_log)/np.sqrt(np.imag(mu_EE_log)*np.
    ↪imag(mu_WW_log)), 'bo', label=r'$R(\omega)$')
```

```
R_long_time = 0.87
plt.plot([1e-2, 1e4], [R_long_time]*2, 'k--')
plt.text(2e2, R_long_time+0.02, r'$R=$' f'{R_long_time}', va='center')
plt.xlim(1e-1,1e4)
plt.ylim(0, 1)
plt.xscale('log')
plt.xlabel(r'Angular frequency, $\omega$ [1/ns]')
plt.
 ↪ylabel(r'$R(\omega)=\frac{\Im\mu_{EW}(\omega)}{\sqrt{\Im\mu_{EE}(\omega)\Im\mu_{WW}(\omega)

plt.show()
```



[24]:
```
# Plot the frequency dependent scaling exponent
plt.figure(figsize=(5, 5))
plt.plot(omega_log, np.imag(mu_EW_log)/np.imag(mu_EE_log), 'bo',␣
 ↪label=r'$\gamma(\omega)$')
plt.plot([1e-2, 1e4], [gamma_long_time]*2, 'k--')
```

```
plt.text(2e2, gamma_long_time+0.2, r'$\gamma=$' f'{gamma_long_time}',␣
 ↪va='center')
plt.text(0.05, 0.93, '(b)', transform=plt.gca().transAxes)
plt.xlim(1e-1,1e4)
plt.ylim(0, 8)
plt.xscale('log')
plt.xlabel(r'Angular frequency, $\omega$ [1/ns]')
plt.ylabel(r'$\gamma(\omega)=\frac{\Im\mu_{EW}(\omega)}{\Im\mu_{EE}(\omega)}$')
plt.savefig('gamma_WU_response.pdf', bbox_inches='tight')
plt.savefig('gamma_WU_response.png', bbox_inches='tight')
plt.show()
```