Full analysis trajectory_using_Dyacine_do_not_touch

September 3, 2021

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib as mpl
from scipy.io import loadmat, savemat
from mpl_toolkits.mplot3d import Axes3D
from scipy.optimize import curve_fit, minimize, least_squares
from scipy.integrate import trapz
from scipy.stats import norm, kurtosis
from matplotlib.ticker import ScalarFormatter
```

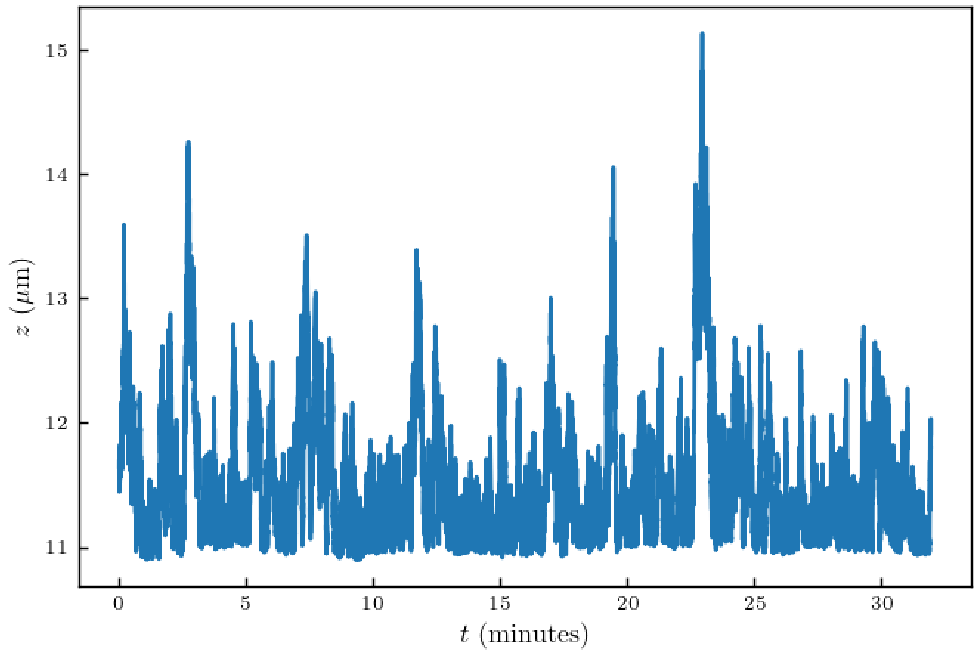
[2]:
```
mpl.rcParams["xtick.direction"] = "in"
mpl.rcParams["ytick.direction"] = "in"
mpl.rcParams["lines.markeredgecolor"] = "k"
mpl.rcParams["lines.markeredgewidth"] = 0.1
mpl.rcParams["figure.dpi"] = 130
from matplotlib import rc
rc('font', family='serif')
rc('text', usetex=True)
rc('xtick', labelsize='x-small')
rc('ytick', labelsize='x-small')
def cm2inch(value):
    return value/2.54
```

We load the data

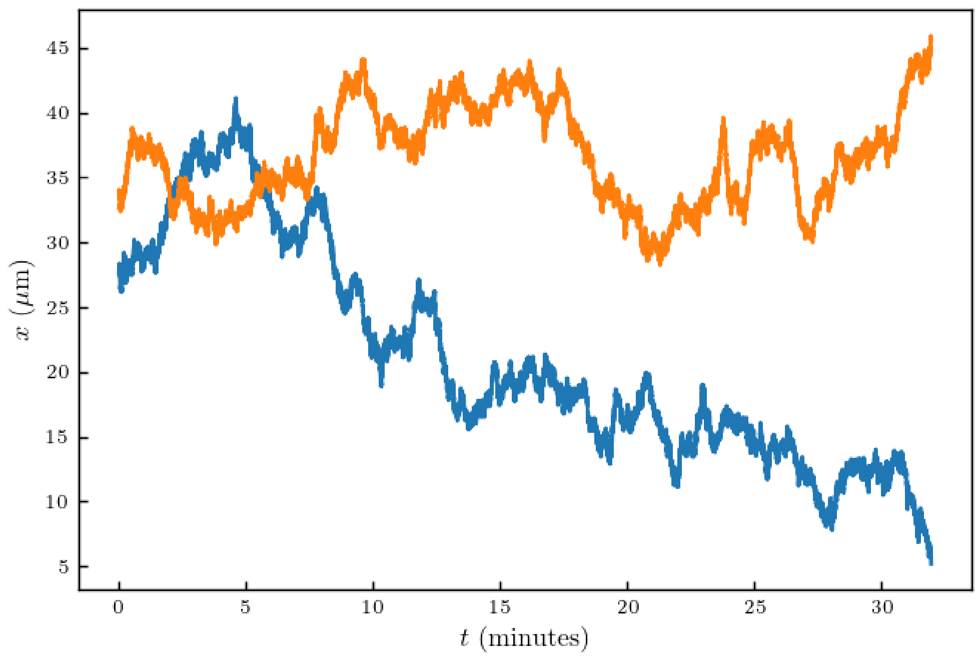
[3]:
```
raw_data = loadmat('../data/
 ↪fit_result_dur_27052020_n_r_fix_0p0513_wav_532_r_1p516_n_1.597.
 ↪mat')["data"][:,0:3]
r = 1.516*1e-6
n_part =  1.597
fps = 60
time = np.arange(0,np.shape(raw_data)[0])/fps
dataset={}
dataset["r"] = r
dataset["n"] = n_part
dataset["fps"] = fps
dataset["time"] = time
```

1 Data exploration

[4]:
```
# We put everything in microns
raw_data_m = raw_data
raw_data_m[:,0:3] = raw_data_m[:,0:3] * 0.0513
plt.plot(time/60, raw_data_m[:,2])
x = raw_data_m[:,0]
y = raw_data_m[:,1]
z = raw_data_m[:,2]

plt.xlabel("$t$ (minutes)")
plt.ylabel("$z$ ($\mathrm{\mu m}$)")
plt.show()
```



[5]:
```
plt.plot(time/60, raw_data_m[:,0], label="x")
plt.plot(time/60, raw_data_m[:,1], label="y")
plt.xlabel("$t$ (minutes)")
plt.ylabel("$x$ ($\mathrm{\mu m}$)")
plt.show()
```



2 MSD

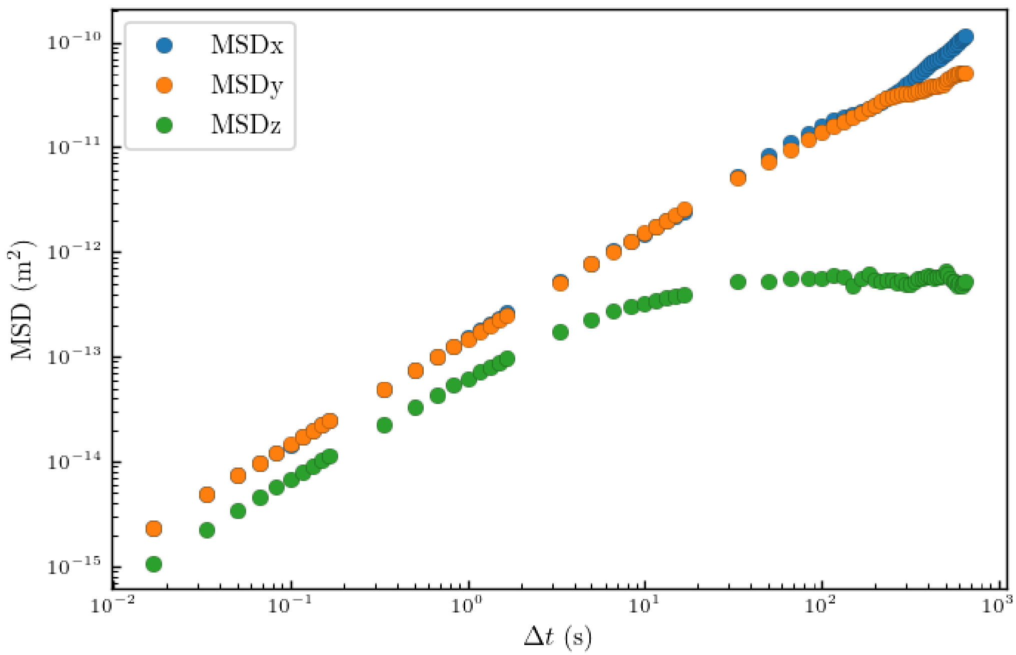
We compute the MSD using the formula:

$$\langle \Delta r_i(t)^2 \rangle_t = \langle [r_i(t + \Delta t) - r_i(t)]^2 \rangle_t \ . \tag{1}$$

[6]:
```
def MSD(x, t):
    MSD = np.zeros(len(t))
    for n,i in enumerate(t):
        MSD[n] = np.nanmean((x[0:-i] - x[i:]) ** 2)
    return MSD
```

[7]:
```
t = np.concatenate((np.arange(1,10, 1),np.arange(10,100, 10), np.
 ↪arange(100,1000, 100),np.arange(1000,40000, 1000)))
MSD_x = MSD(x*1e-6, t) # m² conversion
MSD_y = MSD(y*1e-6, t)
MSD_z = MSD(z*1e-6, t)


plt.loglog(time[t],MSD_x,"o", label = "MSDx")
plt.plot(time[t],MSD_y,"o", label = "MSDy")
plt.plot(time[t],MSD_z,"o", label = "MSDz")
plt.ylabel("MSD ($\mathrm{m^2}$)")
plt.xlabel("$\Delta t$ (s)")
```

