Data Analysis procedure

[1]:
```
%load_ext lab_black
# Import important tools
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
from matplotlib import rc
```

[ ]:
```

```

[2]:
```
mpl.rcParams["xtick.direction"] = "in"
mpl.rcParams["ytick.direction"] = "in"
mpl.rcParams["lines.markeredgecolor"] = "k"
mpl.rcParams["lines.markeredgewidth"] = 1
mpl.rcParams["figure.dpi"] = 130
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
```

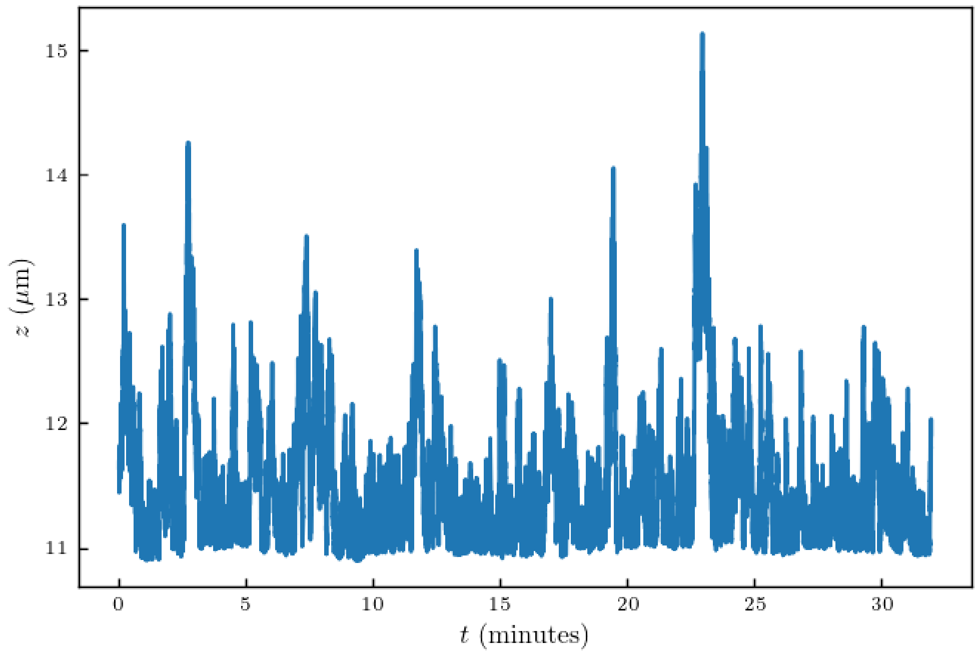
We load the data

[3]:
```
raw_data = loadmat(
    "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
```

```python
dataset = {}
dataset["r"] = r
dataset["n"] = n_part
dataset["fps"] = fps
dataset["time"] = time
```

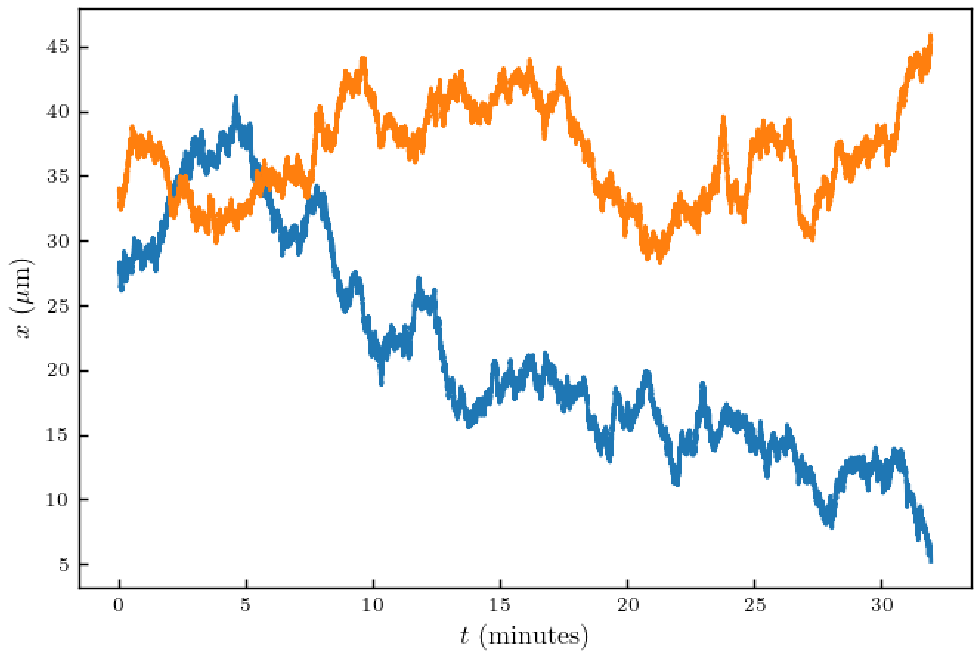
1 Data exploration

[4]:
```python
# 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 / fps, 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]:
```python
plt.plot(time / fps, raw_data_m[:, 0], label="x")
plt.plot(time / fps, raw_data_m[:, 1], label="y")
plt.xlabel("$t$ (minutes)")
plt.ylabel("$x$ ($\mathrm{\mu m}$)")
```

