diffusion_langevin_1d

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1 Simulating diffusion with the Langevin equation

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1.1.1 last updated 2018-05-27

In [283]:
```
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
from scipy import stats
import scipy
```

In [284]:
```
# fix random number seed for reproducibility
# np.random.seed(123456789)
```

In [285]:
```
def LangevinPropagator_vectorized(sampleTimes, m, a = 0.0,
                                  sigma = 1.0, dt = 1.0e-3,
                                  x0 = 0.0):
    '''
    Vectorized version of the LangevinPropagator function, making use of
    numpy's vectorization possibilities.
    '''
    nSamples = len(sampleTimes)
    iterations = (sampleTimes / dt).astype(int)
    iterations[1:] = iterations[1:] - iterations[0:-1]
    totalIterations = (np.cumsum(iterations))[-1]

    # make sure that the noise amplitude is calculated outside the
    # for loops below to save computation time
    # square roots are numerically quite expensive
    noise = sigma * np.sqrt(2.0 * dt) # noise amplitude
    drift = a * dt

    out = np.zeros((nSamples, m))

    X = x0 * np.ones((1, m)) # row element

    for k in range(nSamples):
```

```
        for i in range(iterations[k]):

            X += drift * X + noise * np.random.normal(0.0, 1.0, m)

        out[k, :] = X

    return out

def LangevinPropagatorReflectiveBC_vectorized(sampleTimes, m, a = 0.0,
                                              sigma = 1.0, dt = 1.0e-3,
                                              x0 = 2.0):

    nSamples = len(sampleTimes)
    iterations = (sampleTimes / dt).astype(int)
    iterations[1:] = iterations[1:] - iterations[0:-1]
    totalIterations = (np.cumsum(iterations))[-1]

    # make sure that the noise amplitude is calculated outside the
    # for loops below to save computation time
    # square roots are numerically quite expensive
    noise = sigma * np.sqrt(2.0 * dt) # noise amplitude

    out = np.zeros((nSamples, m))

    X = x0 * np.ones((1, m))

    for k in range(nSamples):

        for i in range(iterations[k]):

            X += noise * np.random.normal(0.0, 1.0, m)

            # reflective boundary condition at x = 0.0
            mask = np.argwhere(X < 0.0)
            X[0, mask] = -1.0 * X[0, mask]

        out[k, :] = X

    return out

def LangevinPropagatorReflectiveBC_overshoot_vectorized(sampleTimes, \
    m, a = 0.0, sigma = 1.0, dt = 1.0e-3, x0 = 2.0):

    nSamples = len(sampleTimes)
    iterations = (sampleTimes / dt).astype(int)
    iterations[1:] = iterations[1:] - iterations[0:-1]
    totalIterations = (np.cumsum(iterations))[-1]
```

```
            # make sure that the noise amplitude is calculated outside the
            # for loops below to save computation time
            # square roots are numerically quite expensive
            noise = sigma * np.sqrt(2.0 * dt) # noise amplitude

            out = np.zeros((nSamples, m))

            X = x0 * np.ones((1, m))

            for k in range(nSamples):

                for i in range(iterations[k]):

                    X += noise * np.random.normal(0.0, 1.0, m)

                    # reflective boundary condition at x = 0.0
                    mask = np.argwhere(X < 0.0)
                    X[0, mask] = 0.0

                out[k, :] = X

            return out

        def getMoments(X):
            '''
            Computes the first moments and the MSD of a given set of trajectories.
            '''
            mu = np.mean(X, axis = 1)
            MSD = np.zeros((X.shape[0],))
            for i in range(X.shape[0]):
                MSD[i] = np.mean(np.square((X[i, : ] - mu[i])))

            return mu, MSD
```

In [286]:
```
        def Mean_ReflectiveBC(t, x0):
            tmp = np.exp(-x0 ** 2 / (4.0 * t)) * np.sqrt(4.0 * t / np.pi)
            return tmp + x0 * scipy.special.erf(x0 / np.sqrt(4.0 * t))

        def MSD_ReflectiveBC(t, x0):
            c = 4.0 * t
            tmp = 2.0 * t + x0 ** 2
            tmp -= (2.0 * np.exp(- x0 ** 2 / c) * np.sqrt(t/np.pi) + x0 * \
                   scipy.special.erf(x0 / (2.0 * np.sqrt(t))) ) ** 2
            return tmp
```

In [287]:
```
        def plotPositionPDF_free(X, t, D = 1.0, x0 = 0.0):
            f, ax = plt.subplots(1)
```

```
    f.set_size_inches(5.0, 3.5)

    labelfontsize = 10.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    plt.hist(X, density = True, bins = 15)

    xVals = np.linspace(-12.0, 12.0, 500)
    yVals = stats.norm.pdf(xVals, x0, np.sqrt(2.0 * D * t))
    labelString = r'$p(x,t = %.1f)$' %(t)
    ax.plot(xVals, yVals, lw = 2.0, color = 'C3', label = labelString)

    ax.set_xlabel('position $x$', fontsize = 18)
    ax.set_ylabel(r'$p(x,t|x_0, t_0)$', fontsize = 18)

    ax.set_xlim(-10.5, 10.5)
    ax.set_ylim(0.0, 0.41)

    leg = ax.legend(fontsize = 12)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)

    return None

def plotPositionPDF_lrBC(X, t, D = 1.0, x0 = 0.0):
    f, ax = plt.subplots(1)
    f.set_size_inches(5.0, 3.5)

    labelfontsize = 10.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    plt.hist(X, density = True, bins = 15)

    xVals = np.linspace(0.0, 14.0, 500)
    yVals = stats.norm.pdf(xVals, x0, np.sqrt(2.0 * D * t)) + \
            stats.norm.pdf(-xVals, x0, np.sqrt(2.0 * D * t))
    labelString = r'$p(x,t = %.1f)$' %(t)
    ax.plot(xVals, yVals, lw = 2.0, color = 'C3', label = labelString)

    ax.set_xlabel('position $x$', fontsize = 18)
    ax.set_ylabel(r'$p(x,t|x_0, t_0)$', fontsize = 18)
```

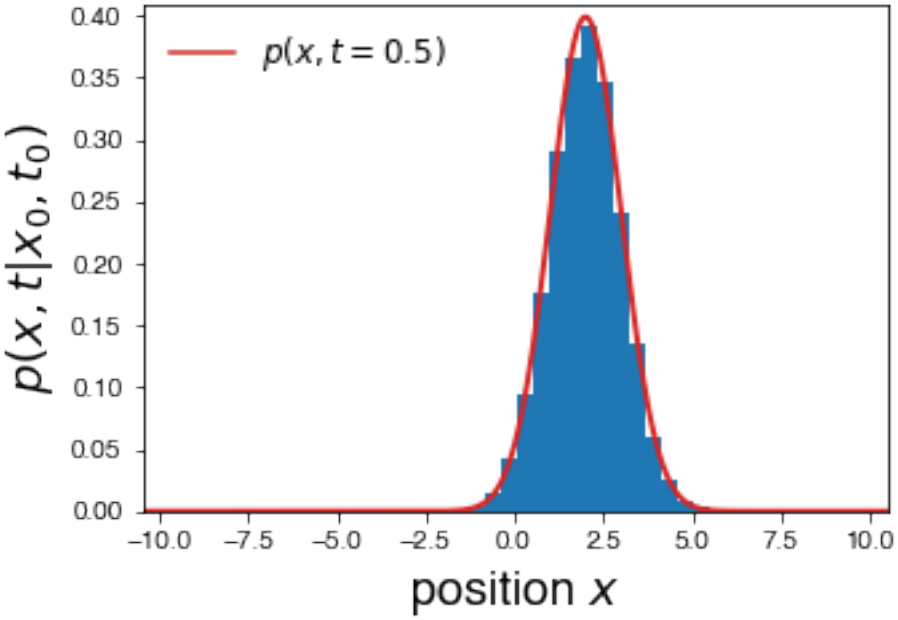
```
    ax.set_xlim(0.0, 12.25)
    ax.set_ylim(0.0, 0.41)

    leg = ax.legend(fontsize = 12)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)

    return None

def plotFirstMoments(X, Y, x0 = 0.0):

    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('time $t$', fontsize = 18)
    ax.set_ylabel(r'first moment $\langle x \rangle(t)$', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    ax.plot([-2.0, 12.0], [x0, x0],
            dashes = [8.0, 5.0],
            lw = 0.5,
            color = 'k',
            label = r'$x = x_0$')
    ax.scatter(X, Y, color = 'k', s = 45)

    ax.set_xlim(-0.5, 11.2)
    ax.set_ylim(1.45, 2.55)

    leg = ax.legend(scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None

def plotMSD(X, Y, t, D = 1.0):

    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)
```

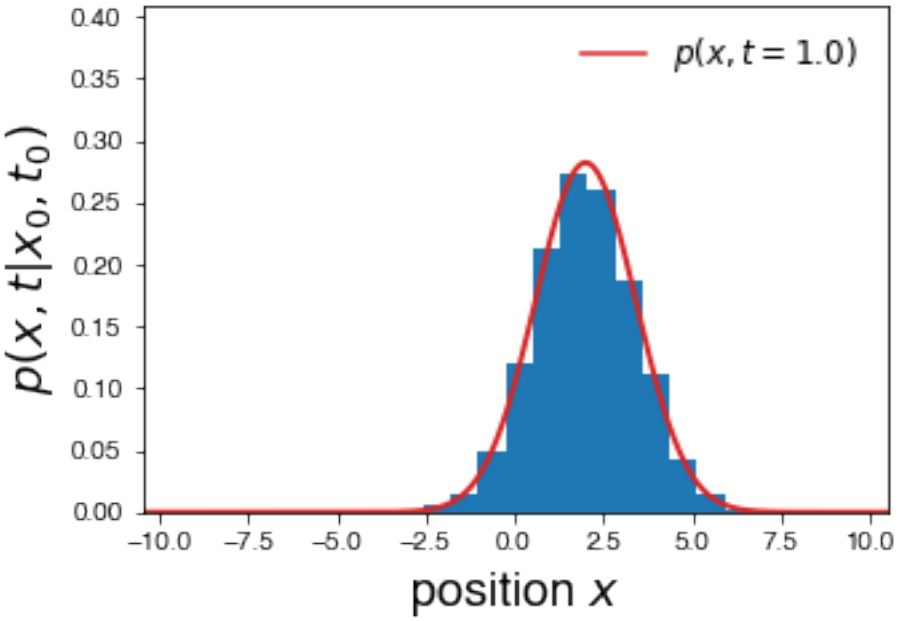
```
    ax.set_xlabel('time $t$', fontsize = 18)
    ax.set_ylabel(r'MSD(t)', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    ax.plot([-2.0, 12.0], [2.0 * D * (-2.0), 2.0 * D * (12.0)],
            lw = 1.0, color = 'C3', label = r'MSD(t) = 2Dt')
    ax.scatter(X, Y, color = 'k', s = 45, label = r'BD (numeric)')

    ax.set_xlim(-0.5, 11.2)
    ax.set_ylim(-1.0, 22.5)

    leg = ax.legend(scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None
```

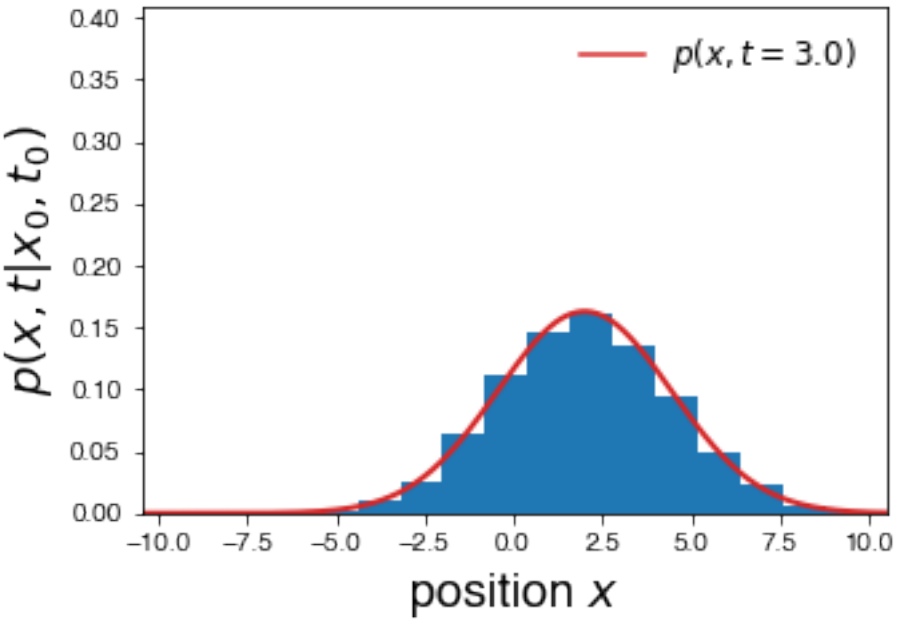
1.2 Simulate free diffusion trajectories in one dimension