```
plt.legend()

dataset["MSD_x_tot"] = MSD_x
dataset["MSD_y_tot"] = MSD_y
dataset["MSD_z_tot"] = MSD_z
dataset["MSD_time_tot"] = time[t]
```



We fit the short time MSD with and average diffusion coefficient such as:

$$\langle \Delta r_i(t)^2 \rangle_t = 2 \langle D_i \rangle \Delta t \ , \tag{2}$$

[8]:
```
Do = 4e-21/(6 * np.pi * 0.001 * r)
f = lambda x,a,noiselevel : 2 * Do * a * x + (noiselevel * 1e-9) ** 2
popt_1 , pcov_1 = curve_fit(f,time[t[0:5]],MSD_x[0:5], p0 = [1, 30])
popt_2 , pcov_1 = curve_fit(f,time[t[0:5]],MSD_y[0:5], p0 = [1, 30])
popt_3 , pcov_1 = curve_fit(f,time[t[0:5]],MSD_z[0:5], p0 = [1, 30])

dataset["x_MSD_fit"] = time[t[0:5]]

dataset["MSD_x"] = MSD_x[0:5]
dataset["MSD_y"] = MSD_y[0:5]
dataset["MSD_z"] = MSD_z[0:5]
```

```
C:\Users\m.lavaud\.conda\envs\holopy\lib\site-
```

```
packages\scipy\optimize\minpack.py:828: OptimizeWarning: Covariance of the
parameters could not be estimated
  warnings.warn('Covariance of the parameters could not be estimated',
```

[9]:
```
print("We measure a reduced mean diffusion coefficient of {:.3f} for the␣
↪perpendicular motion and of {:.3f} for the parallel motion".
↪format((popt_1[0]+popt_2[0])/2, popt_3[0]))
```

```
We measure a reduced mean diffusion coefficient of 0.522 for the perpendicular
motion and of 0.243 for the parallel motion
```

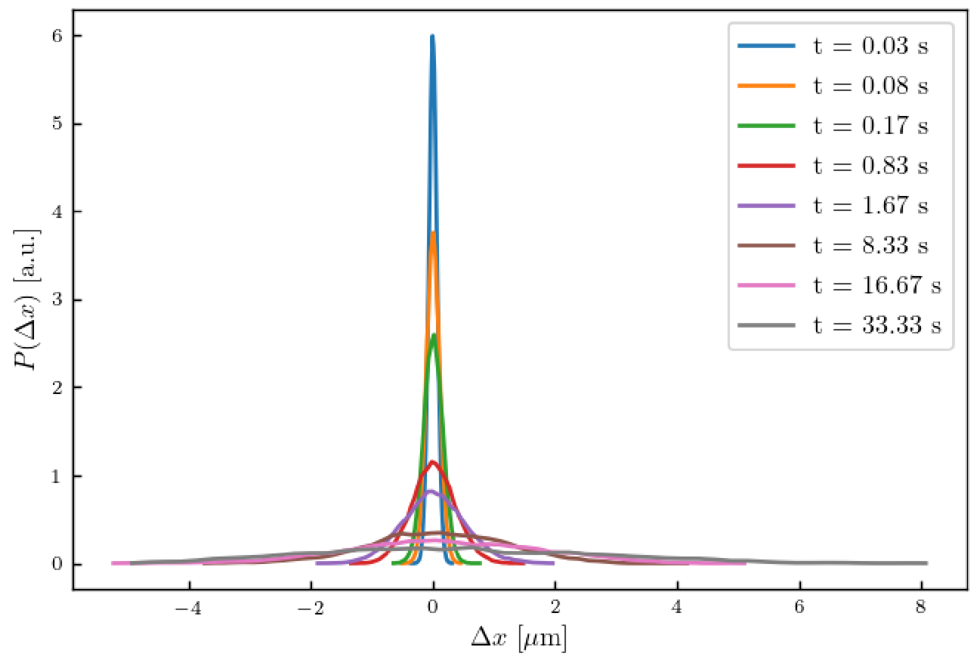
3 Displacement distributions

3.1 Δx distributions

[10]:
```
def pdf(data, bins = 10, density = True):
    """
    function to automatize the computations of experimental probability density␣
↪functions.
    """

    pdf, bins_edge = np.histogram(data, bins = bins, density = density)
    bins_center = (bins_edge[0:-1] + bins_edge[1:]) / 2

    return pdf, bins_center
```

[11]:
```
I = [2, 5 , 10, 50 ,100,500, 1000,2000]

for i in I:

    Dezs = x[0:-i] - x[i:]
    hist, bins_center = pdf(Dezs, bins = 50)

    plt.plot(bins_center, hist, label = " t = {:.2f} s".format(time[i]))

plt.legend()
plt.ylabel("$P(\Delta x)$ [a.u.]")
plt.xlabel("$\Delta x$ [$\mathrm{\mu m}$]")
```

[11]:
```
Text(0.5, 0, '$\\Delta x$ [$\\mathrm{\\mu m}$]')
```



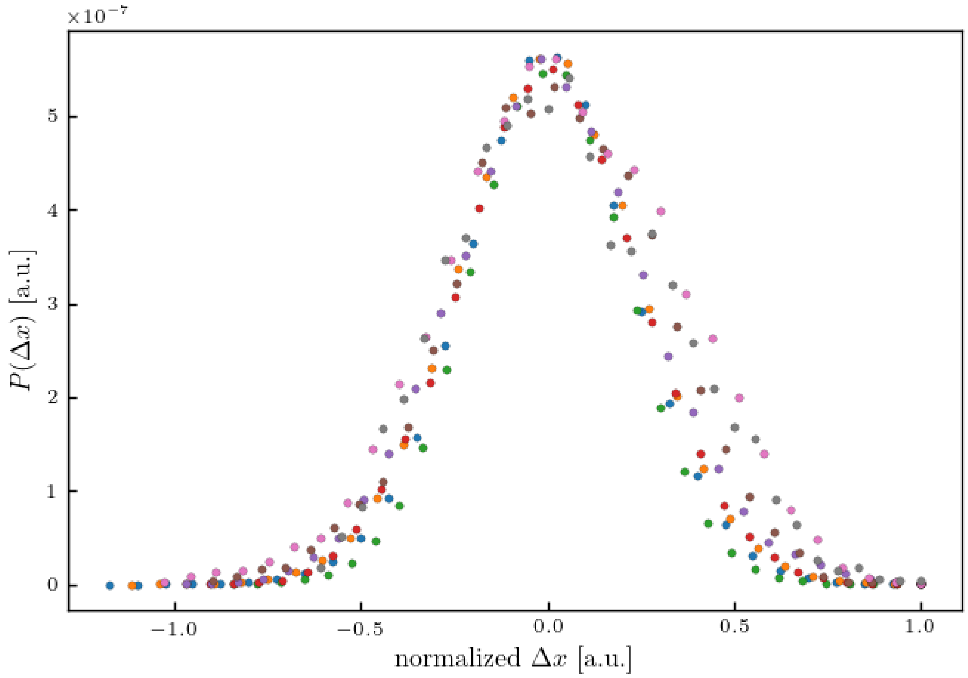
If we now normalize by the standard deviation

[12]:
```
def gauss_function(x, a, x0, sigma):
    return a*np.exp(-(x-x0)**2/(2*sigma**2))
```

[13]:
```
for n,i in enumerate(I):

    Dezs = (x[0:-i] - x[i:])
    Dezs = Dezs / np.sqrt(2 * Do * time[i])
    hist, bins_center = pdf(Dezs, bins = 30)