```
plt.show()
```



2 MSD

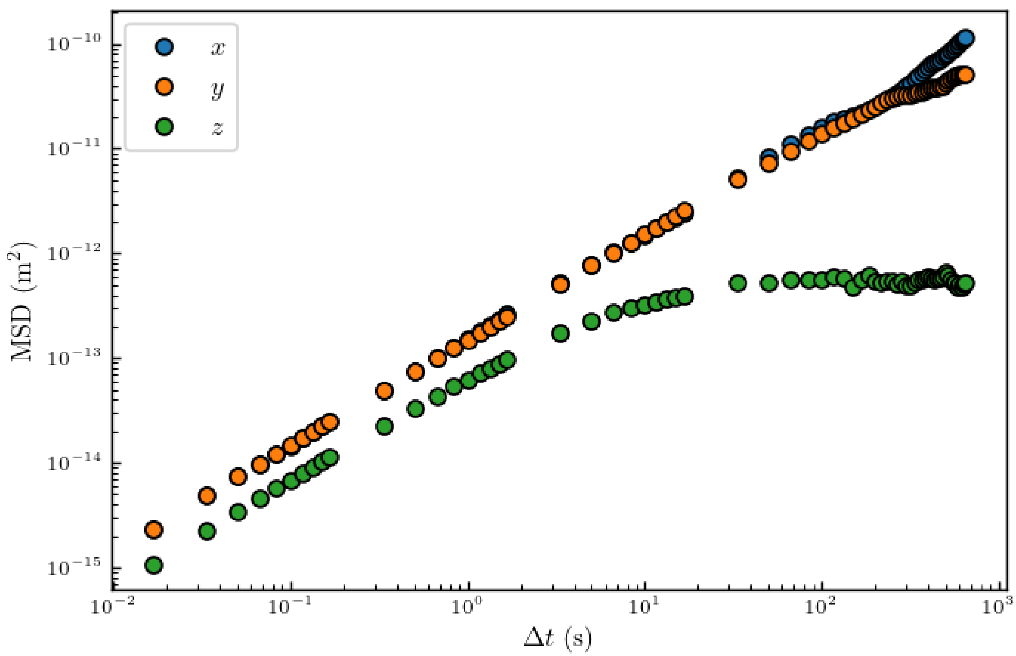
We compute the MSD using the formula:

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

[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.array(
    [
        *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="$x$")
plt.plot(time[t], MSD_y, "o", label="$y$")
plt.plot(time[t], MSD_z, "o", label="$z$")
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\analyse\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]
    )
)
```

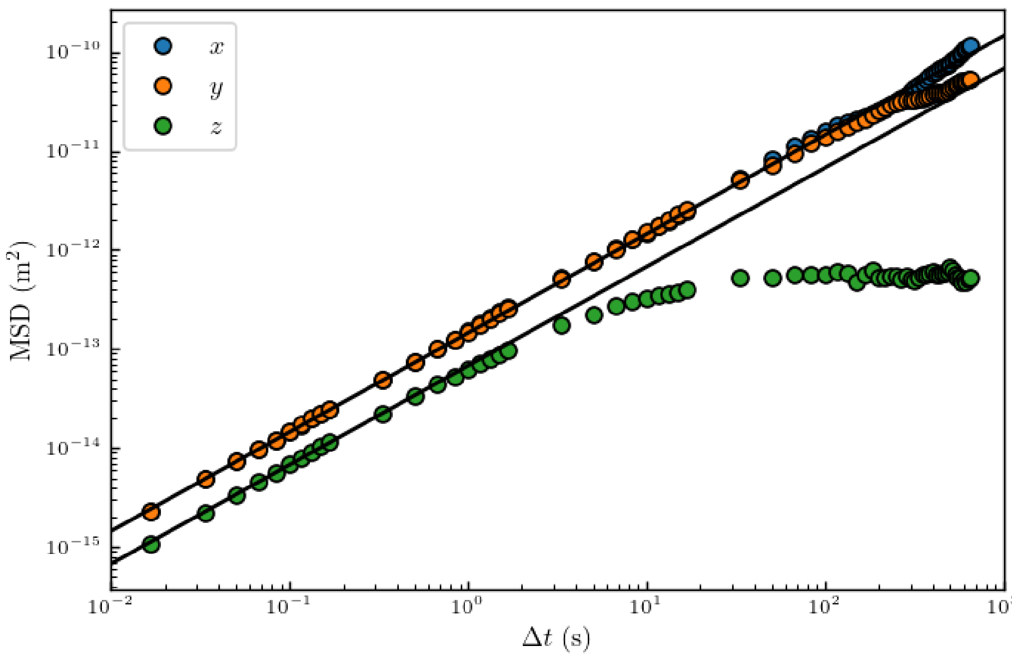
```
We measure a reduced mean diffusion coefficient of 0.522 for the perpendicular
motion and of 0.243 for the parallel motion
```

[10]:

```
plt.loglog(time[t], MSD_x, "o", label="$x$")
plt.plot(time[t], MSD_y, "o", label="$y$")
plt.plot(time[t], MSD_z, "o", label="$z$")
plt.ylabel("MSD ($\mathrm{m^2}$)")
plt.xlabel("$\Delta t$ (s)")
tt = np.linspace(1e-2, 1e3)
plt.plot(tt, f(tt, *popt_1), color="k")
plt.plot(tt, f(tt, *popt_3), color="k")

plt.xlim((1e-2, 1e3))
plt.legend()
```

[10]:

```
<matplotlib.legend.Legend at 0x27a80c0b700>
```



3 Displacement distributions

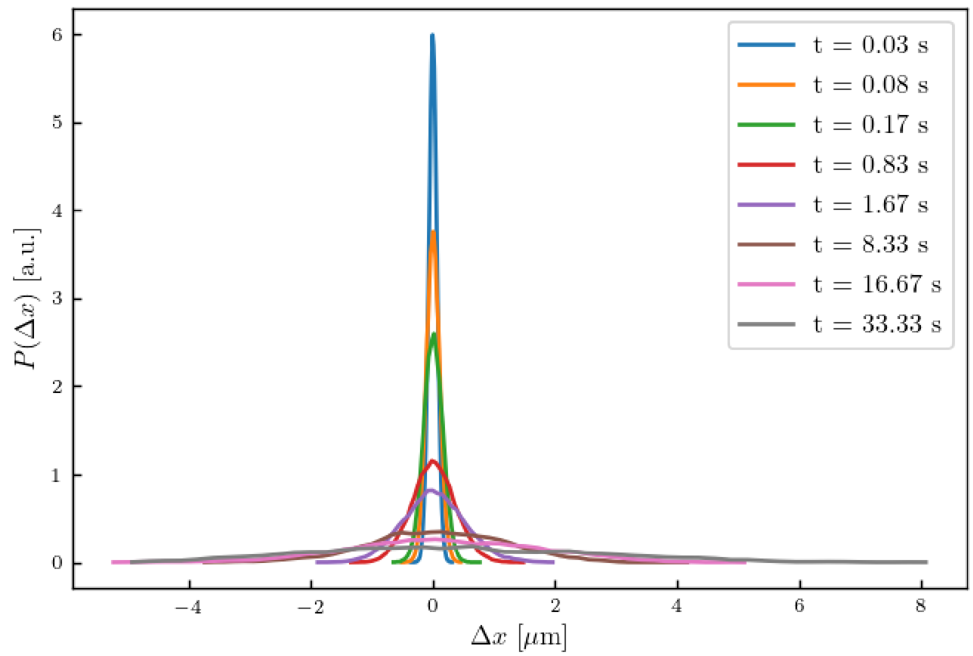
3.1 Δx distributions

[11]:
```
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
```

[12]:
```
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("$\Delta x$ [$\mathrm{\mu m}$]")
```