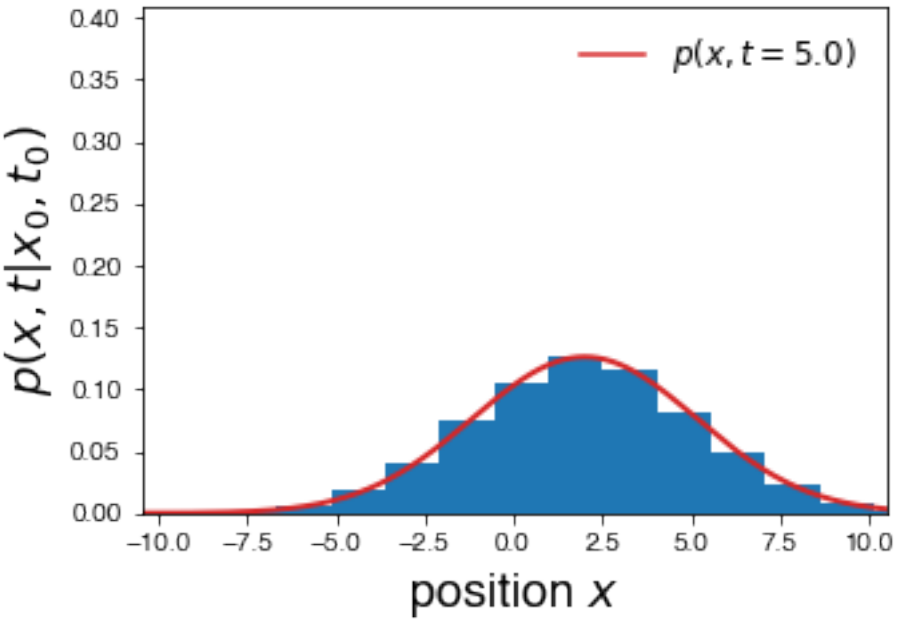
```
In [288]: # set simulation parameters here
          D = 1.0
          dt = 1.0e-3
          x0 = 2.0
          sampleTimes = np.array([0.5 , 1.0, 3.0, 5.0, 10.0])
          m = 10000

In [289]: %%time
          X = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                            m = m,
                                            x0 = x0)

CPU times: user 5.52 s, sys: 36.2 ms, total: 5.55 s
Wall time: 5.66 s


In [290]: print(X.shape)

(5, 10000)


In [291]: plotPositionPDF_free(X[0, :], 0.5, x0 = x0)
          plotPositionPDF_free(X[1, :], 1.0, x0 = x0)
```

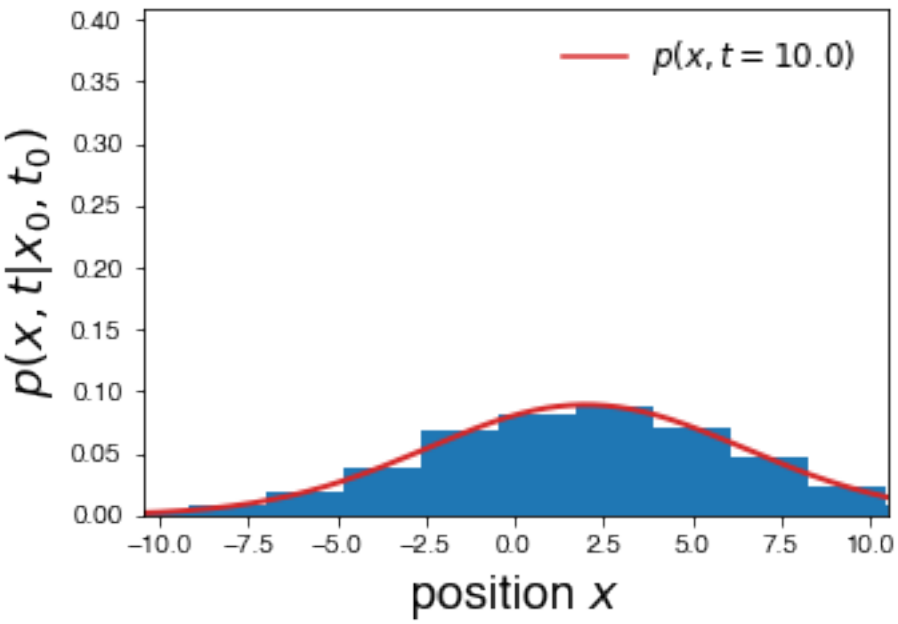
```
plotPositionPDF_free(X[2, :], 3.0, x0 = x0)
plotPositionPDF_free(X[3, :], 5.0, x0 = x0)
plotPositionPDF_free(X[4, :], 10.0, x0 = x0)
```





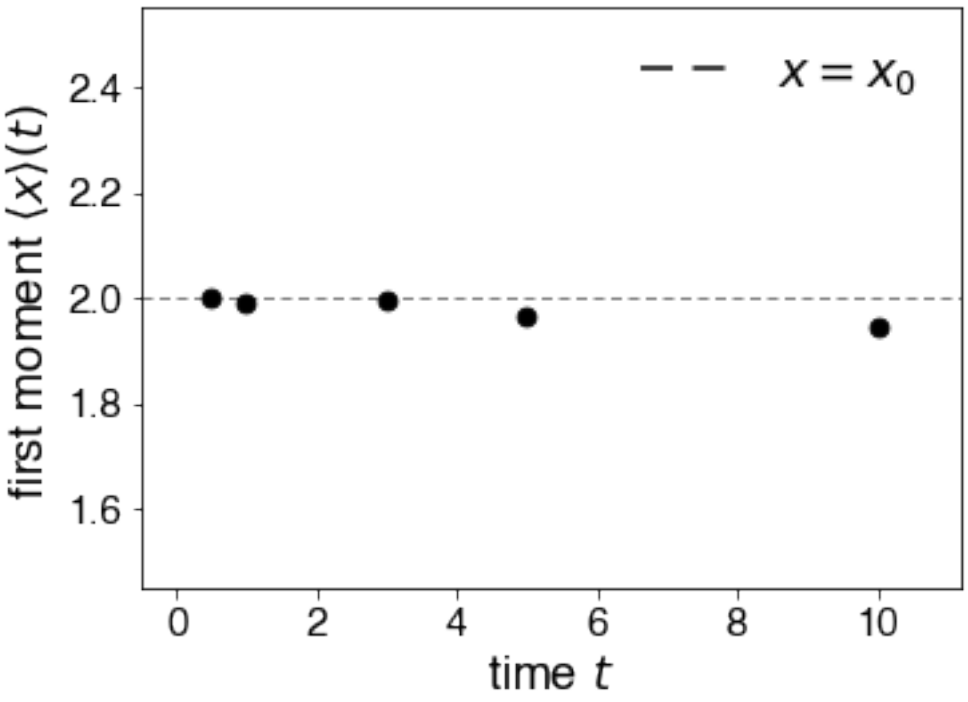

$p(x, t = 3.0)$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

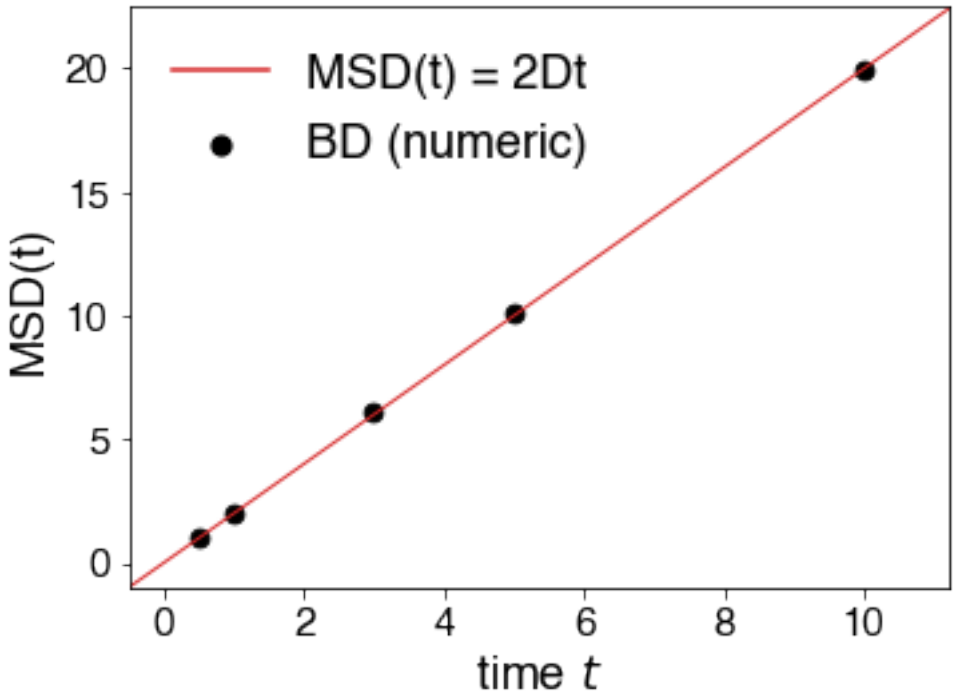

$p(x, t = 5.0)$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0



In [292]:
```
# compute the first moments and the MSD for the trajectories stored in X
mu, MSD = getMoments(X)
```

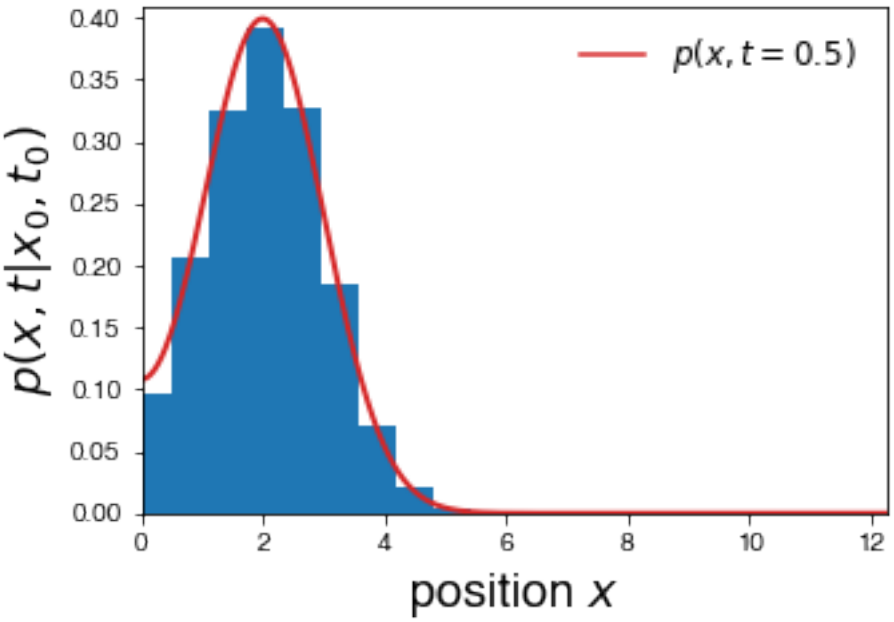
In [293]:
```
plotFirstMoments(sampleTimes, mu, x0 = x0)
plotMSD(sampleTimes, MSD, 1.0, D)
```