    #if i == I[0]:
    #    popt, pcov = curve_fit(gauss_function, bins_center/np.
 ↪max(bins_center), hist, p0 = [1, np.mean(hist), np.std(hist)])
    #    plt.plot(bins_center/np.max(bins_center), gauss_function(bins_center,␣
 ↪*popt), label = "fit at t = {:.2f} s".format(time[i]))
    #    plt.plot(bins_center/np.max(bins_center), hist, "x",label = " t = {:.
 ↪2f} s".format(time[i]),color = "tab:blue")
    #    continue

    plt.plot(bins_center/np.max(bins_center), hist, ".",label = " $Delta$t = {:.
 ↪2f} s".format(time[i]))



plt.ylabel("$P(\Delta x)$ [a.u.]")
```

```
plt.xlabel("normalized $\Delta x$ [a.u.]")
```

[13]: Text(0.5, 0, 'normalized $\\Delta x$ [a.u.]')



[14]:
```
(3.5e-22)**(1/3)
```

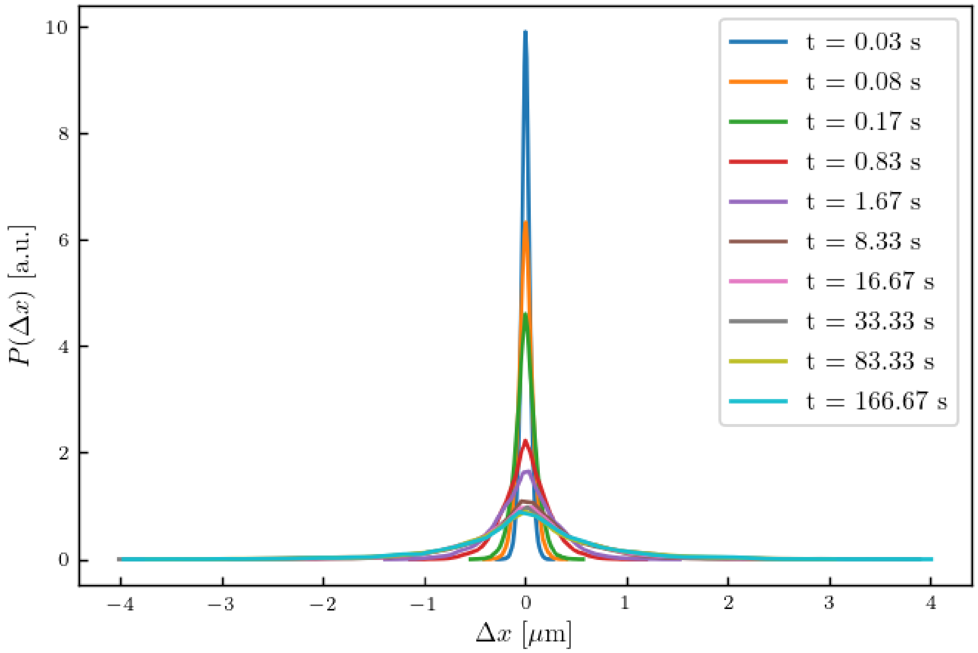
[14]: 7.047298732064899e-08

We can see a clear change but we would need to average on different trajectectories to have consitant results.

3.2 Δz distributions

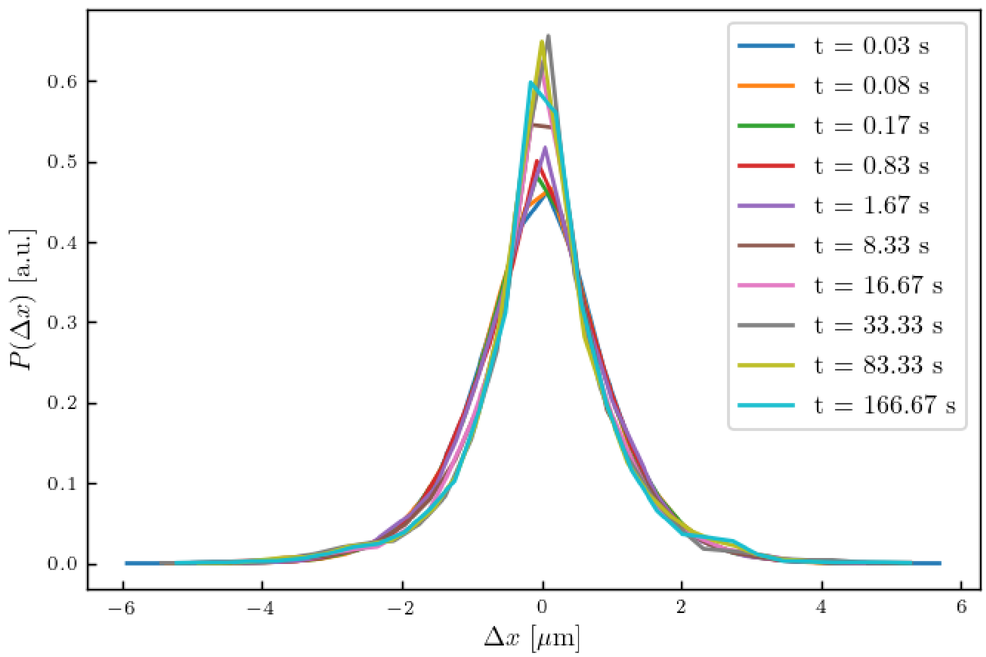
[15]:
```
I = [2, 5 , 10, 50 ,100,500, 1000, 2000, 5000, 10000]

for i in I:

    Dezs = z[0:-i] - z[i:]
    hist, bins_center = pdf(Dezs[~np.isnan(Dezs)], bins = 50)

    plt.plot(bins_center, hist, label = " t = {:.2f} s".format(time[i]))

plt.legend()
plt.ylabel("$P(\Delta x)$ [a.u.]")
plt.xlabel("$\Delta x$ [$\mathrm{\mu m}$]")
```

```
[15]: Text(0.5, 0, '$\\Delta x$ [$\\mathrm{\\mu m}$]')
```




```
[16]: for i in I:

          Dezs = (z[0:-i] - z[i:])
          Dezs = Dezs / np.nanstd(Dezs)
          hist, bins_center = pdf(Dezs[~np.isnan(Dezs)], bins = 30)

          plt.plot(bins_center, hist, label = " t = {:.2f} s".format(time[i]))

      plt.legend()
      plt.ylabel("$P(\Delta x)$ [a.u.]")
      plt.xlabel("$\Delta x$ [$\mathrm{\mu m}$]")
```

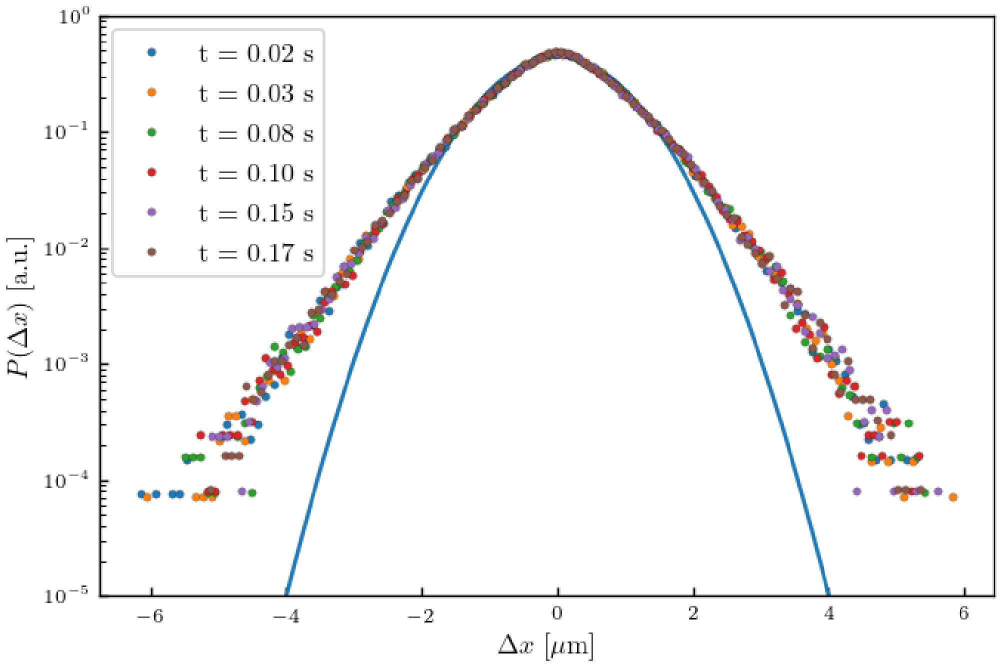
```
[16]: Text(0.5, 0, '$\\Delta x$ [$\\mathrm{\\mu m}$]')
```



3.2.1 Short time distributions

[17]:
```
I = [1,2,5,6,9,10]

for i in I:

    Dezs = (z[0:-i] - z[i:])
    Dezs = Dezs / np.std(Dezs)
    hist, bins_center = pdf(Dezs[~np.isnan(Dezs)], bins = 100)

    if i == I[0]:
        popt, pcov = curve_fit(gauss_function, bins_center, hist, p0 = [1, np.
↪mean(hist), np.std(hist)])
        plt.plot(bins_center, gauss_function(bins_center, *popt))
        plt.plot(bins_center, hist, ".",label = " t = {:.2f} s".
↪format(time[i]),color = "tab:blue")
        continue
    plt.semilogy(bins_center, hist, "." ,label = " t = {:.2f} s".
↪format(time[i]))