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



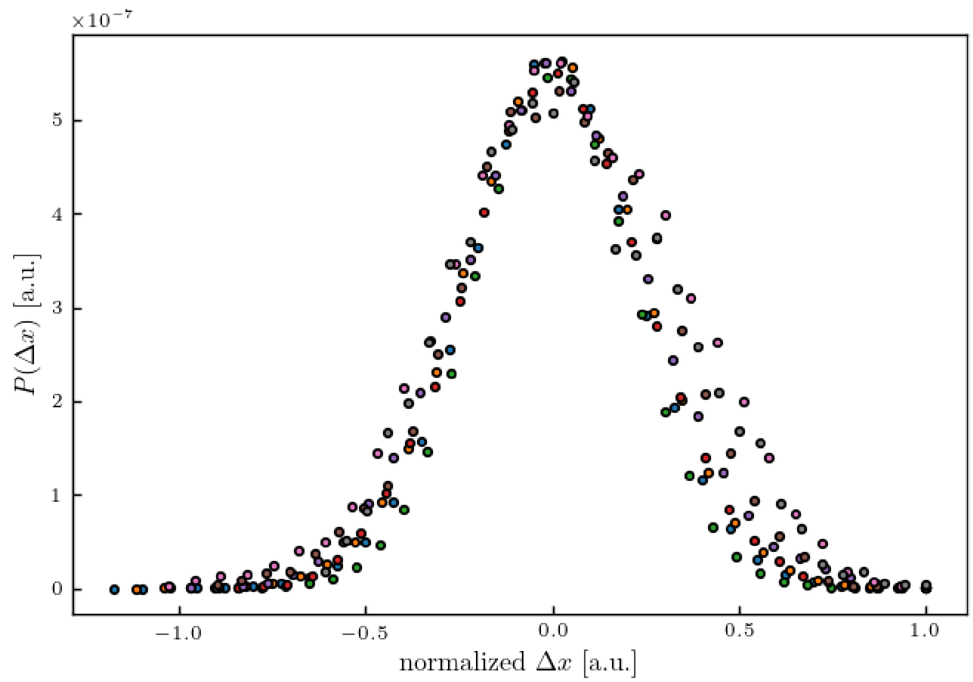
If we now normalize by the standard deviation

[13]:
```
def gauss_function(x, a, x0, sigma):
    return a * np.exp(-((x - x0) ** 2) / (2 * sigma ** 2))
```

[14]:
```
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.]")
```

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



[15]:
```
(3.5e-22) ** (1 / 3)
```

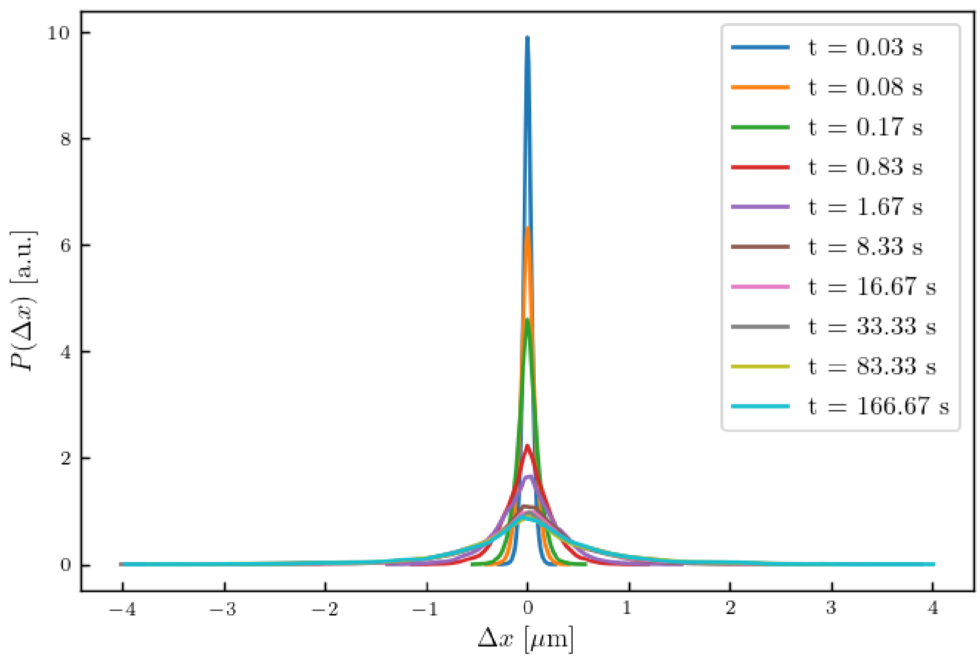
[15]: 7.047298732064899e-08

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

3.2 Δz distributions

[16]:
```
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("$\Delta x$ [$\mathrm{\mu m}$]")
```

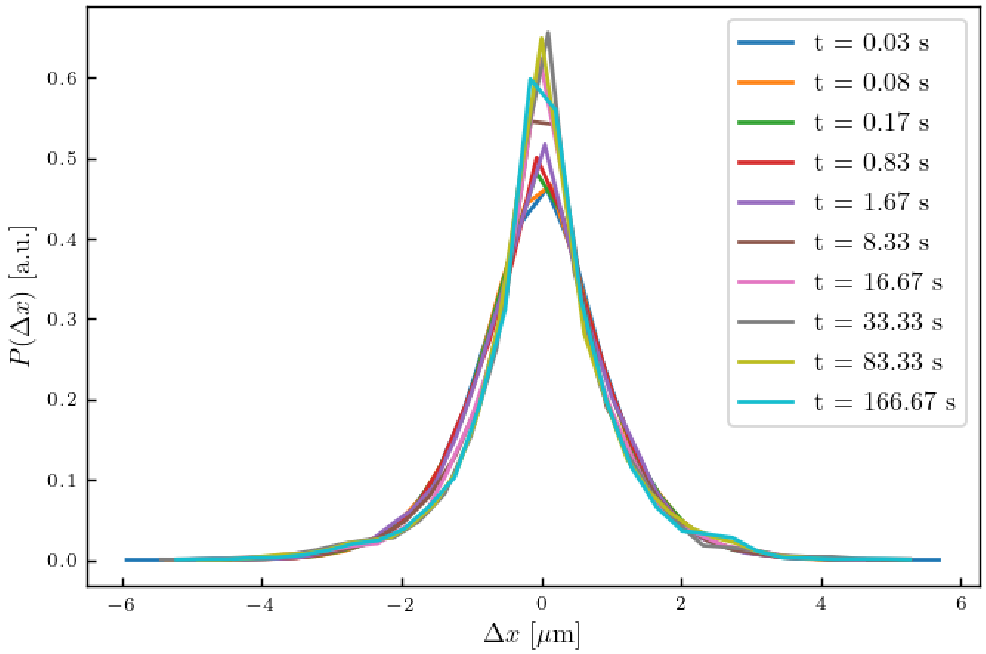
[16]:
```
Text(0.5, 0, '$\\Delta x$ [$\\mathrm{\\mu m}$]')
```