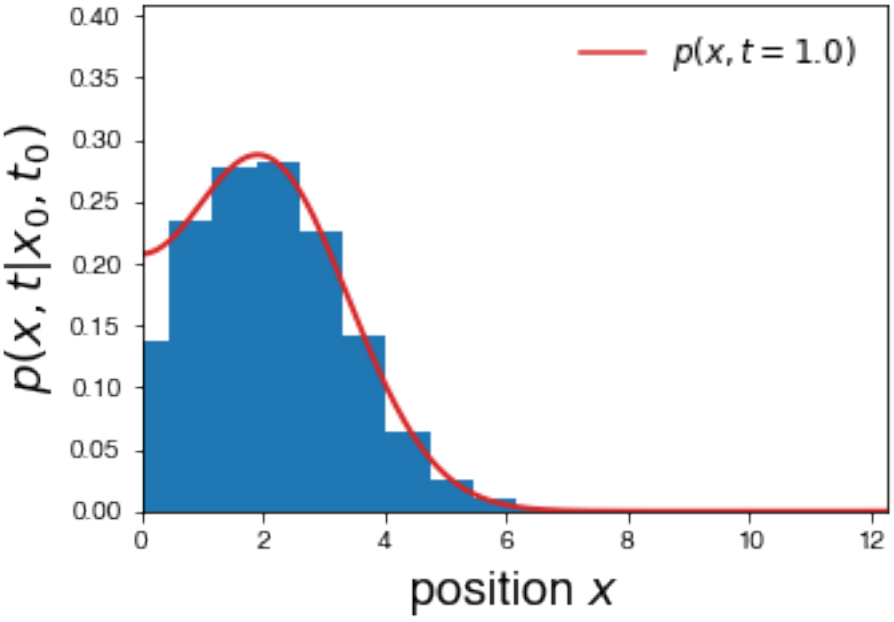


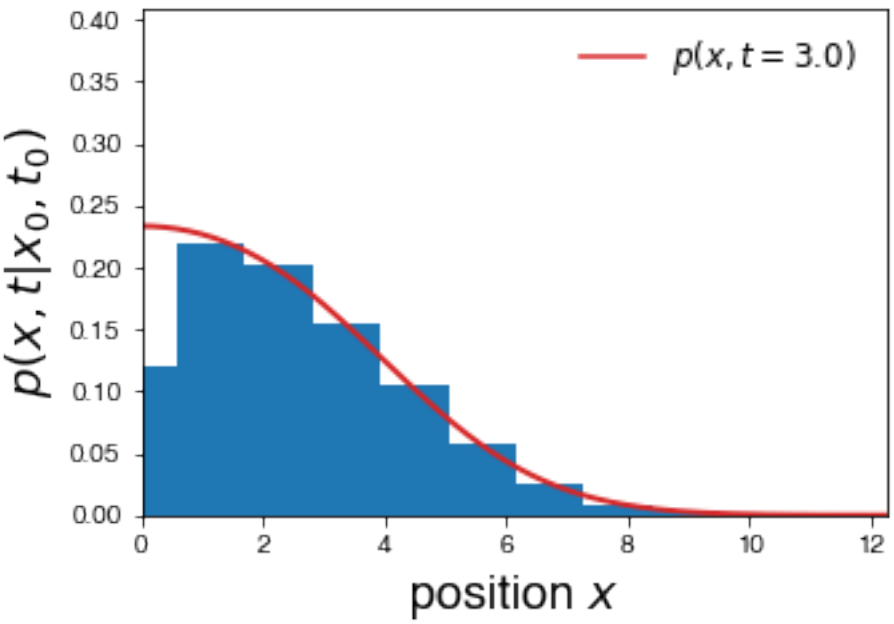


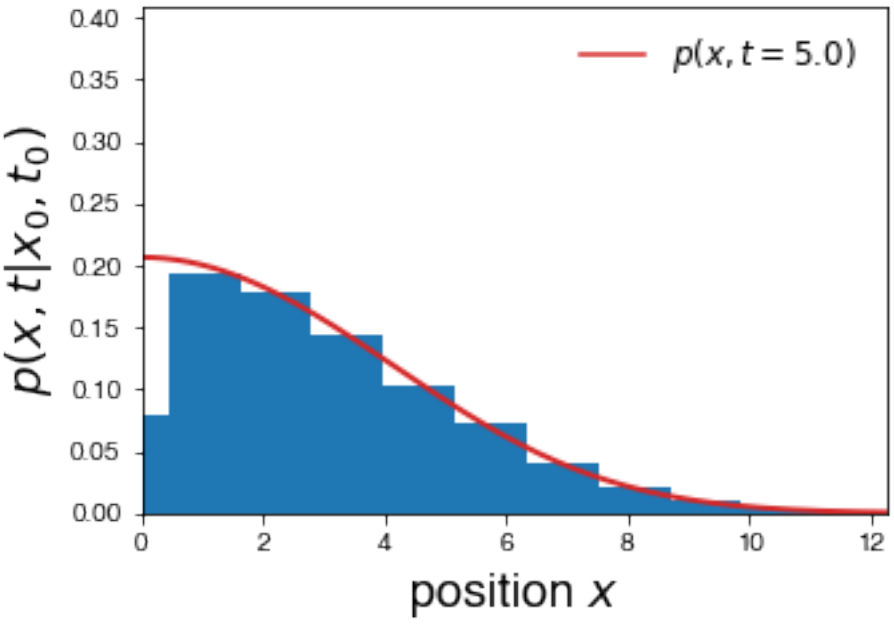
1.3 Diffusion with a reflecting boundary to the left

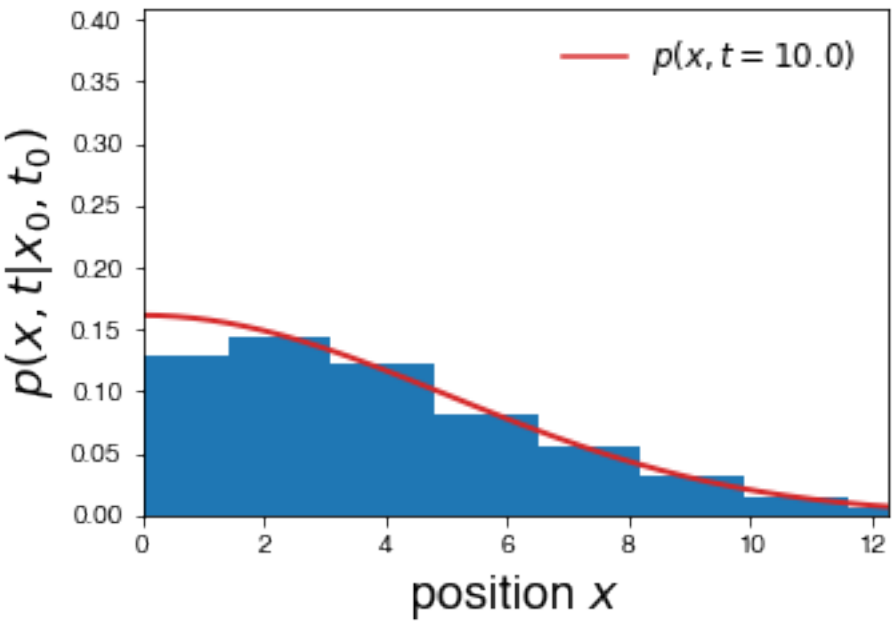
```
In [294]: %%time
          Xl = LangevinPropagatorReflectiveBC_vectorized(sampleTimes = sampleTimes,
                                                         m = m,
                                                         x0 = x0)

CPU times: user 6.04 s, sys: 53.5 ms, total: 6.1 s
Wall time: 6.28 s


In [296]: print(Xl.shape)

(5, 10000)


In [297]: plotPositionPDF_lrBC(Xl[0, :], 0.5, x0 = x0)
          plotPositionPDF_lrBC(Xl[1, :], 1.0, x0 = x0)
          plotPositionPDF_lrBC(Xl[2, :], 3.0, x0 = x0)
          plotPositionPDF_lrBC(Xl[3, :], 5.0, x0 = x0)
          plotPositionPDF_lrBC(Xl[4, :], 10.0, x0 = x0)
```


$p(x, t = 0.5)$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 1.0)$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 3.0)$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12


$p(x, t = 5.0)$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12



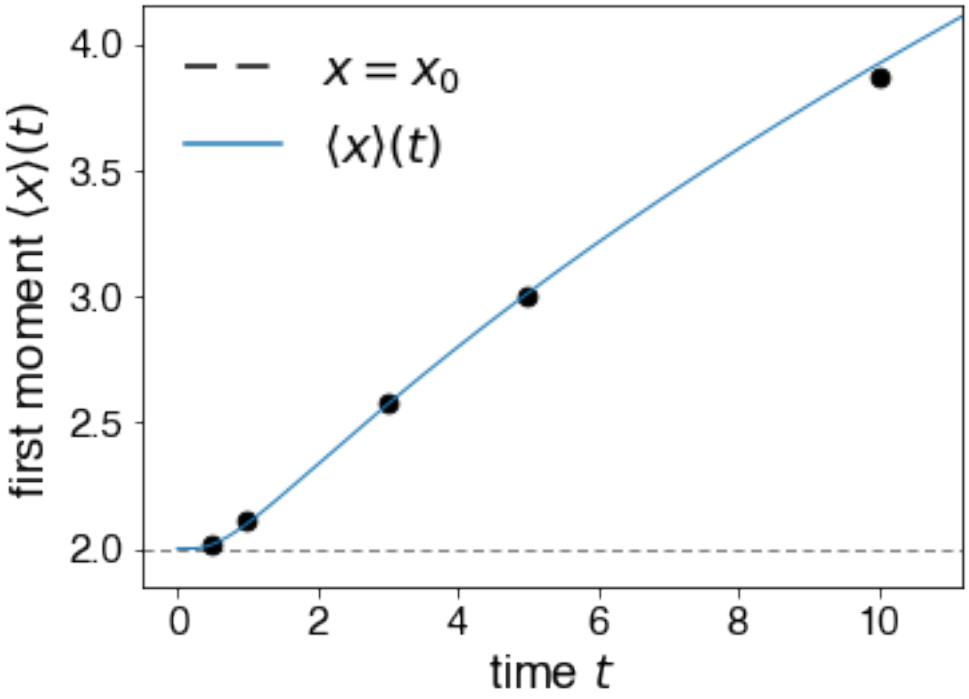
In [298]:
```
# compute the first moments and the MSD for the trajectories stored in X
mul, MSDl = getMoments(Xl)
```