plt.legend()
plt.ylabel("$P(\Delta x)$ [a.u.]")
plt.xlabel("$\Delta x$ [$\mathrm{\mu m}$]")
axes = plt.gca()
axes.set_ylim([1e-5,1])
```

[17]: (1e-05, 1)



[18]:
```
popt
```

[18]: array([0.44423242, 0.00136534, 0.86463018])

The non Gaussianity is due to the fact that the diffusion coefficient vary as a funtion of the height, thus it vary during the diffusion (diffusing diffusivity) process knowing that one can write :

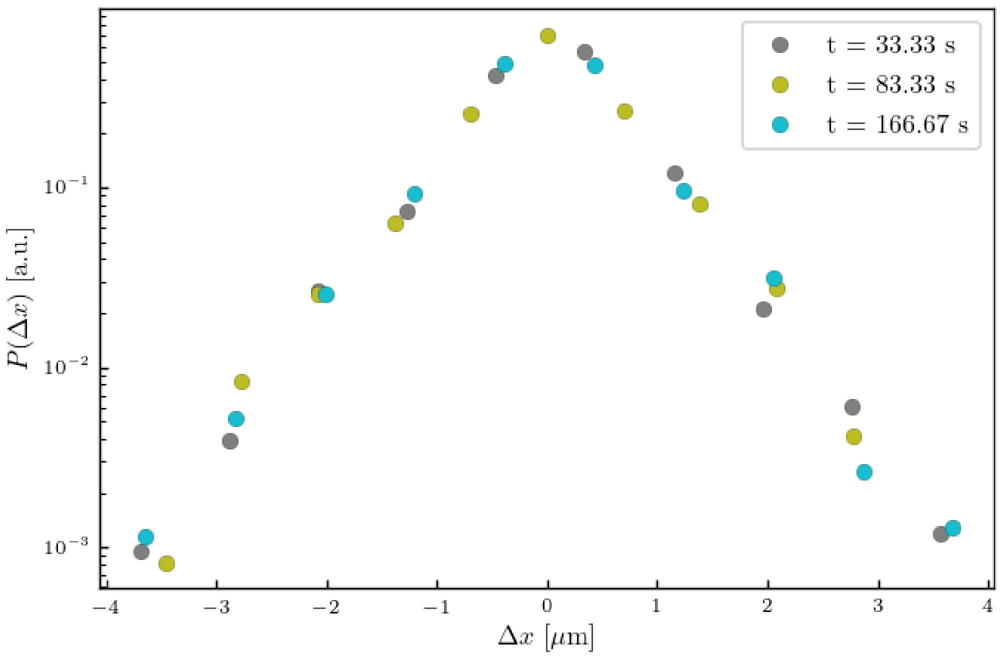
$$P(\Delta z, \Delta t) = \int_0^\infty \mathrm{d}D P(D) \frac{1}{\sqrt{4\pi D \Delta t}} \exp\left[\frac{-\Delta z^2}{4D\Delta t}\right] \quad . \tag{3}$$

3.2.2 Long time distributions

[19]:
```
I = [2000, 5000, 10000]

color_long_time = ["tab:gray","tab:olive","tab:cyan"]
for n,i in enumerate(I):

    Dezs = z[0:-i] - z[i:]
    hist, bins_center = pdf(Dezs[~np.isnan(Dezs)],  bins = 10)

    plt.semilogy(bins_center, hist, "o",label = " t = {:.2f} s".
 ↪format(time[i]), color = color_long_time[n])

plt.legend()
```

```
plt.ylabel("$P(\Delta x)$ [a.u.]")
plt.xlabel("$\Delta x$ [$\mathrm{\mu m}$]")
```

[19]: Text(0.5, 0, '$\\Delta x$ [$\\mathrm{\\mu m}$]')



Indeed at long time it becomes exponential and it's no longer dependent on Δt

At very long time intervals Δt each position measurment can be seen as random measurment on the le Boltzman distribution. Thus, one can write the probability distribution as :

$$P(\Delta z) = \int_{-\infty}^{\infty} dz P_B(z) P_B(z + \Delta z), \tag{4}$$

with :

$$P_B(z) = A e^{\left(B exp\left(-\frac{z}{l_d}\right) - \frac{z}{l_b}\right)} \tag{5}$$

Also, $P_B(z < 0)$

giving at long time step :

$$P(\Delta z) = A' exp\left[B exp\left[-\frac{z}{l_d}\right](1 + exp[-\frac{\Delta z}{l_d}]) - \frac{2z + \Delta z}{l_b}\right] \tag{6}$$

3.3 Analysis of pdf of the Δz at large time step

To have a better data set we are going to measure the pdf of the Δz for a lot of different time step and we arge going to average them. But first of all we need to get rid of the drifts at long time.

The best way to do that is to a moving average, taking a box long enough to assume that the mean value should be equal to the equilibrium mean value. We can estimate the time over wich we have to average with the MSD of z and the time it takes to reach the plateau. Here we will look at times > at 30s

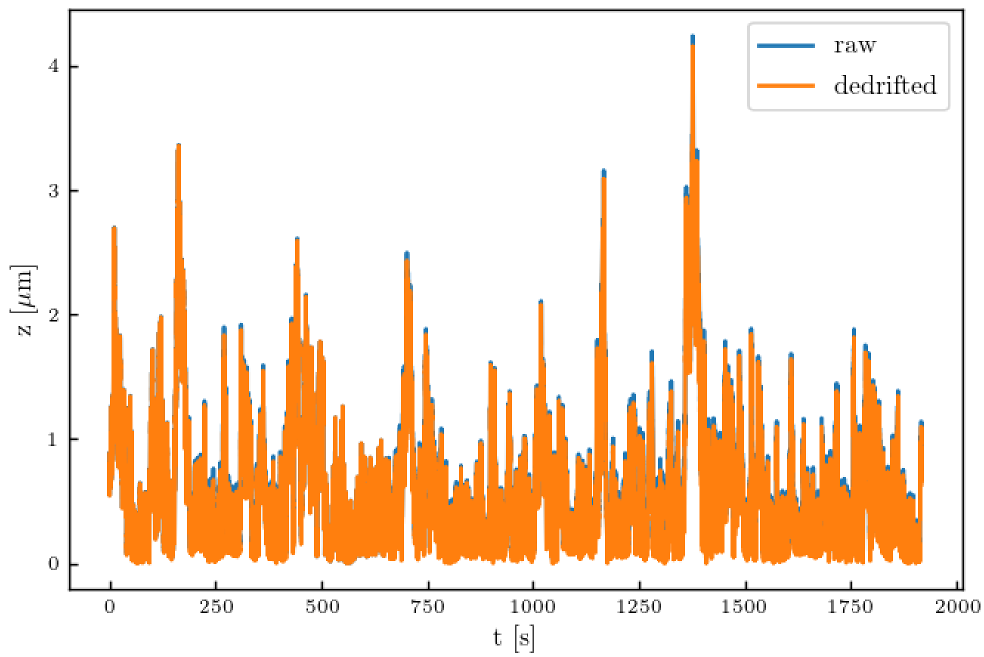
3.4 Dedrifting the z trajectory

[20]:
```
def movmin(datas, k):
    result = np.empty_like(datas)
    start_pt = 0
    end_pt = int(np.ceil(k / 2))

    for i in range(len(datas)):
        if i < int(np.ceil(k / 2)):
            start_pt = 0
        if i > len(datas) - int(np.ceil(k / 2)):
            end_pt = len(datas)
        result[i] = np.min(datas[start_pt:end_pt])
        start_pt += 1
        end_pt += 1

    return result
```

[21]:
```
z_dedrift = z - movmin(z,10000)
```

[22]:
```
# Fig for comparing the two

plt.plot(time,z-np.min(z), label = "raw")
plt.plot(time,z_dedrift, label = "dedrifted")
plt.legend()

plt.xlabel("t [s]")
plt.ylabel("z [$\mathrm{\mu m}$]")
```

[22]:
```
Text(0, 0.5, 'z [$\\mathrm{\\mu m}$]')
```

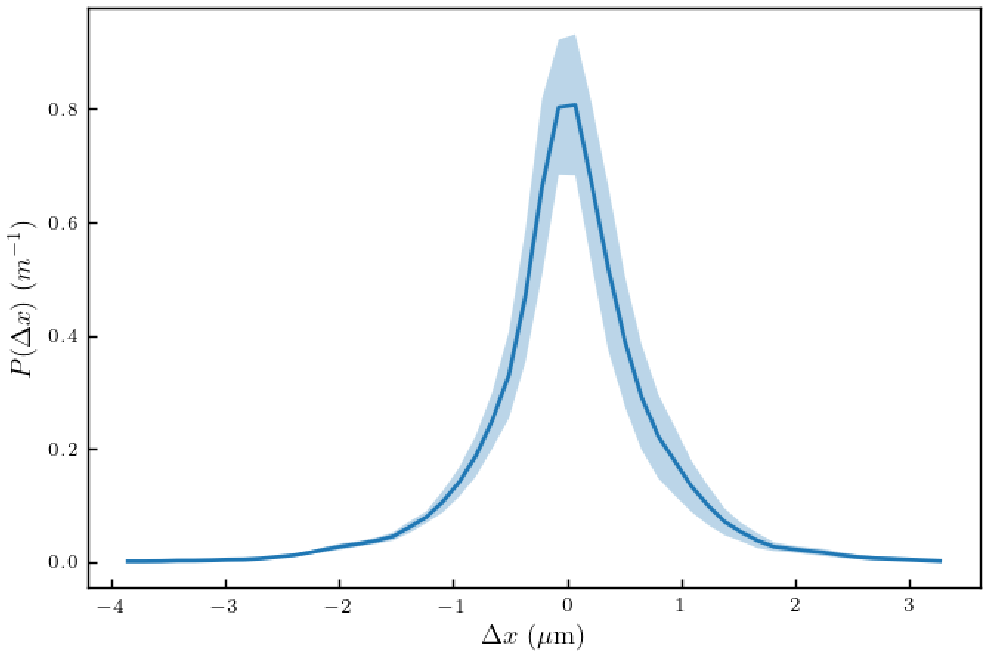


3.4.1 Measuring pdf at large Δt with the dedrifted trajectory and analysing it

[23]:
```
t_start = 25
t_end = 30
I = np.arange(t_start*fps,t_end*fps)
bins = 50

hists = np.zeros((bins,len(I)))
bins_centers = np.zeros((bins,len(I)))

for n,i in enumerate(I):