[17]:
```
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("$\Delta x$ [$\mathrm{\mu m}$]")
```

[17]:
```
Text(0.5, 0, '$\\Delta x$ [$\\mathrm{\\mu m}$]')
```

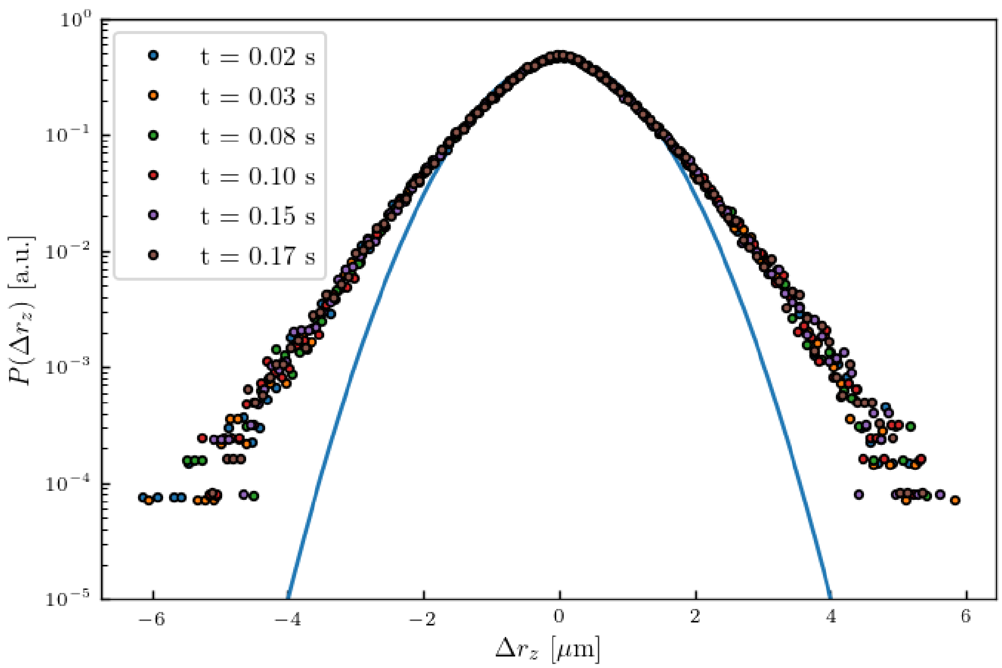


3.2.1 Short time distributions

[18]:
```
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("$P(\Delta r_z)$ [a.u.]")
plt.xlabel("$\Delta r_z$ [$\mathrm{\mu m}$]")
axes = plt.gca()
axes.set_ylim([1e-5, 1])
```

[18]: (1e-05, 1)



The non-Gaussianity is due to the hindered mobility. Taking into account the hindered mobility the PDF of displacement writes:

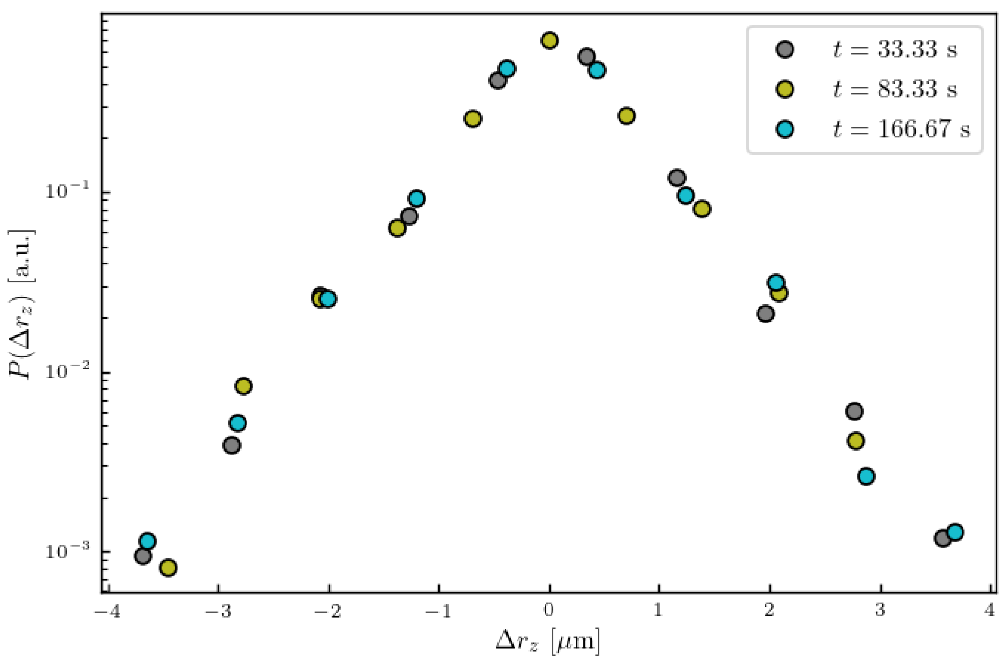
$$P(\Delta r_i, \Delta t) = \int_0^\infty \mathrm{d}D P(D_i) \frac{1}{\sqrt{4\pi D_i \Delta t}} \exp\left[\frac{-\Delta_i r_i^2}{4D_i\Delta t}\right] . \quad (3)$$

This non-Gaussianity can be fitted as done at the end of this appendix and shown in the manuscript.