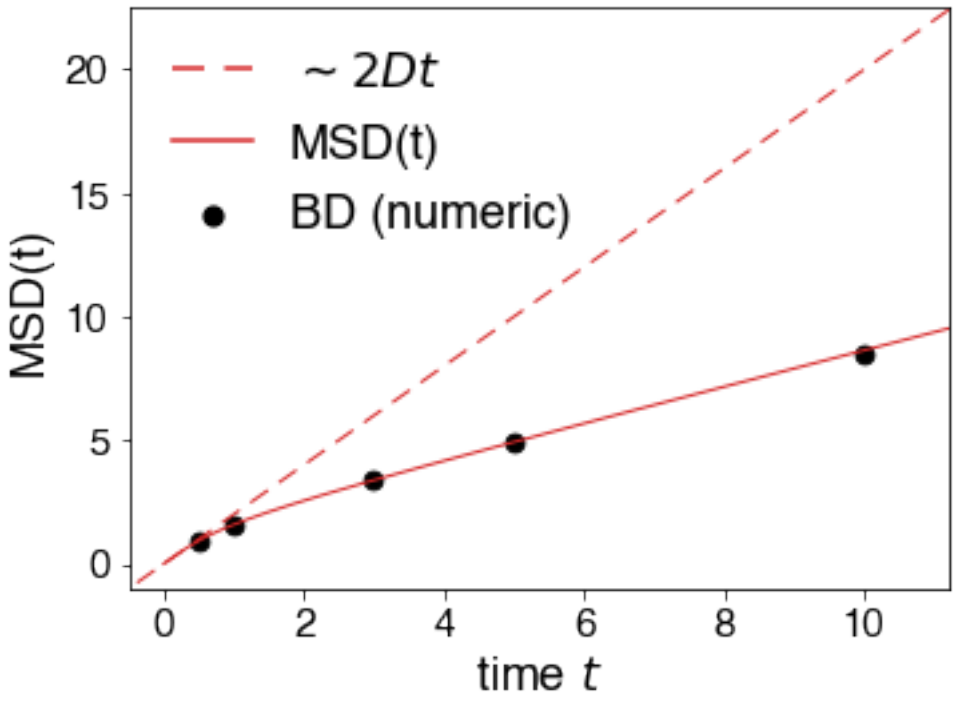
In [299]:
```
def plotFirstMoments_reflective(X, Y, x0 = 0.0):

    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('time $t$', fontsize = 18)
    ax.set_ylabel(r'first moment $\langle x \rangle(t)$', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    ax.plot([-2.0, 12.0], [x0, x0],
            dashes = [8.0, 5.0],
            lw = 0.5,
            color = 'k',
            label = r'$x = x_0$')

    xVals = np.linspace(0.0001, 12.0, 1000)
    yVals = np.array([Mean_ReflectiveBC(t, x0) for t in xVals])
    ax.plot(xVals, yVals,
            lw = 1.0, color = 'C0', label = r'$\langle x \rangle(t)$')
```

```
    ax.scatter(X, Y, color = 'k', s = 45)

    ax.set_xlim(-0.5, 11.2)
    ax.set_ylim(1.85, 4.15)

    leg = ax.legend(scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None

def plotMSD_reflective(X, Y, t, D = 1.0):

    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('time $t$', fontsize = 18)
    ax.set_ylabel(r'MSD(t)', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    ax.plot([-2.0, 12.0], [2.0 * D * (-2.0), 2.0 * D * (12.0)],
            lw = 1.0, color = 'C3', label = r'$\sim 2Dt$',
           dashes = [8.0, 5.0])

    xVals = np.linspace(0.0001, 12.0, 1000)
    yVals = np.array([MSD_ReflectiveBC(t, x0) for t in xVals])
    ax.plot(xVals, yVals,
            lw = 1.0, color = 'C3', label = r'MSD(t)')

    ax.scatter(X, Y, color = 'k', s = 45, label = r'BD (numeric)')

    ax.set_xlim(-0.5, 11.2)
    ax.set_ylim(-1.0, 22.5)

    leg = ax.legend(loc = 'upper left',
                    scatterpoints = 1,
                    markerscale = 1.0,
                    handlelength = 1.65,
                    ncol = 1,
                    fontsize = 18)
```

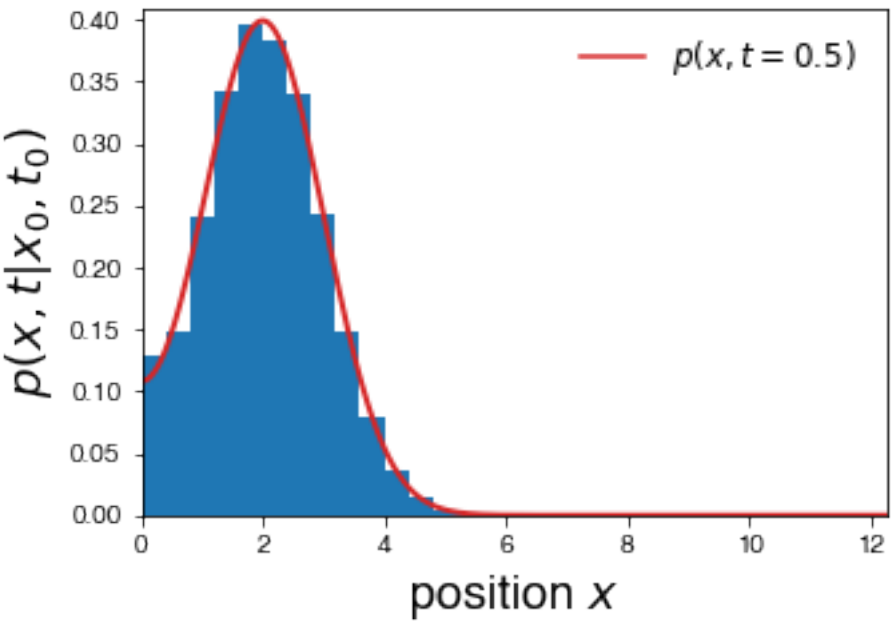
```
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None
```

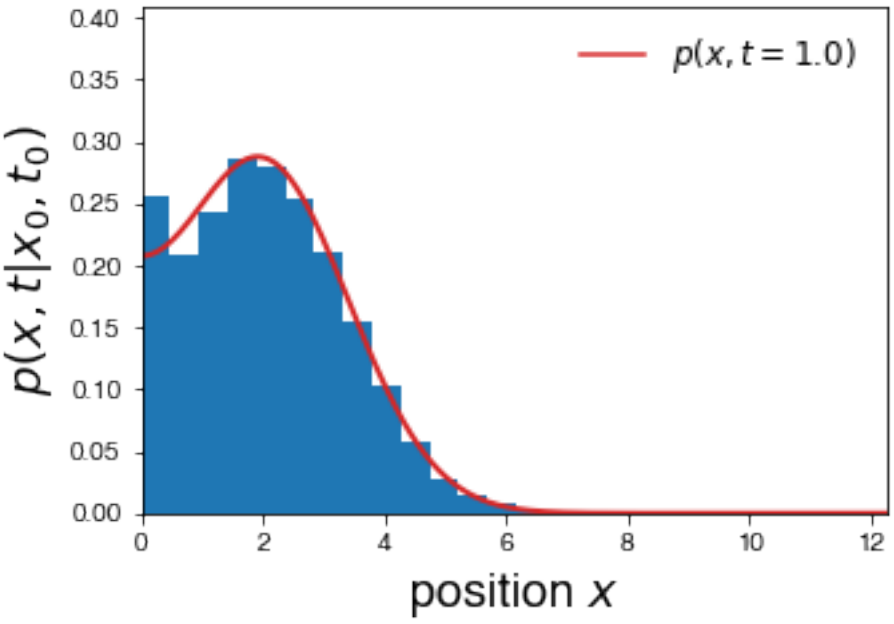
In [255]:
```
plotFirstMoments_reflective(sampleTimes, mul, x0 = x0)
plotMSD_reflective(sampleTimes, MSDl, 1.0, D)
```

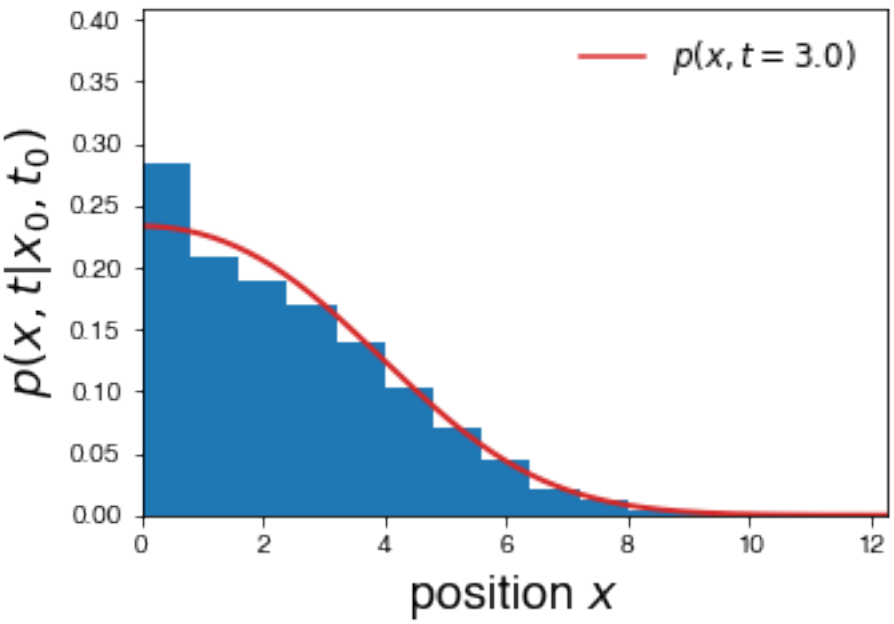


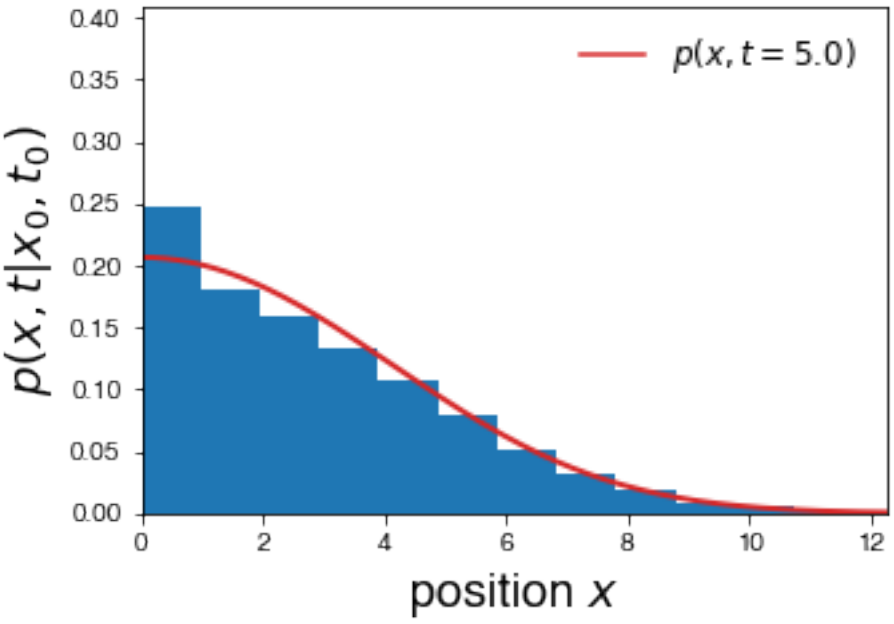


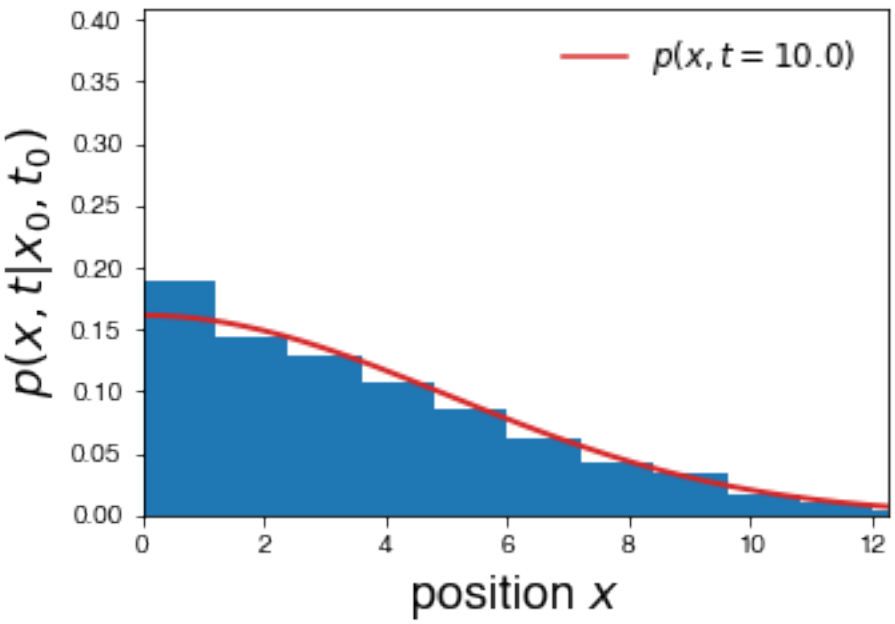

```
In [300]: %%time
          m = 20000
          Xl_over = LangevinPropagatorReflectiveBC_overshoot_vectorized(\
                      sampleTimes = sampleTimes,
                      m = m,
                      x0 = x0,
                      dt = 1.0e-1)

CPU times: user 155 ms, sys: 4.72 ms, total: 160 ms
Wall time: 173 ms


In [301]: print(Xl_over.shape)

(5, 20000)


In [302]: plotPositionPDF_lrBC(Xl_over[0, :], 0.5, x0 = x0)
          plotPositionPDF_lrBC(Xl_over[1, :], 1.0, x0 = x0)
          plotPositionPDF_lrBC(Xl_over[2, :], 3.0, x0 = x0)
          plotPositionPDF_lrBC(Xl_over[3, :], 5.0, x0 = x0)
          plotPositionPDF_lrBC(Xl_over[4, :], 10.0, x0 = x0)
```