    Dezs = z_dedrift[0:-i] - z_dedrift[i:]
    hist, bins_center = pdf(Dezs[~np.isnan(Dezs)],  bins = bins)

    hists[:,n] = hist
    bins_centers[:,n] = bins_center


pdf_long_t = np.mean(hists, axis = 1)
bins_centers_long_t = np.mean(bins_centers, axis = 1)
err_long_t = np.std(hists, axis = 1)
err_bins_centers = np.std(bins_centers, axis = 1)
```

[24]:
```
plt.plot(bins_centers_long_t,pdf_long_t)
plt.fill_between(bins_centers_long_t, pdf_long_t-err_long_t,␣
 ↪pdf_long_t+err_long_t, alpha = 0.3)
plt.ylabel("$P(\Delta x)$ ($m^{-1}$)")
plt.xlabel("$\Delta x$ ($\mathrm{\mu m}$)")
```

[24]:
```
Text(0.5, 0, '$\\Delta x$ ($\\mathrm{\\mu m}$)')
```



We are now going to code the function

$$P(\Delta z) = \int_{-\infty}^{\infty} A' exp\left[Bexp\left[-\frac{z}{l_d}\right](1 + exp[-\frac{\Delta z}{l_d}]) - \frac{2z + \Delta z}{l_b}\right] \tag{7}$$

Noting that coding the form :

$$P(\Delta z) = \int_{-\infty}^{\infty} dz P_B(z) P_B(z + \Delta z), \tag{8}$$

Will be easier and P_B will be reused later on. Also since $P_B(z < 0) = 0$:

$$P(\Delta z) = \int_{0}^{\infty} dz P_B(z) P_B(z + \Delta z), \tag{9}$$

with :

$$P_B(z) = Ae^{\left(Bexp\left(-\frac{z}{l_d}\right) - \frac{z}{l_b}\right)} \tag{10}$$

[25]:
```python
def P_b(z, A, B, ld, lb):
    P_b = A * np.exp(-B * np.exp(-z / (ld)) - z / lb)
    P_b[z < 0] = 0
    return P_b

def dPdeltaz_long(z, DZ, A, B, ld, lb):
    return P_b(z, A, B, ld, lb) * P_b(z + DZ, A, B, ld, lb)

def P_computation(DZ, A, B, ld, lb):
    z = np.linspace(0, 20e-6, 1000)
    dP = dPdeltaz_long(z, DZ, A, B, ld, lb)
    P = trapz(dP,z)
    return P

def Pdeltaz_long(DZ, B, ld, lb):
    if type(DZ) == float:
        return P_computation(i, 1, B, ld, lb)

    pdf = np.array([P_computation(i, 1, B, ld*1e-9, lb*1e-9) for i in DZ])

    # normalisation of the PDF to not use A

    A = trapz(pdf,DZ*1e6)

    return np.array([P_computation(i, 1, B, ld*1e-9, lb*1e-9) for i in DZ]) / A
```

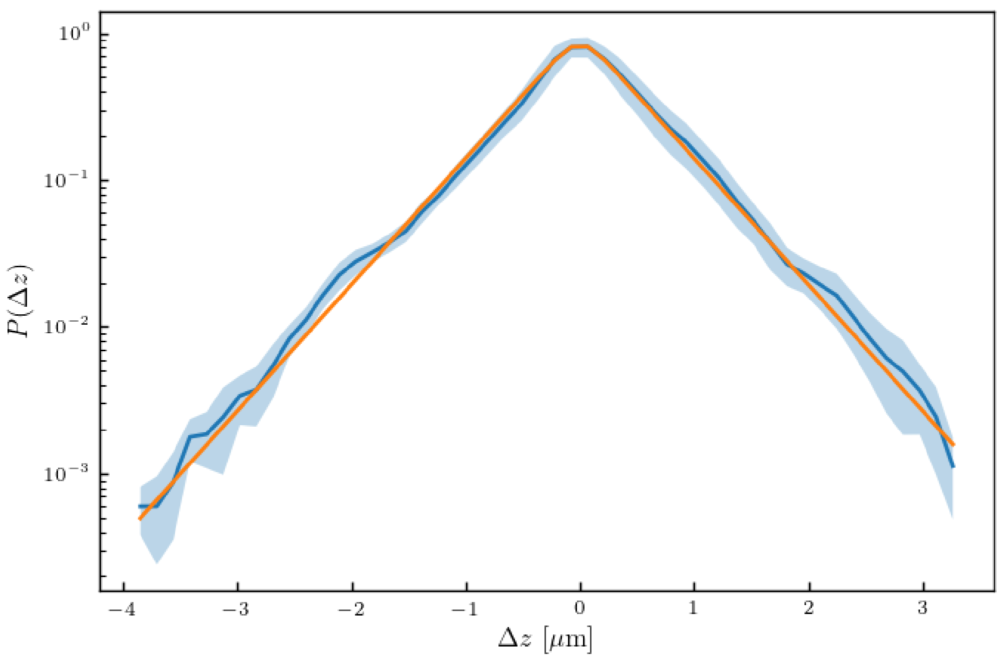
[26]:
```python
A = 0.14e8
B = 4
ld = 70
lb = 500
p1 = [B, ld, lb]

# Normalisation fo the pdf

pdf_long_t = pdf_long_t / trapz(pdf_long_t,bins_centers_long_t)


popt, pcov = curve_fit(Pdeltaz_long, bins_centers_long_t * 1e-6,pdf_long_t,p0 =␣
↪p1)
dataset["pdf_longtime"] = pdf_long_t
dataset["x_pdf_longtime"] = bins_centers_long_t * 1e-6
```

```
<ipython-input-25-da5e4a6111f0>:2: RuntimeWarning: overflow encountered in exp
  P_b = A * np.exp(-B * np.exp(-z / (ld)) - z / lb)
```

[27]:
```python
A = 0.14e8
B = 400
```

```
ld = 70
lb = 500
p0 = [B, ld, lb]


plt.semilogy(bins_centers_long_t,pdf_long_t, label = "experimantal pdf")
plt.fill_between(bins_centers_long_t, pdf_long_t-err_long_t,␣
 ↪pdf_long_t+err_long_t, alpha = 0.3)

plt.plot(bins_centers_long_t,Pdeltaz_long(bins_centers_long_t*1e-6, *popt),␣
 ↪label = "fit")
plt.ylabel("$P(\Delta z)$")
plt.xlabel("$\Delta z$ [$\mathrm{\mu m}$]")
```

[27]: Text(0.5, 0, '$\\Delta z$ [$\\mathrm{\\mu m}$]')



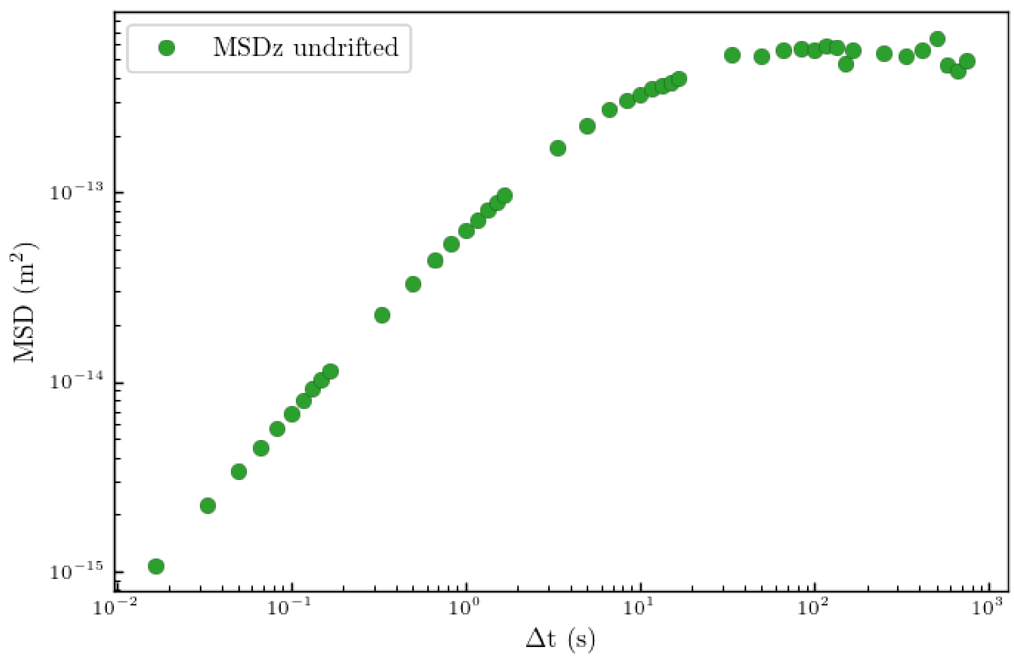
[28]:
```
print("We measure, B = {:.2f}, ld = {:.2f} nm, lb = {:.2f} nm".format(*popt))
B, ld, lb = popt
```

We measure, B = 20.71, ld = 71.84 nm, lb = 504.78 nm

3.5 Analyse of the MSD z plateau

[29]:
```
t = np.concatenate((np.arange(1,10, 1),np.arange(10,100, 10), np.
↪arange(100,1000, 100),np.arange(1000,10000, 1000),np.arange(10000,50000,␣
↪5000)))