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

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



Indeed at long time it becomes exponential and it's no longer dependent on Δt At very long time intervals Δt each position measurement can be seen as random measurement on the Boltzmann distribution. Thus, one can write the probability distribution as a convolution of two PDF:

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

with :

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

Also, $P_B(z < 0)$ giving at long time step :

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

3.4 Analysis of pdf of the Δz at large time step

To have a better measurement we average the PDF of displacement Δr_z over different time-step Δt . But, first of all, we need to get rid of the drifts at long time. We do that by taking a moving minimum.

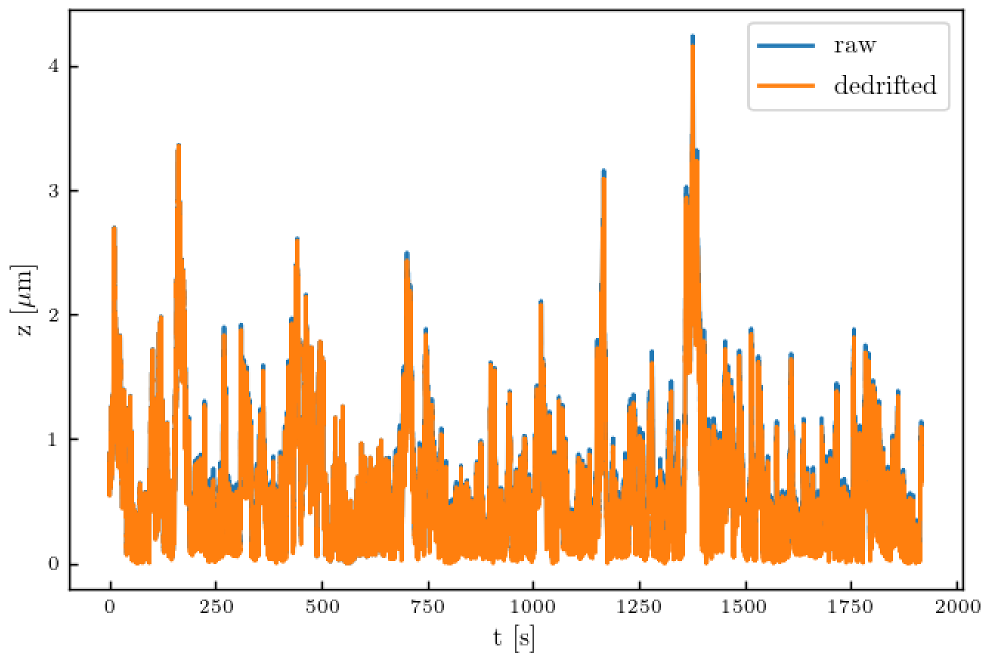
3.5 Dedrifting the z trajectory

[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 [$\\mathrm{\\mu m}$]')
```

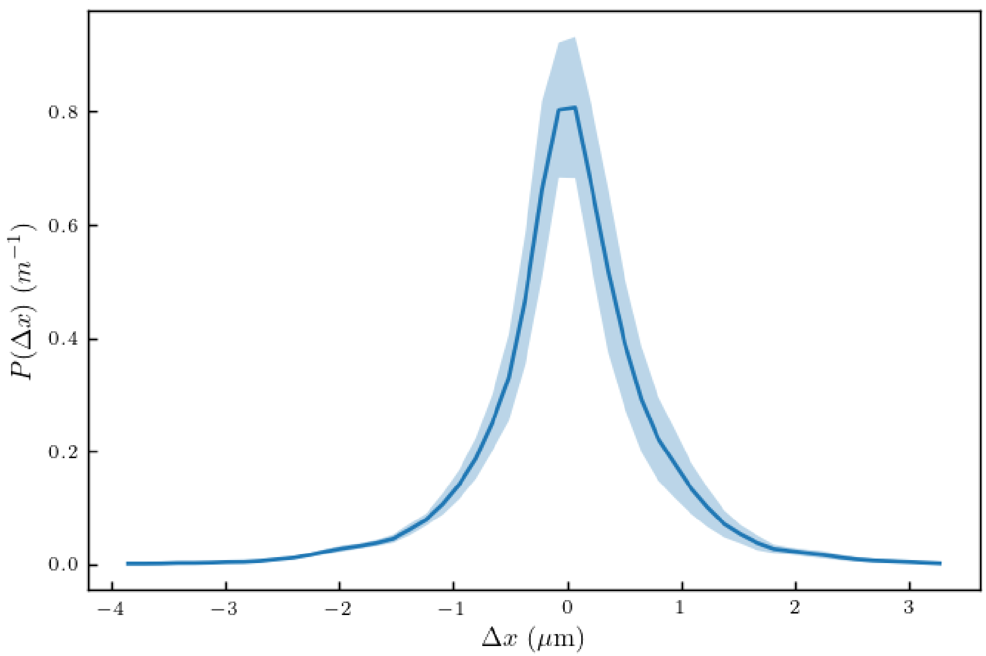


3.5.1 Measuring pdf at large Δt with the dedrifted trajectory and analysing it

[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 :

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

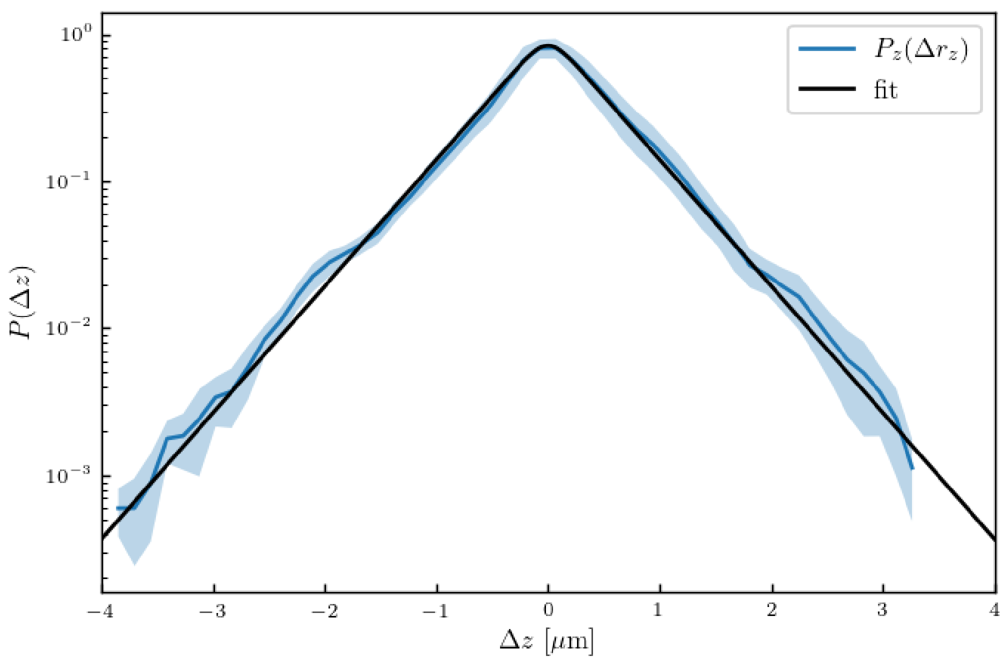
[25]:
```
def P_b(z, A, B, ld, lb):
    P_b = A * np.exp(-B * np.exp(-z / (ld)) - z / lb)
    P_b[z < 0] = 0
    return P_b