$p(x, t = 0.5)$
$p(x, t|x_0, t_0)$
position x

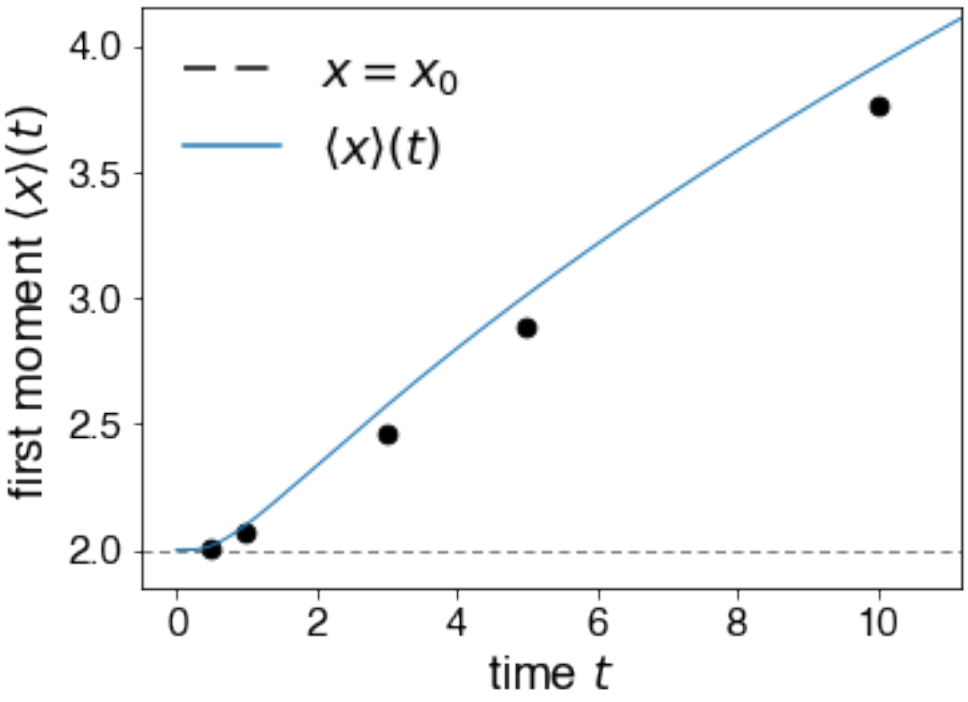

$p(x, t = 1.0)$
$p(x, t|x_0, t_0)$
position x

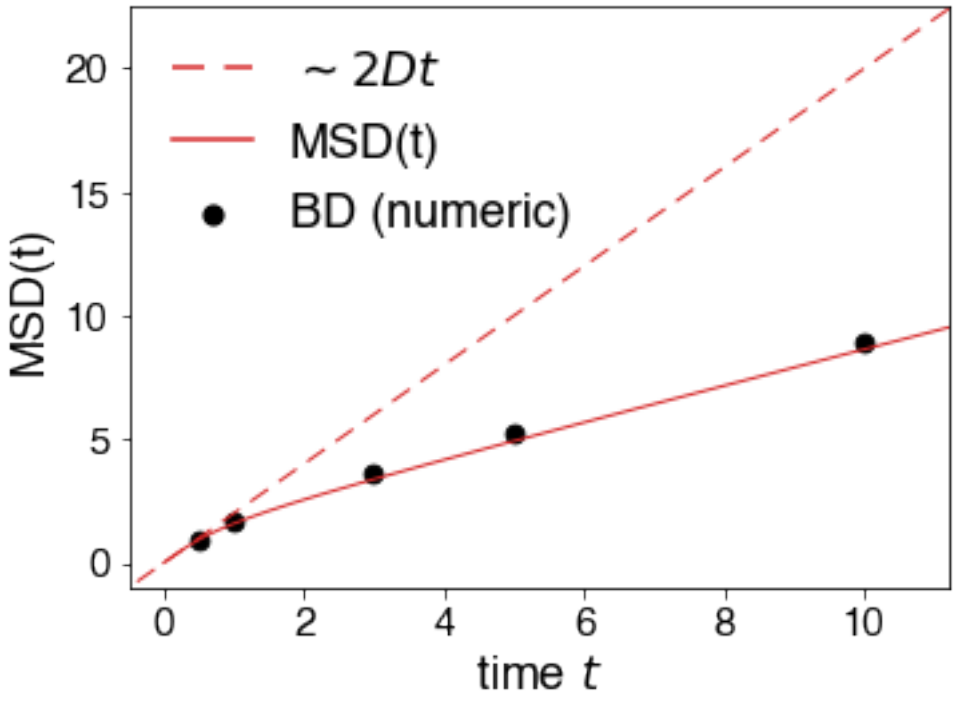

$p(x, t = 3.0)$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12


$p(x, t = 5.0)$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12



In [303]:
```
# compute the first moments and the MSD for the trajectories stored in X
mul, MSDl = getMoments(Xl_over)

plotFirstMoments_reflective(sampleTimes, mul, x0 = x0)
plotMSD_reflective(sampleTimes, MSDl, 1.0, D)
```



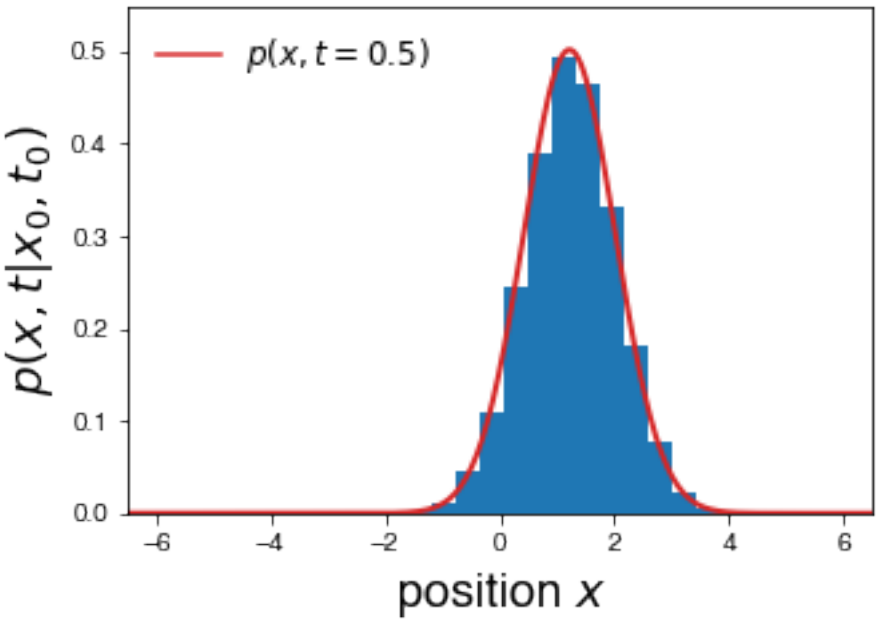


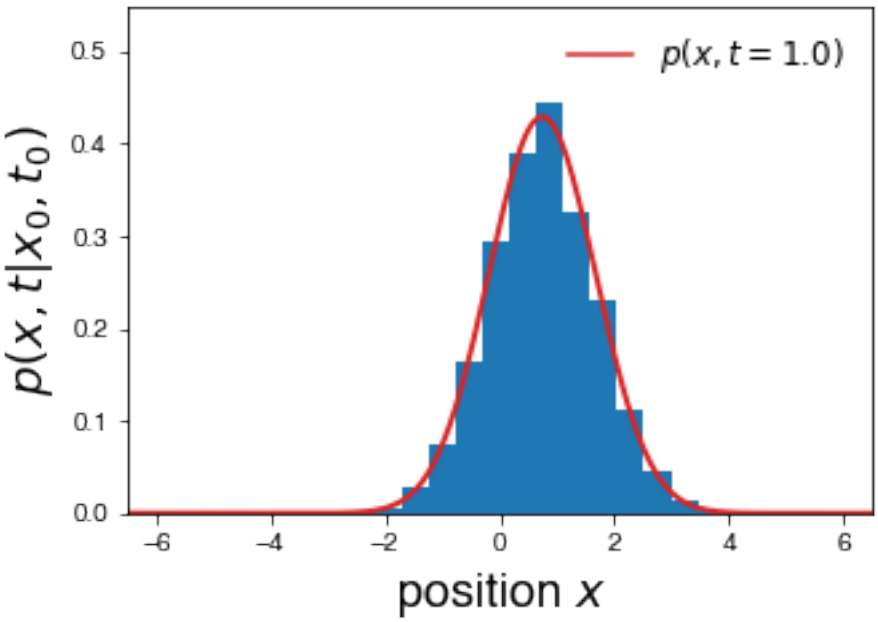
1.4 Diffusion in a harmonic potential

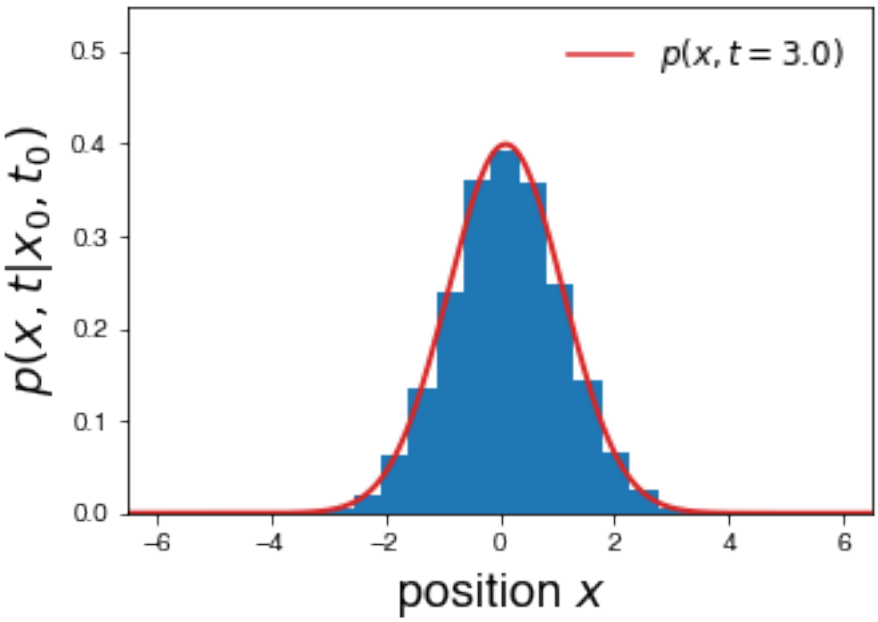
```
In [304]: x0 = 2.0
          m = 10000

In [305]: %%time
          Xh = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                             m = m,
                                             x0 = x0,
                                             a = -1.0)

CPU times: user 5.22 s, sys: 43.6 ms, total: 5.26 s
Wall time: 5.34 s


In [306]: print(Xh.shape)

(5, 10000)


In [307]: def plotPositionPDF_harmonic(X, t, D = 1.0, x0 = 0.0):
              f, ax = plt.subplots(1)
```