MSD_z_dedrift = MSD(z_dedrift*1e-6, t)

plt.loglog(time[t],MSD_z_dedrift,"o", label = "MSDz undrifted", color = "tab:
↪green")
plt.legend()
plt.ylabel("MSD (m$^2$)")
plt.xlabel("$\Delta$t (s)")
```

[29]:
```
Text(0.5, 0, '$\\Delta$t (s)')
```

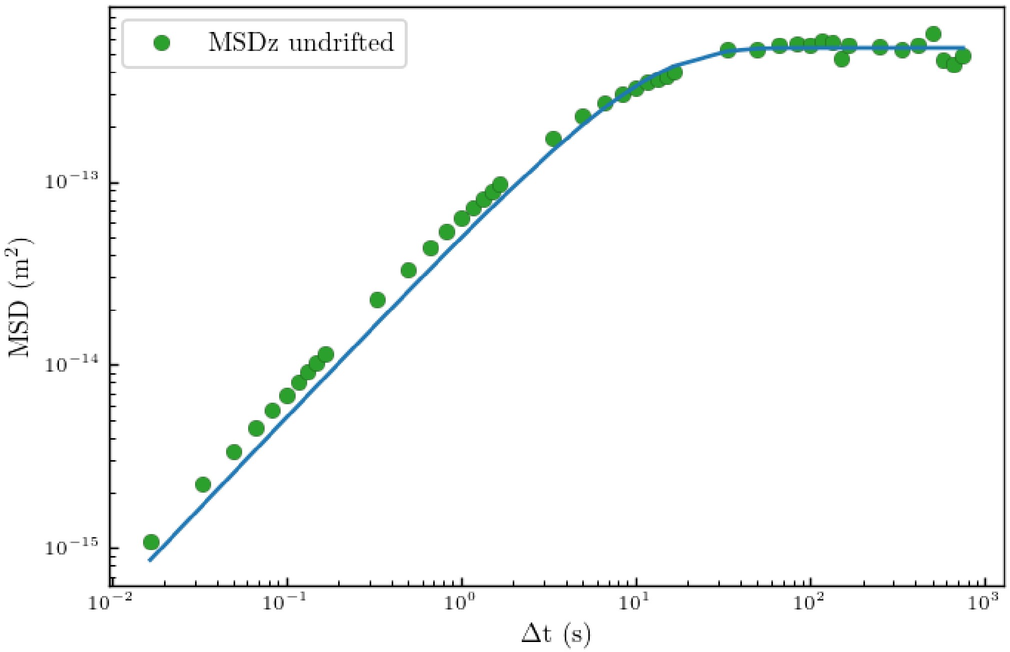


[30]:
```
def func_plateau(x,P,tau):
    return P * (1 - np.exp(-x/tau))

popt, pcov = curve_fit(func_plateau, time[t], MSD_z_dedrift, p0 = [1e-12, 100])
```

[31]:
```
plt.loglog(time[t],MSD_z_dedrift,"o", label = "MSDz undrifted", color = "tab:
↪green")
plt.plot(time[t], func_plateau(time[t], *popt))
plt.legend()
```

```
plt.ylabel("MSD (m$^2$)")
plt.xlabel("$\Delta$t (s)")
```

[31]: Text(0.5, 0, '$\\Delta$t (s)')



[32]:
```
np.mean(MSD_z_dedrift[time[t]>1e2])
```

[32]: 5.348018604759325e-13

[33]:
```
#dataset["plateau_MSD"] = popt[0]
dataset["plateau_MSD"] =np.mean(MSD_z_dedrift[time[t]>1e2])
print("Measured plateau : {:e}".format(popt[0]))
```

Measured plateau : 5.387309e-13

The MSD plateau is theoritically given by:

$$Plateau = \int_{-\infty}^{+\infty} \Delta z^2 P_{\Delta z, t \to +\infty}(\Delta z, B, l_d, l_b) d\Delta z \tag{11}$$

[34]:
```
x_Th_Plateau = bins_centers_long_t*1e-6

def Theoritical_Plateau(B,ld,lb):
    x = dataset["x_pdf_longtime"]
    P = Pdeltaz_long(x, B, ld, lb) / trapz(Pdeltaz_long(x, B, ld, lb),x)
```

```
    res = trapz((x ** 2) * P,x)
    return res
```

[35]:
```
def minimize_plateau(x):
    B = x[0]
    ld = x[1]
    lb = x[2]
    return (np.log(Theoritical_Plateau(B,ld,lb)) - np.
 ↪log(dataset["plateau_MSD"])) ** 2 / np.log(Theoritical_Plateau(B,ld,lb))**2
```

[36]:
```
res_plateau = minimize(minimize_plateau,x0=[B,ld,lb])
print("We measure, B = {:.2f}, ld = {:.2f} nm, lb = {:.2f} nm".
 ↪format(*res_plateau.x))
```

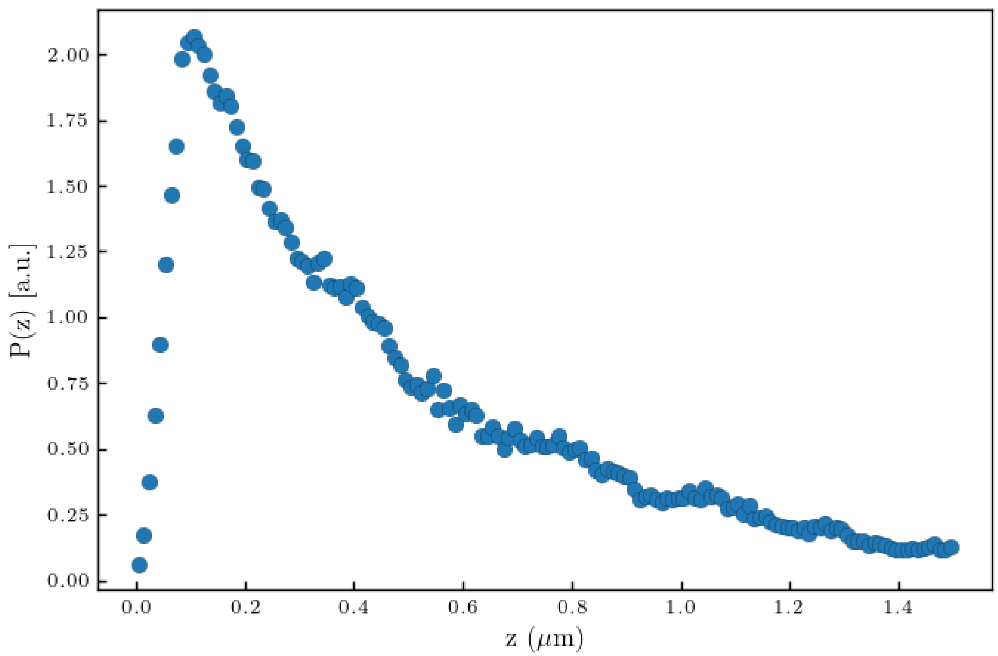
```
We measure, B = 20.71, ld = 71.84 nm, lb = 504.78 nm
```

3.6 PDF of heights

[37]:
```
def logarithmic_hist(data,begin,stop,num = 50,base = 2):

    if begin == 0:
        beg = stop/num
        bins = np.logspace(np.log(beg)/np.log(base), np.log(stop)/np.log(base),␣
 ↪num-1, base=base)
        widths = (bins[1:] - bins[:-1])
        bins = np.cumsum(widths[::-1])
        bins = np.concatenate(([0],bins))
        widths = (bins[1:] - bins[:-1])

    else:
        bins = np.logspace(np.log(begin)/np.log(base), np.log(stop)/np.
 ↪log(base), num, base=base)
        widths = (bins[1:] - bins[:-1])

    hist,bins = np.histogram(data, bins=bins,density=True)
    # normalize by bin width
    bins_center = (bins[1:] + bins[:-1])/2