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]:
```
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-d08630fe76fc>:2: RuntimeWarning: overflow encountered in exp
  P_b = A * np.exp(-B * np.exp(-z / (ld)) - z / lb)
```

[27]:
```
A = 0.14e8
B = 400
ld = 70
lb = 500
p0 = [B, ld, lb]


plt.semilogy(bins_centers_long_t, pdf_long_t, label="$P_z(\Delta r_z)$")
plt.fill_between(
    bins_centers_long_t, pdf_long_t - err_long_t, pdf_long_t + err_long_t,␣
 ↪alpha=0.3
)

zz = np.linspace(-4, 4, 1000)
plt.plot(zz, Pdeltaz_long(zz * 1e-6, *popt), label="fit", color="k")
plt.xlim(-4, 4)
plt.legend()
plt.ylabel("$P(\Delta z)$")
plt.xlabel("$\Delta z$ [$\mathrm{\mu m}$]")
```

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



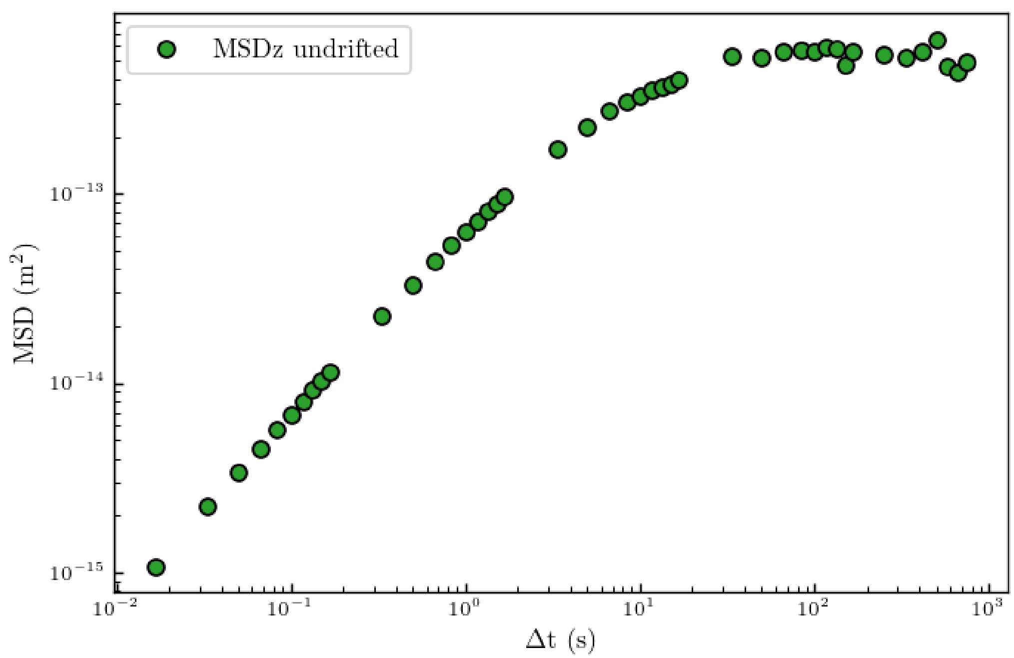
[28]:
```
print("We measure, B = {:.2f}, ld = {:.2f} nm, lb = {:.2f} nm".format(*popt))
B, ld, lb = popt
```

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

3.6 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)")
```

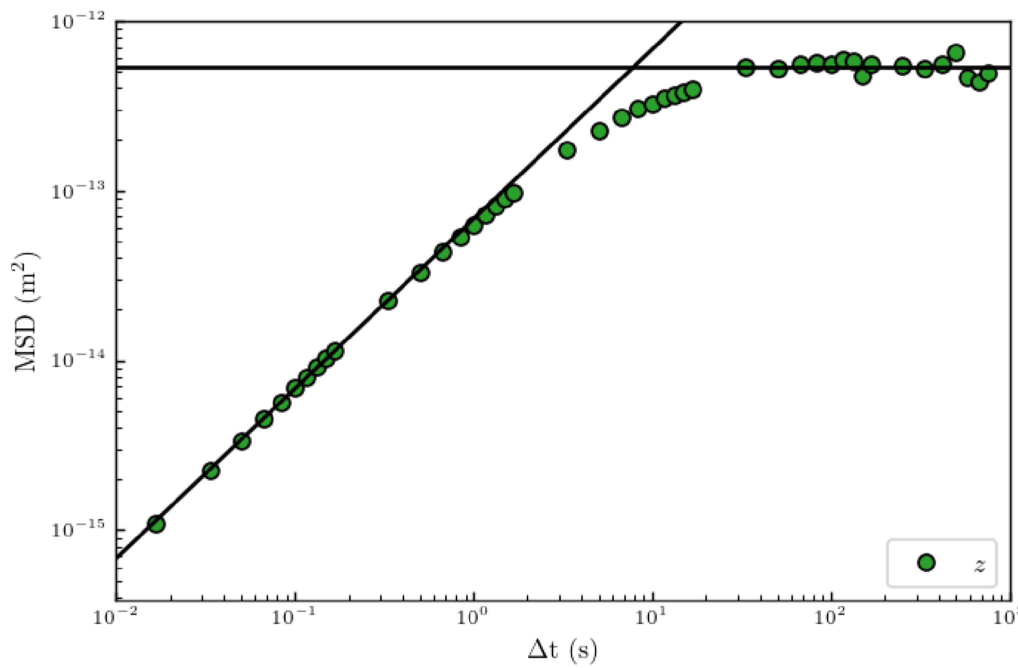
[29]:
```
Text(0.5, 0, '$\\Delta$t (s)')
```



[30]:
```
plateau = np.mean(MSD_z_dedrift[time[t] > 1e2])
```

[31]:
```
plt.loglog(time[t], MSD_z_dedrift, "o", label="$z$", color="tab:green")
plt.plot(tt, [plateau] * len(tt), "k")
plt.plot(tt, f(tt, *popt_3), color="k")
plt.xlim((1e-2, 1e3))
plt.ylim((None, 1e-12))
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 : 2.070536e+01
```

The MSD plateau is theoritically given by:

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