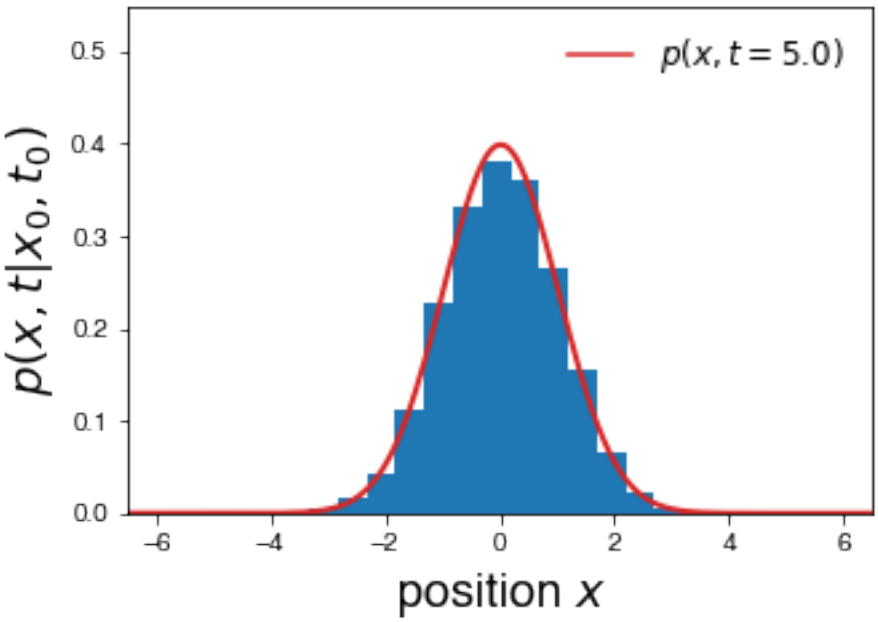
```
    f.set_size_inches(5.0, 3.5)

    labelfontsize = 10.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    plt.hist(X, density = True, bins = 15)

    xVals = np.linspace(-12.0, 12.0, 500)
    yVals = stats.norm.pdf(xVals, \
        x0 * np.exp(-t), np.sqrt(D * (1.0 - np.exp(-2.0 * t))))
    labelString = r'$p(x,t = %.1f)$' %(t)
    ax.plot(xVals, yVals, lw = 2.0, color = 'C3', label = labelString)

    ax.set_xlabel('position $x$', fontsize = 18)
    ax.set_ylabel(r'$p(x,t|x_0, t_0)$', fontsize = 18)

    ax.set_xlim(-6.5, 6.5)
    ax.set_ylim(0.0, 0.55)

    leg = ax.legend(fontsize = 12)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)

    return None
```

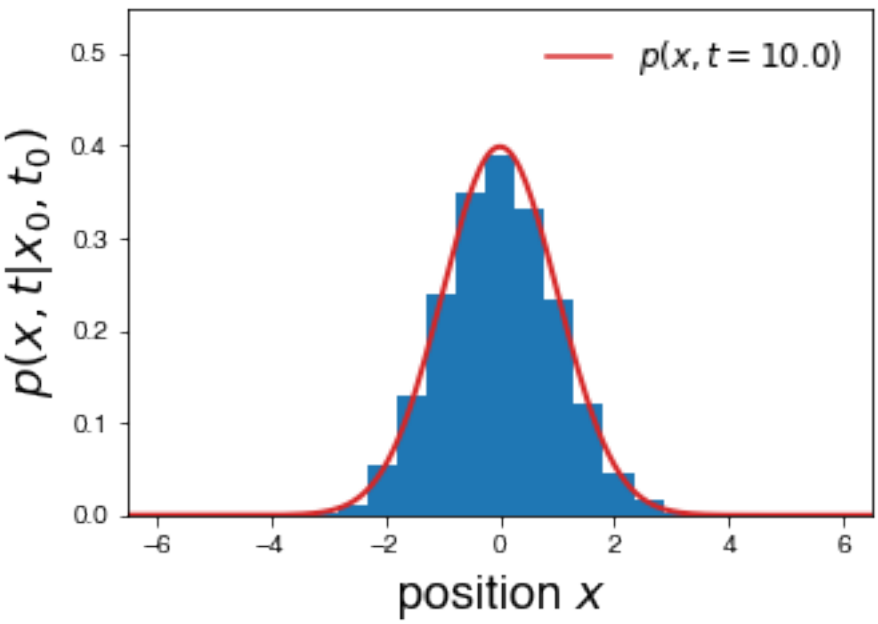
In [309]:
```
plotPositionPDF_harmonic(Xh[0, :], 0.5, x0 = x0)
plotPositionPDF_harmonic(Xh[1, :], 1.0, x0 = x0)
plotPositionPDF_harmonic(Xh[2, :], 3.0, x0 = x0)
plotPositionPDF_harmonic(Xh[3, :], 5.0, x0 = x0)
plotPositionPDF_harmonic(Xh[4, :], 10.0, x0 = x0)
```


$p(x, t = 0.5)$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 1.0)$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 3.0)$
$p(x, t|x_0, t_0)$
position x
0.0
0.1
0.2
0.3
0.4
0.5
−6
−4
−2
0
2
4
6


$p(x, t = 5.0)$
$p(x, t|x_0, t_0)$
position x
0.0
0.1
0.2
0.3
0.4
0.5
−6
−4
−2
0
2
4
6



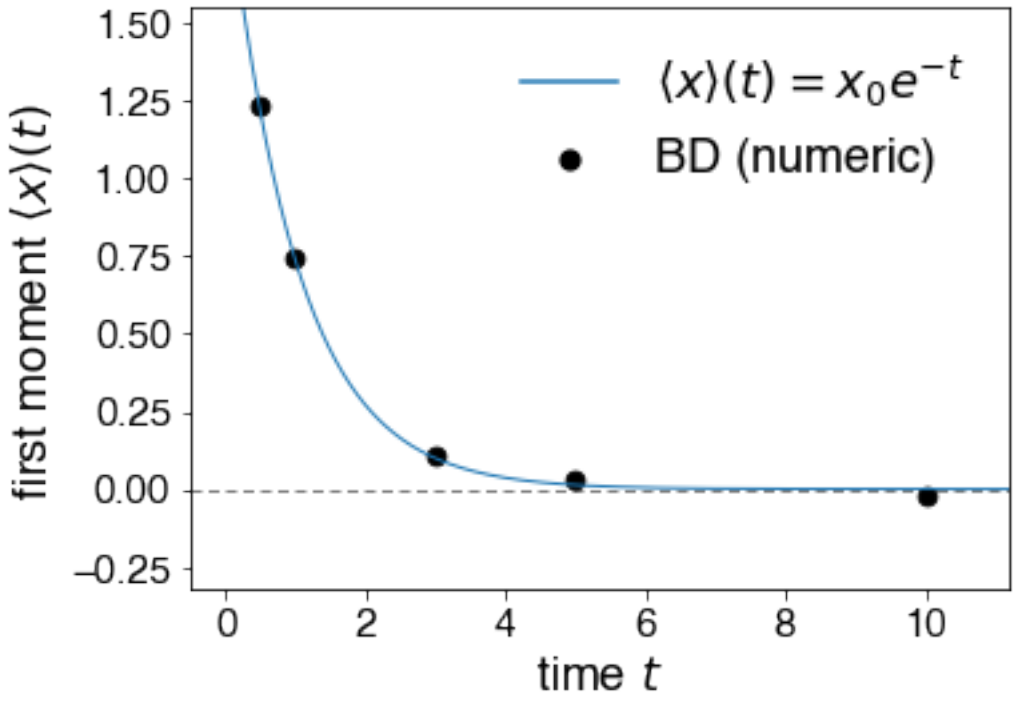
In [310]:
```
# compute the first moments and the MSD for the trajectories stored in Xh2
muh, MSDh = getMoments(Xh)
```

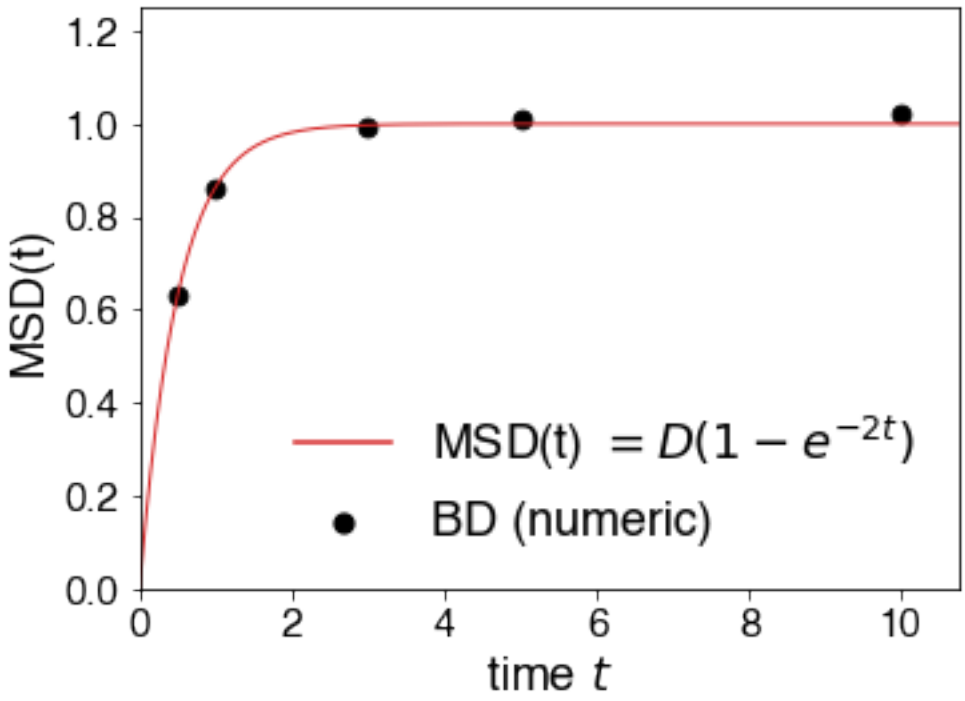
In [311]:
```
def plotFirstMomentsOU(X, Y, x0 = 0.0):
    ''' first moment of a Ornstein-Uhlenbeck process'''
    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('time $t$', fontsize = 18)
    ax.set_ylabel(r'first moment $\langle x \rangle(t)$', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    ax.plot([-2.0, 12.0], [0.0, 0.0],
            dashes = [8.0, 5.0],
            lw = 0.5,
            color = 'k')

    xVals = np.linspace(0.0, 12.5, 500)
    yVals = np.array([x0 * np.exp(-t) for t in xVals])
    ax.plot(xVals, yVals, lw = 1.0, color = 'C0',
            label = r'$\langle x\rangle(t) = x_0e^{-t}$')
```

```
    ax.scatter(X, Y,
               color = 'k',
               s = 45,
               label = r'BD (numeric)')

    ax.set_xlim(-0.5, 11.2)
    ax.set_ylim(-0.32, 1.55)

    leg = ax.legend(scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None

def plotMSD_harmonic(X, Y, D = 1.0):

    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('time $t$', fontsize = 18)
    ax.set_ylabel(r'MSD(t)', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)


    xVals = np.linspace(0.0, 12.0, 500)
    yVals = np.array([D * (1.0 - np.exp(-2.0 * t)) for t in xVals])

    ax.plot(xVals, yVals, lw = 1.0, color = 'C3',
            label = r'MSD(t) $= D(1-e^{-2t})$')
    ax.scatter(X, Y, color = 'k', s = 45, label = r'BD (numeric)')

    ax.set_xlim(0.0, 10.75)
    ax.set_ylim(0.0, 1.25)

    leg = ax.legend(loc = 'lower right',
                    scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
```

```
        leg.draw_frame(False)
        return None
```

In [312]:
```
plotFirstMomentsOU(sampleTimes, muh, x0 = 2.0)
plotMSD_harmonic(sampleTimes, MSDh, D = 1.0)
```





1.5 Analyze the accuracy of $p(x,t)$ for free diffusion as a function of the time step Δt

```
In [313]: # set simulation parameters here
          D = 1.0
          x0 = 2.0
          sampleTimes = np.array([3.0])
          m = 10000

In [314]: %%time
          X1 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                             m = m,
                                             x0 = x0,
                                             dt = 1.0)
          X2 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                             m = m,
                                             x0 = x0,
                                             dt = 0.1)
          X3 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                             m = m,
                                             x0 = x0,
                                             dt = 0.01)
          X4 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                             m = m,
                                             x0 = x0,
```