    return bins_center,widths, hist
```

[38]:
```
pdf_z, bins_center_pdf_z = pdf(z_dedrift[z_dedrift < 1.5],  bins = 150)
plt.plot(bins_center_pdf_z,pdf_z, "o")
plt.xlabel("z ($\mathrm{\mu m}$)")
plt.ylabel("P(z) [a.u.]")
```

[38]:
```
Text(0, 0.5, 'P(z) [a.u.]')
```



The idea now is to find where the substrate is, to do this we will use a first method which consist to adjust the PDF with an offset to make it fit with the measured mean Diffusion coefficient. With :

$$< D_i >= \int_{-\infty}^{\infty} dz D_i(z) P(z) \tag{12}$$

For z we are going to use the Padé approx :

$$D_z(z) \approx D_0 \left(\frac{6z^2 + 2rz}{6z^2 + 9rz + 2r^2} \right) \tag{13}$$

For x we are going to use the Faxen formula :

$$D_x(z) \approx D_0 \left[1 - \frac{9}{16} \left(\frac{r}{z} \right) + \frac{1}{8} \left(\frac{r}{z} \right)^3 - \frac{45}{236} \left(\frac{r}{z} \right)^4 - \frac{1}{16} \left(\frac{r}{z} \right)^5 \right] \tag{14}$$

To do this we will fit the PDF with an offset, adjust it with the mean value of z. Let's first do it over z

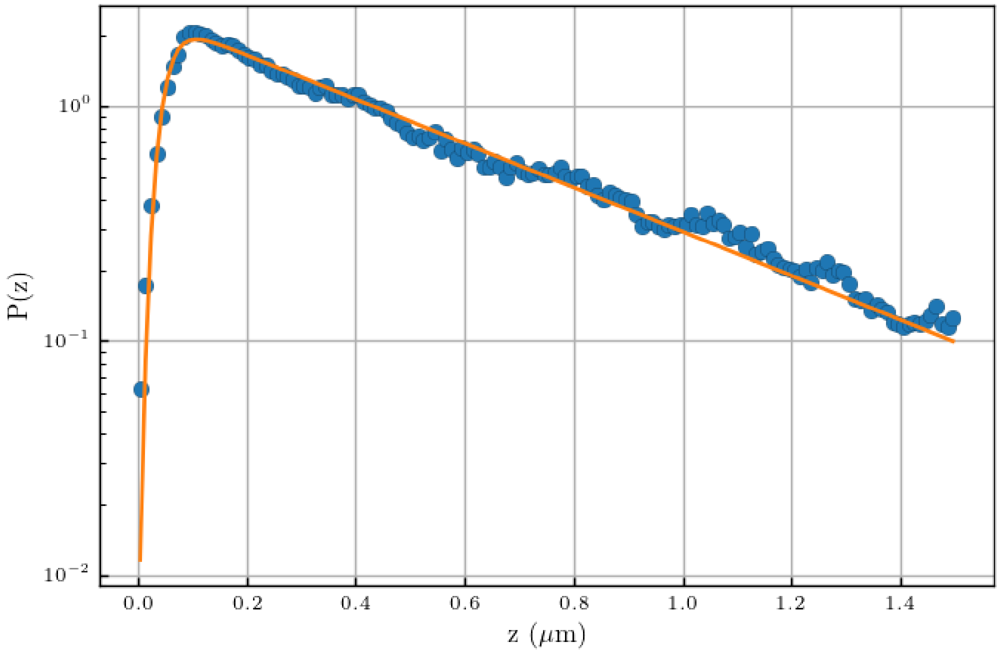
[39]:
```
def P_b_off(z,z_off,  B, ld, lb):
    z_off = z_off * 1e-6
    lb = lb * 1e-9
    ld = ld * 1e-9
    z = z - z_off
    P_b = np.exp(-B * np.exp(-z / (ld)) - z / lb)
    P_b[z < 0] = 0
```

```python
    # Normalization of P_b

    A = trapz(P_b,z * 1e6)
    P_b = P_b / A


    return P_b
```

[40]:
```python
#Normalization of the PDF

pdf_z = pdf_z / trapz(pdf_z,bins_center_pdf_z)


p2 = [0,B, ld, lb]

popt, pcov = curve_fit(P_b_off, bins_center_pdf_z * 1e-6,pdf_z, p0 = p2)
```

```
<ipython-input-39-635051e60521>:6: RuntimeWarning: overflow encountered in exp
  P_b = np.exp(-B * np.exp(-z / (ld)) - z / lb)
<ipython-input-39-635051e60521>:12: RuntimeWarning: invalid value encountered in
true_divide
  P_b = P_b / A
```

[41]:
```python
plt.semilogy(bins_center_pdf_z,pdf_z, "o")
plt.plot(bins_center_pdf_z,P_b_off(bins_center_pdf_z*1e-6,*popt))

plt.xlabel("z $\mathrm{(\mu m)}$")
plt.ylabel("P(z)")
plt.grid()
```



[42]:
```
mean_Dx = (popt_1[0]+popt_2[0])/2
mean_Dz = popt_3[0]
print("We measure a mean diffusion coefficient of {:.3f}D0 for the␣
↪perpendicular motion and of {:.3f}D0 for the parallel motion".
↪format((popt_1[0]+popt_2[0])/2, popt_3[0]))


dataset["D_para"] = mean_Dx
dataset["D_perp"] = mean_Dz
```

```
We measure a mean diffusion coefficient of 0.522D0 for the perpendicular motion
and of 0.243D0 for the parallel motion
```

[43]:
```
Do = 4e-21/(6*np.pi*0.001*r)

def Dz_z(z):
    result = ((6*z*z + 2*r*z) / (6*z*z + 9*r*z + 2*r*r))
    return result

def Dx_z(z):
    result = (1 - 9/16*(r/(z+r)) + 1/8*(r/(z+r))**3 - 45/256*(r/(z+r))**4 - 1/
↪16*(r/(z+r))**5)
    return result
```

```
[44]: def minimizer(z_off):
          Dx_pdf = trapz(Dx_z(bins_center_pdf_z*1e-6) *␣
       ↪P_b_off(bins_center_pdf_z*1e-6,z_off,*popt[1:]),bins_center_pdf_z)
          Dz_pdf = trapz(Dz_z(bins_center_pdf_z*1e-6) *␣
       ↪P_b_off(bins_center_pdf_z*1e-6,z_off,*popt[1:]),bins_center_pdf_z)

          return np.abs((1 - mean_Dx/Dx_pdf) + (1 - mean_Dx/Dx_pdf))


      res = minimize(minimizer, 0, method='nelder-mead')
```

```
[45]: offset = res
```

```
[46]: offset = np.mean(res["final_simplex"][0])
      print("From the measurement of the mean diffusion coefficient, we measure an␣
       ↪offset of {:.3f} um".format(offset))
```

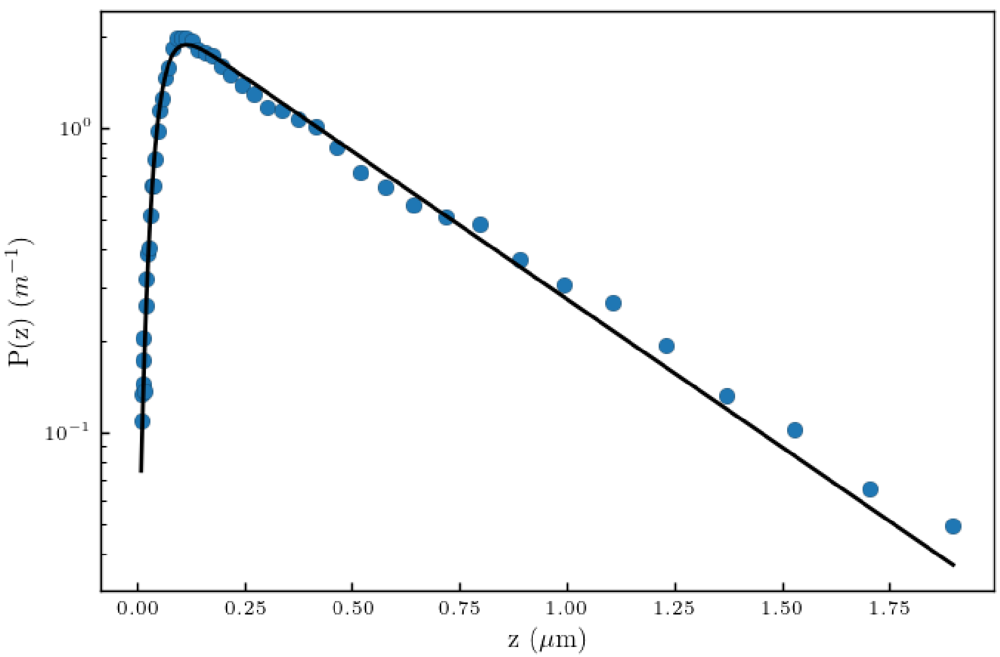
```
From the measurement of the mean diffusion coefficient, we measure an offset of
0.005 um
```