```
[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
```

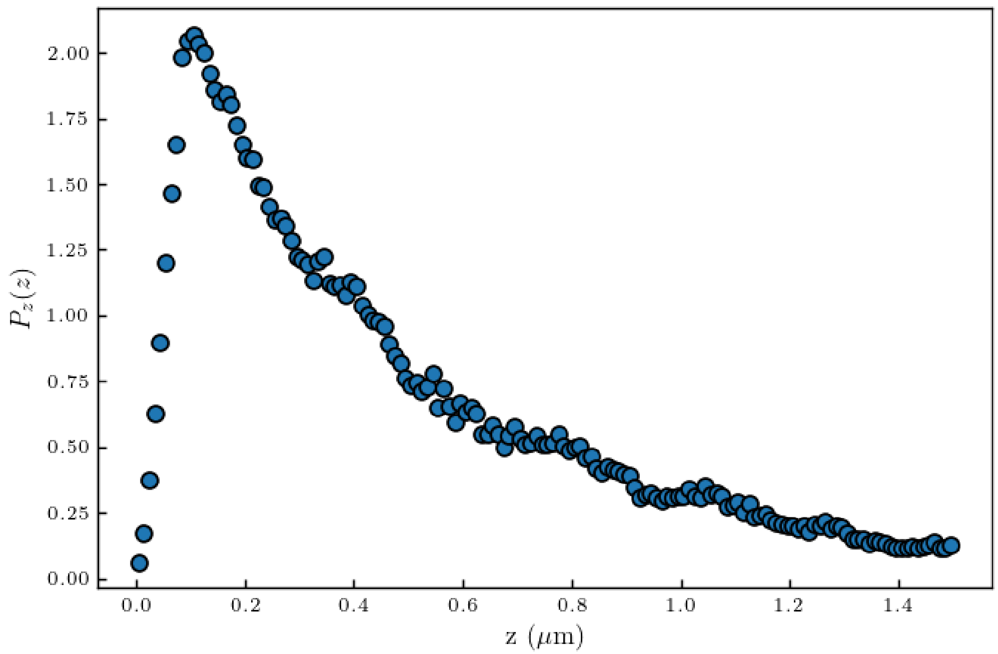
3.7 PDF of heights

```
[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)
```

```python
    # normalize by bin width
    bins_center = (bins[1:] + bins[:-1]) / 2

    return bins_center, widths, hist
```

[38]:
```python
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("$P_z(z)$")
```

[38]: Text(0, 0.5, '$P_z(z)$')



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 :

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

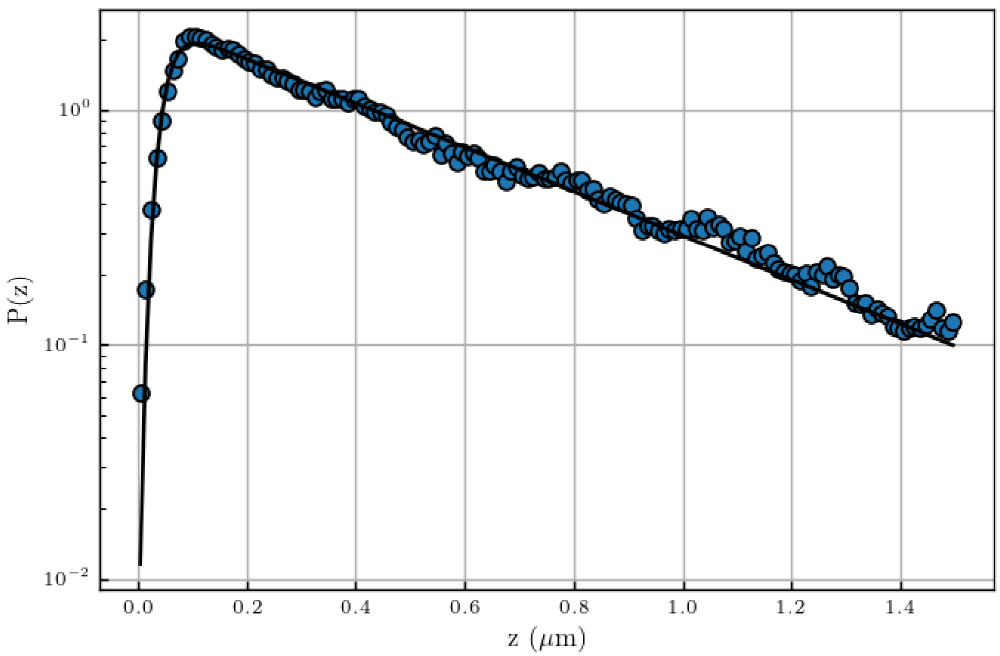
To do this we will fit the PDF with an offset, adjust it with the mean value of z. Let's first do it over z

[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

    # Normalization of P_b

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

    return P_b
```

[40]:
```
# 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-f5e0b340e678>:6: RuntimeWarning: overflow encountered in exp
  P_b = np.exp(-B * np.exp(-z / (ld)) - z / lb)
<ipython-input-39-f5e0b340e678>:12: RuntimeWarning: invalid value encountered in
true_divide
  P_b = P_b / A
```

[41]:
```
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), "k")

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
    )
)
```