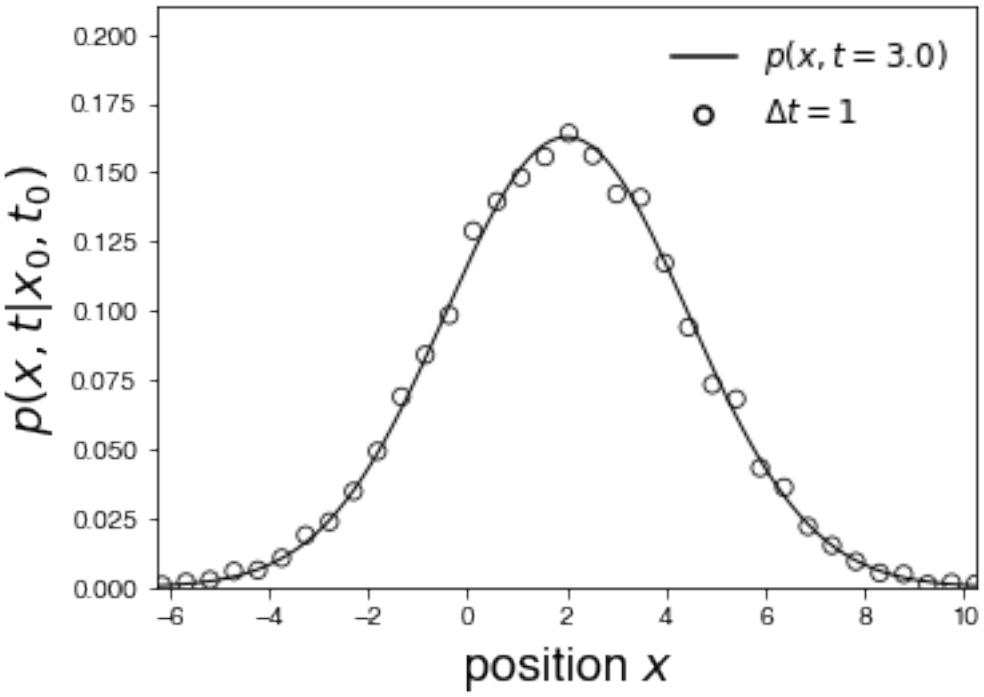
```
                                                dt = 0.001)
        print(X1.shape)
        print(X2.shape)
        print(X3.shape)
        print(X4.shape)
```

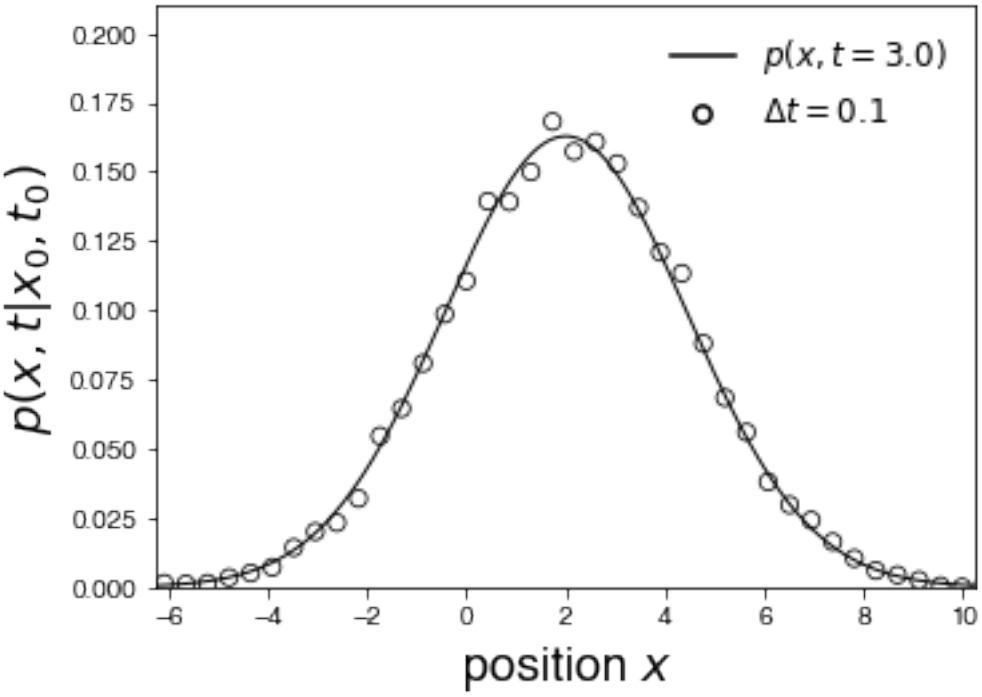
```
(1, 10000)
(1, 10000)
(1, 10000)
(1, 10000)
CPU times: user 2.04 s, sys: 29.5 ms, total: 2.07 s
Wall time: 2.15 s
```

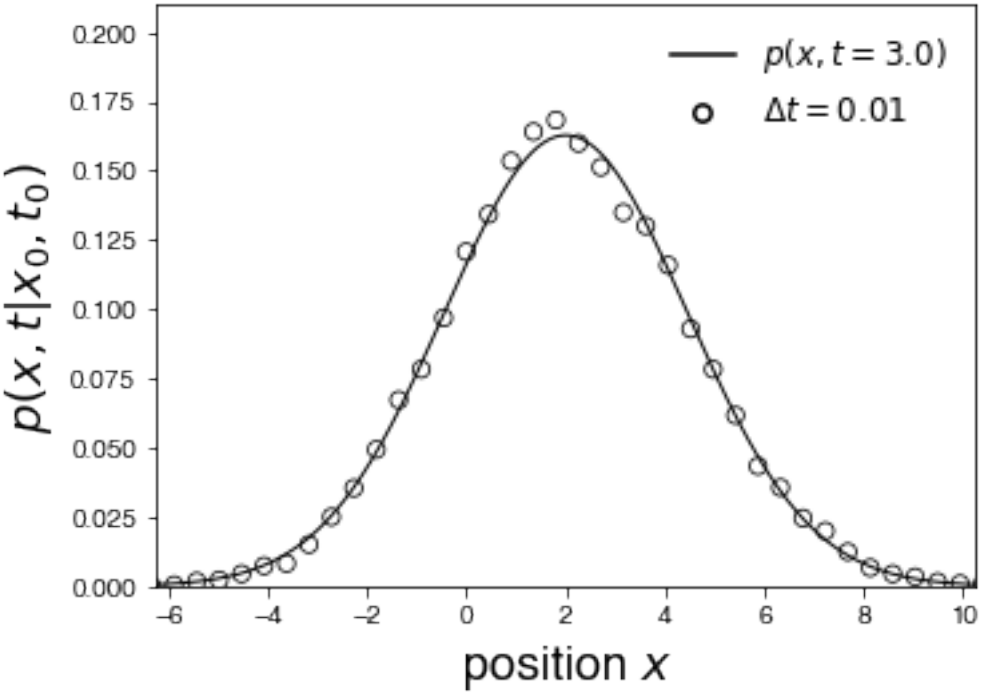
```
In [315]: def plot_PDF_free_mk2(X, t, label, x0 = 0.0, D = 1.0,):
              f, ax = plt.subplots(1)
              f.set_size_inches(5.5, 4.0)

              labelfontsize = 10.0
              for tick in ax.xaxis.get_major_ticks():
                  tick.label.set_fontsize(labelfontsize)
              for tick in ax.yaxis.get_major_ticks():
                  tick.label.set_fontsize(labelfontsize)

              counts, bins = np.histogram(X, bins = 40, normed = True)
              binCenters = [0.5 * (bins[k] + bins[k+1]) for k in range(len(counts))]
              binWidth = bins[1] - bins[0]
              ax.scatter(binCenters, counts,
                             s = 40.0,
                             marker = 'o',
                             facecolors = 'None',
                             edgecolors = 'k',
                             linewidth = 0.75,
                             label = label,
                             zorder = 3)

              xVals = np.linspace(-12.0, 12.0, 500)
              yVals = stats.norm.pdf(xVals, x0, np.sqrt(2.0 * D * t))
              labelString = r'$p(x,t = %.1f)$' %(t)
              ax.plot(xVals, yVals, lw = 1.0, color = 'k', label = labelString)

              ax.set_xlabel('position $x$', fontsize = 18)
              ax.set_ylabel(r'$p(x,t|x_0, t_0)$', fontsize = 18)

              ax.set_xlim(-6.25, 10.25)
              ax.set_ylim(0.0, 0.21)

              leg = ax.legend(fontsize = 12)
```

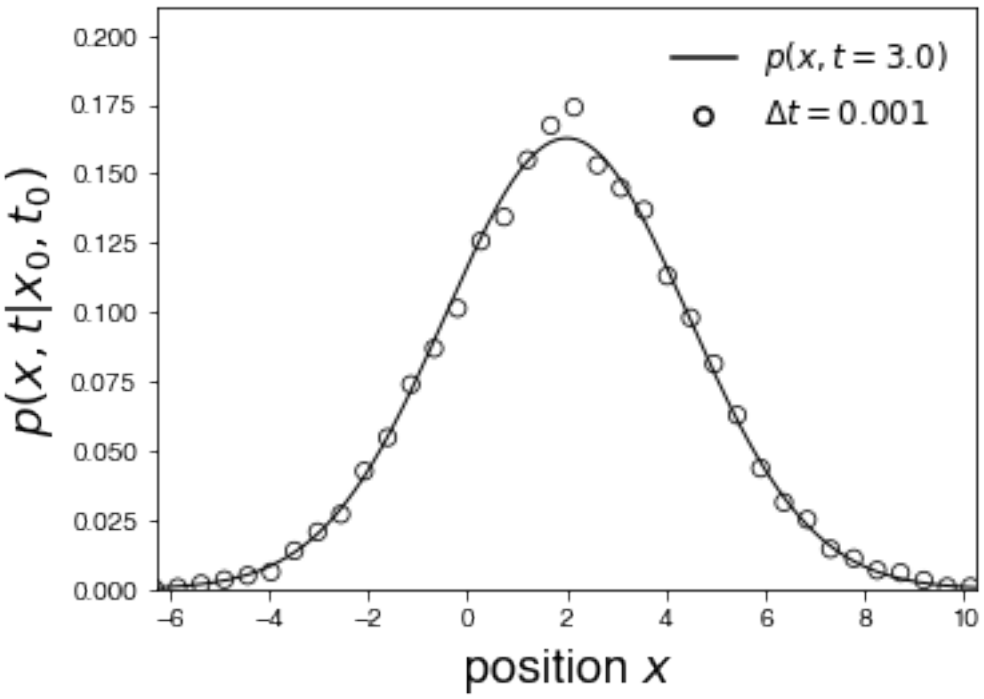
```
        for i, legobj in enumerate(leg.legendHandles):
            legobj.set_linewidth(1.5)
        leg.draw_frame(False)

        return None
```

In [273]:
```
plot_PDF_free_mk2(X1, t = 3.0, label = r'$\Delta t = 1$', x0 = x0)
plot_PDF_free_mk2(X2, t = 3.0, label = r'$\Delta t = 0.1$', x0 = x0)
plot_PDF_free_mk2(X3, t = 3.0, label = r'$\Delta t = 0.01$', x0 = x0)
plot_PDF_free_mk2(X4, t = 3.0, label = r'$\Delta t = 0.001$', x0 = x0)
```




$p(x, t = 3.0)$
$\Delta t = 0.1$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 3.0)$
$\Delta t = 0.01$
$p(x, t|x_0, t_0)$
position x



1.6 Analyze the accuracy of $p(x,t)$ for diffusion in a harmonic potential as a function of the time step Δt

```
In [316]: # set simulation parameters here
          D = 1.0
          x0 = 2.0
          sampleTimes = np.array([3.0])
          m = 10000

In [317]: %%time
          Xh1 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                              m = m,
                                              a = -1.0,
                                              sigma = 1.0,
                                              dt = 1.0,
                                              x0 = x0)

          Xh2 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                              m = m,
                                              a = -1.0,
                                              sigma = 1.0,
                                              dt = 0.1,
                                              x0 = x0)
```