```
[47]: def logarithmic_hist(data,begin,stop,num = 50,base = 2):
          """
          Function to make logarithmic histograms to have more points
          near the surface and where the particle spend the most of its time.
          """
          if begin == 0:
              beg = stop/num
              bins = np.logspace(np.log(beg)/np.log(base), np.log(stop)/np.log(base),␣
       ↪num-1, base=base)
              widths = (bins[1:] - bins[:-1])
              bins = np.cumsum(widths[::-1])
              bins = np.concatenate(([0],bins))
              widths = (bins[1:] - bins[:-1])

          else:
              bins = np.logspace(np.log(begin)/np.log(base), np.log(stop)/np.
       ↪log(base), num, base=base)
              widths = (bins[1:] - bins[:-1])

          hist,a= np.histogram(data, bins=bins,density=True)
          # normalize by bin width
          bins_center = (bins[1:] + bins[:-1])/2

          return bins_center,widths, hist
```

```
bins_center_pdf_z,widths, pdf_z = logarithmic_hist(z_dedrift,0.01,2,num =␣
↪50,base = 12)

p2 = [0, B, ld, lb]
popt_pdf, pcov_pdf = curve_fit(P_b_off, bins_center_pdf_z * 1e-6,pdf_z, p0 = p2)
dataset["pdf_z"] = pdf_z
dataset["x_pdf_z"] = bins_center_pdf_z * 1e-6

plt.semilogy(bins_center_pdf_z,pdf_z, "o")
plt.plot(bins_center_pdf_z,P_b_off(bins_center_pdf_z*1e-6,*popt_pdf), color =␣
↪"black")

plt.xlabel("z ($\mathrm{\mu m}$)")
plt.ylabel("P(z)  ($m^{-1}$)")
```

```
<ipython-input-39-635051e60521>:6: RuntimeWarning: overflow encountered in exp
  P_b = np.exp(-B * np.exp(-z / (ld)) - z / lb)
<ipython-input-39-635051e60521>:12: RuntimeWarning: invalid value encountered in
true_divide
  P_b = P_b / A
```

[47]: Text(0, 0.5, 'P(z) (m^{-1})')




```
[48]: offset_pdf, B_pdf, ld_offset, lb_offset = popt_pdf
```

We write the diffusion function.

[49]:
```python
def Dz_z(z,off):
    off = off * 1e-6
    z = z - off
    result = ((6*z*z + 2*r*z) / (6*z*z + 9*r*z + 2*r*r))
    return result

def Dx_z_off(z,offset):
    offset = offset * 1e-6
    z = z + offset
    result = (1 - 9/16*(r/(z+r)) + 1/8*(r/(z+r))**3 - 45/256*(r/(z+r))**4 - 1/
 ↪16*(r/(z+r))**5)
    return result
```

3.7 Measuring the diffusion coefficient using the Frishman and Ronceray's method

[50]:
```python
from scipy.io import loadmat
D_yacine = loadmat("../data/diffusionAnalysis.mat")["diffusion"]
dataset["z_D_yacine"] = D_yacine[:,0] + 17.94*1e-9
dataset["z_D_x_yacine"] = (D_yacine[:,1] + D_yacine[:,2])/2
dataset["z_D_z_yacine"] = D_yacine[:,3]
```

[51]:
```python
def c_P_D(B,ld,lb,offset=None):
    if offset == None:
        offset = 0

    z = np.linspace(1e-9,15e-6,1000)

    P_D = Dz_z(z,offset) * Do * P_b_off(z, offset, B, ld, lb)

    return Dz_z(z,offset) * Do, P_D/np.trapz(P_D,z)

def _P_Dz_short_time(Dz,Dt,B,ld,lb,offset=None):
    if offset == None:
        offset = 0

    D_z, P_D = c_P_D(B,ld,lb,offset)

    P = np.trapz(P_D / np.sqrt(4 * np.pi * D_z * Dt) * np.exp(- Dz**2 / (4 *␣
 ↪D_z*Dt)),D_z)

    return P

def P_Dz_short_time(Dz,Dt,B,ld,lb,offset=None):
    if offset == None:
        offset = 0
```

```
    P = [_P_Dz_short_time(i,Dt,B,ld,lb,offset=offset) for i in Dz]
    P = np.array(P)
    P = P / np.trapz(P,Dz)

    return P
```

4 Fit everything in the same time !

Finaly we can fit everything in the same time to recap we have :

- MSD x and MSD y => $< D >$
- MSD z => $< D >$
- mean $< D >$ with the pdf
- Long time pdf $\Delta z => l_d, l_b, B$
- Pdf z => $offset, l_d, l_b, B$
- D parallel, perp => offset

The minimizer χ^2 we are going to optimize can be written as :

$$\chi^2 = \sum_{n=1}^{N} \chi_n^2 \tag{15}$$

$$\chi_n^2 = \sum^{A}(n)_i = 1\frac{1}{\sigma_{ni}}(y_{ni} - y_n(x_{ni}, \boldsymbol{a}))^2 \tag{16}$$

with σ_{ni} the uncertainty (can be set to 1), A the number of point in the dataset for each function, y_n, nth equation, $\boldsymbol{a}$ the fit parameters

We have nonlinear functions so we can use the Marquardt to optimize or Nelder-Mead methods to optimize the minimizer.

[52]:
```
def minimizer_diffusion_coeff(mean_D_para, mean_D_perp, z_off, B, ld, lb):
    #minimization of the mean diffusion coefficient measurement with the PDF␣
 ↪and MSD
    a = trapz(Dx_z_off(bins_center_pdf_z*1e-6, z_off) *␣
 ↪P_b_off(bins_center_pdf_z*1e-6,z_off, B, ld, lb),bins_center_pdf_z)
    b = trapz(Dz_z(bins_center_pdf_z*1e-6, z_off) *␣
 ↪P_b_off(bins_center_pdf_z*1e-6,z_off, B, ld, lb),bins_center_pdf_z)
    at = mean_Dx; bt = mean_Dz
    return (a-at)**2 / at**2 + (b-bt)**2 / bt**2

dataset["z"] = z_dedrift
dataset["x"] = x
dataset["y"] = y



def minimizer_Dz_small_t(B,ld,lb):
    xi = 0
```

```
    for n,i in enumerate([1,2,3]):
        Dezs = (dataset["z"][0:-i] - dataset["z"][i:]) * 1e-6
        Dezs = Dezs# - np.mean(Dezs)

        hist, bins_center = pdf(Dezs[~np.isnan(Dezs)], bins = 30)
        hist = hist/np.trapz(hist,bins_center)

        Dz_th = bins_center
        PPP = P_Dz_short_time(Dz_th,time[i],B,ld,lb)

        #xi = xi + np.nanmean((((np.abs(hist) - (PPP) ) ) ** 2) / ((np.
↪abs(hist)**2)))
        xi = xi + np.nanmean(((hist[hist>0]-PPP[hist>0]) ** 2) /␣
↪hist[hist>0]**2)
    return xi
```

[53]:
```
dataset["D_para"] = mean_Dx
dataset["D_perp"] = mean_Dz



def minimizer(x, *args):
    data = dataset
    ld = x[0]
    lb = x[1]
    B = x[2]
    offset_dif = x[3]
    offset_boltz = 0




    chi_mean_D_pdf = minimizer_diffusion_coeff(dataset["D_para"],␣
↪dataset["D_perp"],offset_boltz, B, ld, lb)
    chi_MSD_plateau = minimize_plateau([B,ld,lb])

    E_longtime_pdf = (Pdeltaz_long(data["x_pdf_longtime"], B, ld, lb)) -␣
↪(data["pdf_longtime"])
    chi_longtime_pdf = np.mean((E_longtime_pdf[E_longtime_pdf > -np.inf] ** 2) /
↪ (((Pdeltaz_long(data["x_pdf_longtime"], B, ld, lb)))**2))

    E_chi_pdf_z = (P_b_off(data["x_pdf_z"], offset_boltz, B, ld, lb) -␣
↪data["pdf_z"])
    chi_pdf_z = np.nanmean((E_chi_pdf_z[E_chi_pdf_z > -np.inf] ** 2) /␣
↪((P_b_off(data["x_pdf_z"], offset_boltz, B, ld, lb))**2))

    E_D_z = (Dz_z(data["z_D_yacine"], offset_dif)) - (data["z_D_z_yacine"] / Do)
```

```
    chi_D_z = np.mean((E_D_z[E_D_z > -np.inf] ** 2) /␣
↪((Dz_z(data["z_D_yacine"], offset_dif))**2))

    E_D_x = (Dx_z_off(data["z_D_yacine"], offset_dif)) - (data["z_D_x_yacine"] /
↪ Do)
    chi_D_x = np.mean((E_D_x[E_D_x > -np.inf]  ** 2) /␣
↪((Dx_z_off(data["z_D_yacine"], offset_dif))**2))

    chi_Dz_small_t = minimizer_Dz_small_t(B,ld,lb)

    summ = chi_mean_D_pdf + chi_MSD_plateau + chi_longtime_pdf + chi_pdf_z +␣
↪chi_D_z + chi_D_x + chi_Dz_small_t

    return  summ
```

[54]:
```
B = 5
ld = ld_offset
x0 = [ld,550,B,0,offset_pdf]
```

[55]:
```
from scipy.optimize import leastsq

options={
    'maxc1or': 30,
    'ftol': 2.2e-10,
    'gtol': 1e-5,
    'eps': 1e-08,
    'maxfun': 15000,
    'maxiter': 15000,
    'maxls': 20,
    'finite_diff_rel_step': None,
}

res = minimize(minimizer,
                   x0,
                   method = "BFGS",
                   tol = 1e-1,
                  )
```

[56]:
```
res.x
results = {
    "ld":res.x[0],
    "lb":res.x[1],
    "B":res.x[2],
    "offset_diffusion":res.x[3],
}

results
```

[56]:
```
{'ld': 25.470469609361395,
 'lb': 549.9705309805663,
 'B': 4.405291114790512,
 'offset_diffusion': 0.019878479897997275}
```

This final result has been used to plot theories, allong the manuscript.