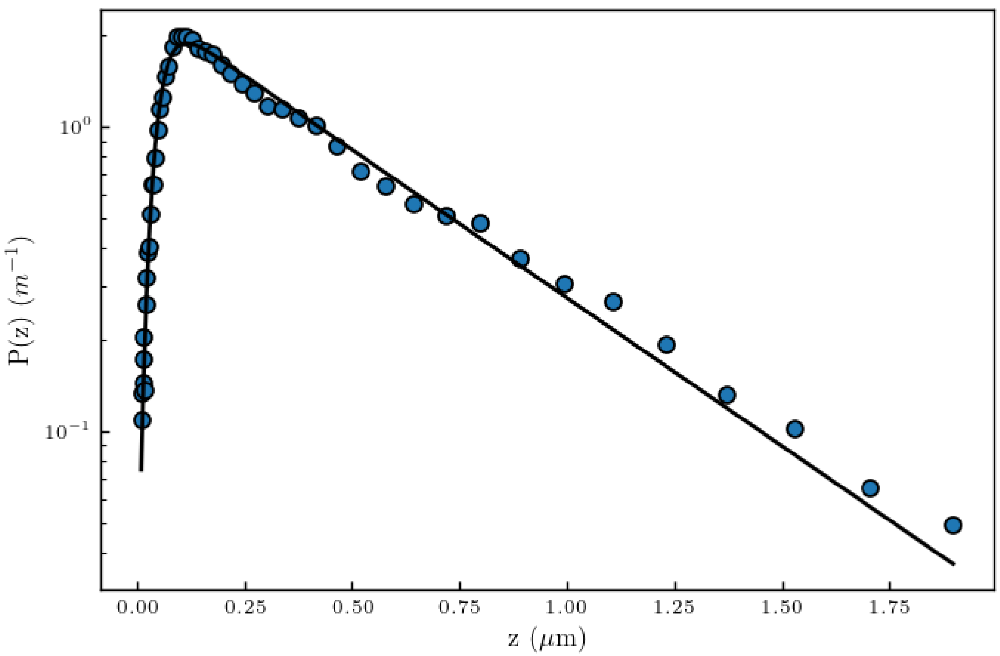
From the measurement of the mean diffusion coefficient, we measure an offset of 0.005 um

[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(
```

```python
            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-f5e0b340e678>:6: RuntimeWarning: overflow encountered in exp
  P_b = np.exp(-B * np.exp(-z / (ld)) - z / lb)
<ipython-input-39-f5e0b340e678>: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.

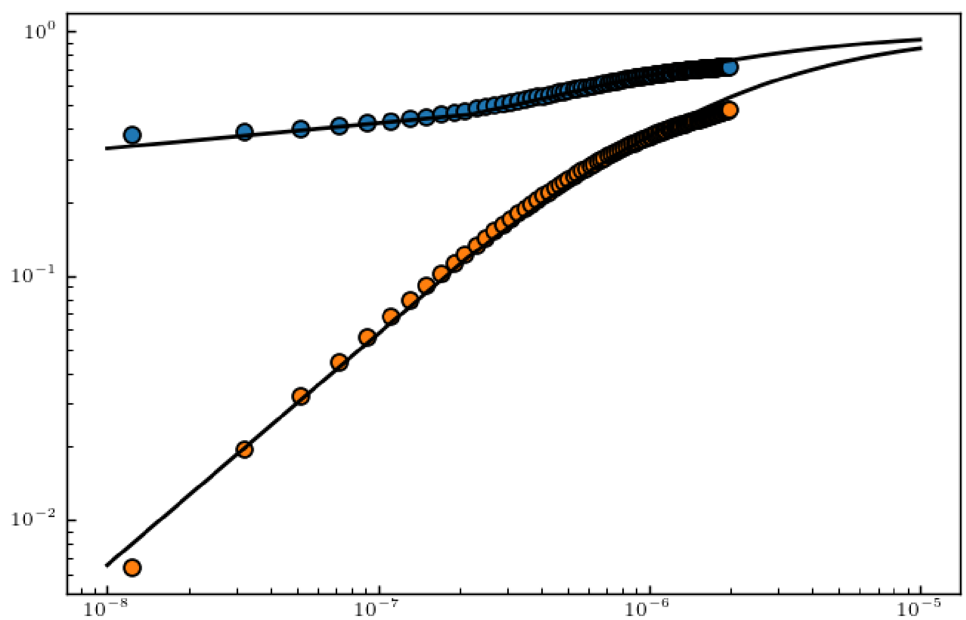
[49]:
```
def Dz_z(z, off):
    off = off * 1e-6
    z = z - off
    result = (6 * z * z + 2 * r * z) / (6 * z * z + 9 * r * z + 2 * r * r)
    return result


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
```

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

[50]:
```
from scipy.io import loadmat

dataset["D_0"] = 4e-21 / (6 * np.pi * 0.001 * dataset["r"])
D = loadmat("diffusionAnalysis.mat")["diffusion"]
dataset["z_D"] = D[:, 0]
dataset["z_D_x"] = (D[:, 1] + D[:, 2]) / 2
dataset["z_D_z"] = D[:, 3]
```

[51]:
```
plt.plot(dataset["z_D"], dataset["z_D_x"] / dataset["D_0"], "o")
plt.loglog(dataset["z_D"], dataset["z_D_z"] / dataset["D_0"], "o")

zz = np.linspace(1e-8, 1e-5)
plt.plot(zz, Dz_z(zz, 0), "k")

plt.plot(zz, Dx_z_off(zz, 0), "k")
```

[51]:
```
[<matplotlib.lines.Line2D at 0x27a85cc7850>]
```



[52]:
```
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 Δz => 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.

[53]:
```
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
```

[54]:

```python
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]

    chi_mean_D_pdf = minimizer_diffusion_coeff(
        dataset["D_para"], dataset["D_perp"], 0, 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"], 0, 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"], 0, B, ld, lb)) ** 2)
    )

    E_D_z = (Dz_z(data["z_D"], offset_dif)) - (data["z_D_z"] / Do)
    chi_D_z = np.mean(
        (E_D_z[E_D_z > -np.inf] ** 2) / ((Dz_z(data["z_D"], offset_dif)) ** 2)
    )

    E_D_x = (Dx_z_off(data["z_D"], offset_dif)) - (data["z_D_x"] / Do)
    chi_D_x = np.mean(
        (E_D_x[E_D_x > -np.inf] ** 2) / ((Dx_z_off(data["z_D"], 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 summm
```

[55]:
```
B = 5
ld = ld_offset
x0 = [ld, 550, B, 0, offset_pdf]
```

[56]:
```
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,
)
```

[57]:
```
res.x
results = {
    "ld": res.x[0],
    "lb": res.x[1],
    "B": res.x[2],
    "offset_diffusion": res.x[3],
}

results
```

[57]:
```
{'ld': 25.53322987706852,
 'lb': 549.9956782843908,
 'B': 4.856896668800334,
 'offset_diffusion': 0.0019089236000464675}
```

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