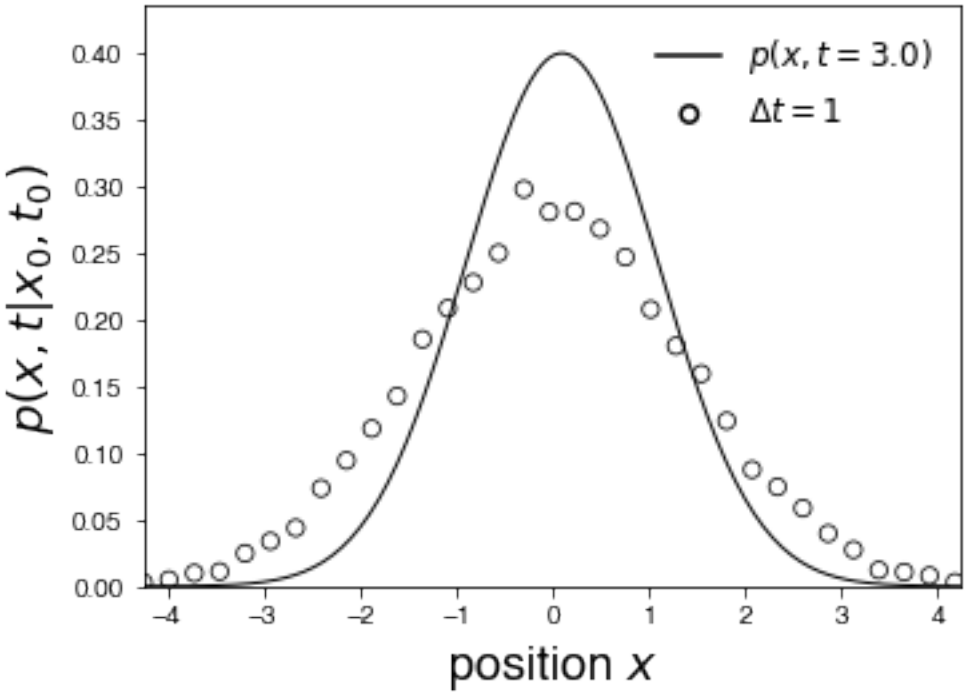
```
        Xh3 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                            m = m,
                                            a = -1.0,
                                            sigma = 1.0,
                                            dt = 0.01,
                                            x0 = x0)

        Xh4 = LangevinPropagator_vectorized(sampleTimes = sampleTimes,
                                            m = m,
                                            a = -1.0,
                                            sigma = 1.0,
                                            dt = 0.001,
                                            x0 = x0)

        print(Xh1.shape)
        print(Xh2.shape)
        print(Xh3.shape)
        print(Xh4.shape)
```

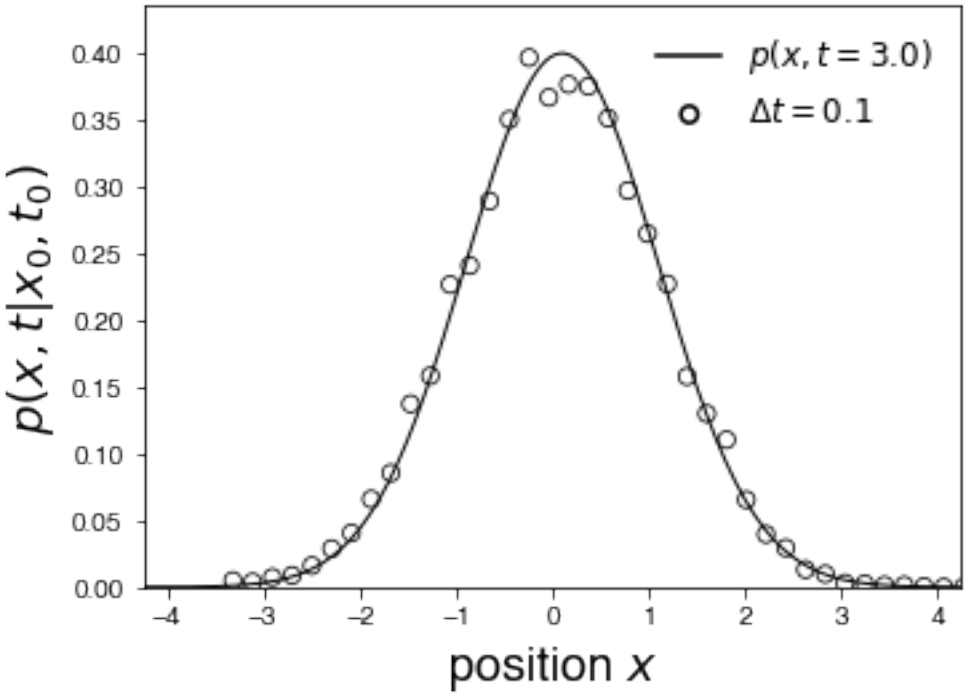
```
(1, 10000)
(1, 10000)
(1, 10000)
(1, 10000)
CPU times: user 1.9 s, sys: 21.6 ms, total: 1.92 s
Wall time: 2 s
```

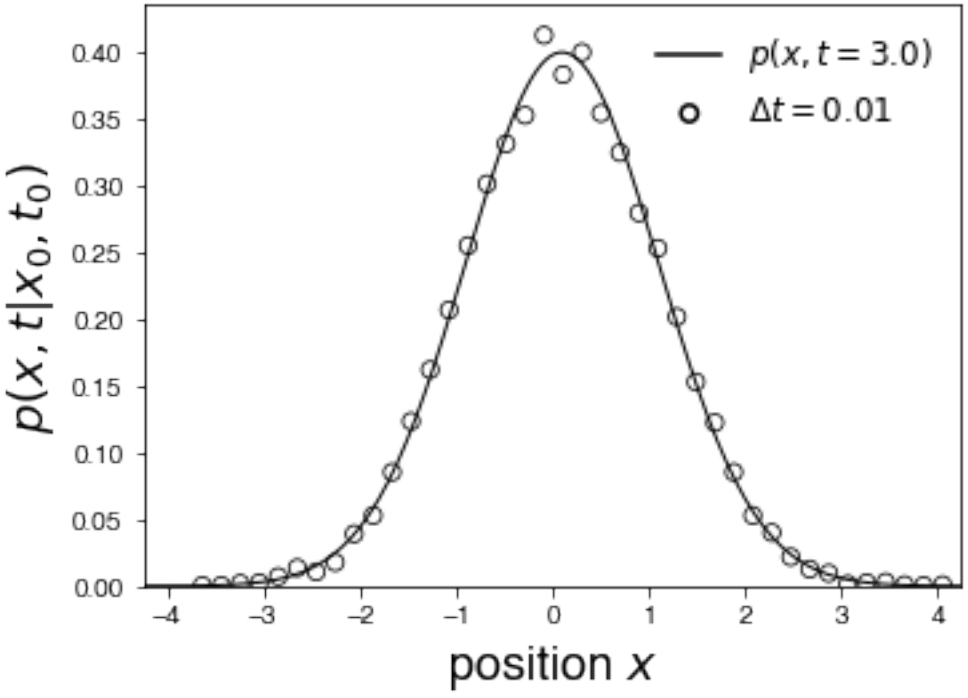
```
In [318]: def plot_PDF_harmonic_mk2(X, t, label, x0 = 0.0, D = 1.0,):
              f, ax = plt.subplots(1)
              f.set_size_inches(5.5, 4.0)

              labelfontsize = 10.0
              for tick in ax.xaxis.get_major_ticks():
                  tick.label.set_fontsize(labelfontsize)
              for tick in ax.yaxis.get_major_ticks():
                  tick.label.set_fontsize(labelfontsize)

              counts, bins = np.histogram(X, bins = 40, normed = True)
              binCenters = [0.5 * (bins[k] + bins[k+1]) for k in range(len(counts))]
              binWidth = bins[1] - bins[0]
              ax.scatter(binCenters, counts,
                             s = 40.0,
                             marker = 'o',
                             facecolors = 'None',
                             edgecolors = 'k',
                             linewidth = 0.75,
                             label = label,
                             zorder = 3)
```

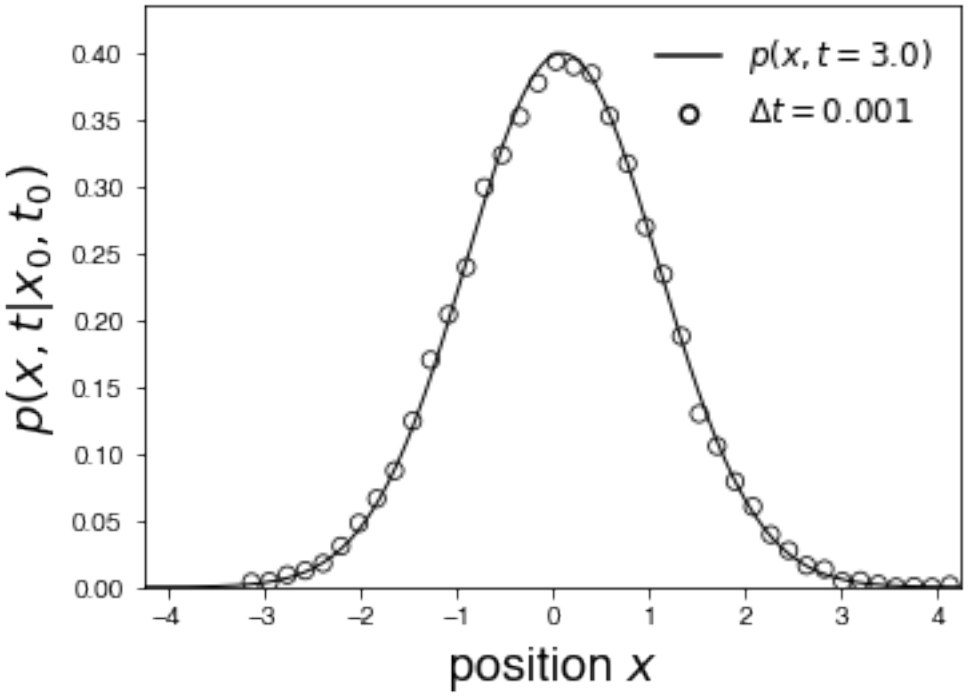
```
    xVals = np.linspace(-12.0, 12.0, 500)
    yVals = stats.norm.pdf(xVals, \
        x0 * np.exp(-t), np.sqrt(D * (1.0 - np.exp(-2.0 * t))))
    labelString = r'$p(x,t = %.1f)$' %(t)
    ax.plot(xVals, yVals, lw = 1.0, color = 'k', label = labelString)

    ax.set_xlabel('position $x$', fontsize = 18)
    ax.set_ylabel(r'$p(x,t|x_0, t_0)$', fontsize = 18)

    ax.set_xlim(-4.25, 4.25)
    ax.set_ylim(0.0, 0.435)

    leg = ax.legend(fontsize = 12)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)

    return None
```

In [319]:
```
plot_PDF_harmonic_mk2(Xh1, t = 3.0, label = r'$\Delta t = 1$', x0 = x0)
plot_PDF_harmonic_mk2(Xh2, t = 3.0, label = r'$\Delta t = 0.1$', x0 = x0)
plot_PDF_harmonic_mk2(Xh3, t = 3.0, label = r'$\Delta t = 0.01$', x0 = x0)
plot_PDF_harmonic_mk2(Xh4, t = 3.0, label = r'$\Delta t = 0.001$', x0 = x0)
```




$p(x, t = 3.0)$
$\Delta t = 0.1$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 3.0)$
$\Delta t = 0.01$
$p(x, t|x_0, t_0)$
position x


$p(x, t = 3.0)$
$\Delta t = 0.001$
$p(x, t|x_0, t_0)$
position x
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−4
−3
−2
−1
0
1
2
3
4