Testing `numba/jit` accelerated `dissipation3` functions

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Redo `Study 26` using `numba/jit`-accelerated functions coded in `dissipationtheory.dissipation3`. The `numba/jit` functions run below are 100 to 200 times faster than their pure-Python counterparts run in `Study 26`, enabling us to plot here a more detailed BLDS spectrum and explore friction and the zero-frequency limit of the BLDS spectrum as a function of many more conductivity points.

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The above header is for creating a nicely-formatted `.html` and `.pdf` documents using the program `quarto` (link). To create nicely-formated `.html` and `.pdf` versions of this notebook, run `quarto` from the command line as follows

```
quarto render dissipation-theory--Study-28.ipynb
```

Other useful information about this notebook:

- Filename: `dissipation-theory--Study-28.ipynb`
- Continued from: `dissipation-theory--Study-26.ipynb`
- Continued to: `dissipation-theory--Study-29.ipynb`

1 Preliminaries

```
import numpy as np
import pandas
```

```
%matplotlib inline
import matplotlib.pylab as plt
import matplotlib.cm as cm
import matplotlib.colors as mcolors
import cycler
```

```
font = {'family' : 'serif',
        'weight' : 'normal',
        'size'   : 12}
```

```
plt.rc('font', **font)
plt.rcParams['figure.figsize'] = 3.25, 3.5
```

```
THIS = 'dissipation-theory--Study-28--'
fig = {}
```

```
from dissipationtheory.constants import ureg, qe, epsilon0
from dissipationtheory.dissipation3 import CantileverModel, SampleModel1, SampleModel2
from dissipationtheory.dissipation3 import CantileverModelJit, SampleModel1Jit, SampleModel2Jit
from dissipationtheory.dissipation3 import theta1norm, gamma_perpendicular
from dissipationtheory.dissipation3 import theta1norm_jit, gamma_perpendicular_jit
from dissipationtheory.dissipation3 import blds_perpendicular, blds_perpendicular_jit
from dissipationtheory.dissipation3 import gamma_perpendicular_approx, BLDSzerohigh, BLDSzerolow, BLD
```

2 Sample object

Set up pure Python objects.

```
cantilever = CantileverModel(
    f_c = ureg.Quantity(75, 'kHz'),
    k_c = ureg.Quantity(2.8, 'N/m'),
    V_ts = ureg.Quantity(1, 'V'),
    R = ureg.Quantity(35, 'nm'),
    d = ureg.Quantity(38, 'nm')
)
```

```
sample1 = SampleModel1(
    cantilever = cantilever,
    h_s = ureg.Quantity(500, 'nm'),
    epsilon_s = ureg.Quantity(complex(3, -0.2), ''),  # <== edit this
    sigma = ureg.Quantity(1E-5, 'S/m'),
    rho = ureg.Quantity(1e21, '1/m^3'),
```

```
    epsilon_d = ureg.Quantity(complex(1e6, 0), ''),
    z_r = ureg.Quantity(300, 'nm')
)
```

```
sample1
```

```
cantilever

      resonance freq = 75.000 kHz
                     = 4.712e+05 rad/s
     spring constant = 2.800 N/m
  tip-sample voltage = 1.000 V
              radius = 35.000 nm
              height = 38.000 nm

semiconductor

             epsilon (real) = 3.000
             epsilon (imag) = -0.200
                  thickness = 500.0 nm
               conductivity = 1.000e-05 S/m
             charge density = 1.000e+21 m^{-3}
           reference height = 3.000e+02 nm

         roll-off frequency = 1.129e+06 Hz
                   mobility = 6.242e-08 m^2/(V s)
         diffusion constant = 1.614e-09 m^2/s
               Debye length = 3.780e+01 nm
          diffusion length = 5.852e+01 nm
   effective epsilon (real) = 3.000
   effective epsilon (imag) = -2.597

dielectric

  epsilon (real) = 1000000.000
  epsilon (imag) = 0.000
       thickness = infinite
```

Magically, set up the jit sample model from the pure Python sample model, as described in `Study 27`.

```
sample1_jit = SampleModel1Jit(**sample1.args())
```

```
sample1_jit.print()
```

```
cantilever
==========
   cantilever freq =  75000.0 Hz
                   =  471238.89803846896 rad/s
```

```
   spring constant =  2.8 N/m
tip-sample voltage =  1.0 V
            radius =  3.5e-08 m
            height =  3.8e-08 m

semiconductor
=============
          epsilon (real) =  3.0
          epsilon (imag) =  -0.2
               thickness =  5.000000000000001e-07 m
            conductivity =  1e-05 S/m
          charge density =  1e+21 m^{{-3}}
        reference height =  3.0000000000000004e-07 m

      roll-off frequency =  1129409.0673730192 Hz
                mobility =  6.241509090043337e-08 m^2/(V s)
      diffusion constant =  1.6135549206567651e-09 m^2/s
            Debye length =  3.7797775481848936e-08 m
        diffusion length =  5.851555252782804e-08 m
effective epsilon (real) =  3.0
effective epsilon (imag) =  -2.5966804779363124

dielectric
==========
 epsilon (real) =  1000000.0
 epsilon (imag) =  0.0
      thickness = infinite
```

3 Example friction calculation

Spot-check the new friction-calculation code by comparing a numba/jit result to a pure-Python result.

First, the numba/jit result.

```
%%time
ans1a = gamma_perpendicular_jit(theta1norm_jit, sample1_jit)
ans1a
```

```
CPU times: user 9.86 ms, sys: 1.98 ms, total: 11.8 ms
Wall time: 13.6 ms
```

$$\left(\quad\right)\ \frac{\text{piconewton}\cdot\text{second}}{\text{meter}}$$

Now the pure Python result.

```
%%time
ans1b = gamma_perpendicular(theta1norm, sample1)
ans1b
```

```
CPU times: user 2.92 s, sys: 30.7 ms, total: 2.95 s
Wall time: 3.15 s
```

$$\left(\quad\right) \frac{\text{piconewton}\cdot\text{second}}{\text{meter}}$$

By inspection we get the same result for the three terms' contribution to the friction. Success!

The numba/jit calculation is 100 to 200 times faster.

4 Example BLDS calculation

Compare the execution time for pure-Python and numba/jit calculations.

```
omega_m = ureg.Quantity(2 * np.pi * np.logspace(1, 2, 2), 'Hz')
```

```
%%time
ans2a = blds_perpendicular_jit(theta1norm_jit, sample1_jit, omega_m)
ans2a
```

```
CPU times: user 20.1 ms, sys: 1.12 ms, total: 21.3 ms
Wall time: 20.8 ms
```

$$\left(\quad\right) \text{ hertz}$$

```
%%time
ans2b = blds_perpendicular(theta1norm, sample1, omega_m)
ans2b
```

```
CPU times: user 7.69 s, sys: 78.3 ms, total: 7.76 s
Wall time: 8.22 s
```

$$\left(\quad\right) \text{ hertz}$$

By inspection we get the same result for the two terms' contribution to the BDLS frequency shift. Success!

The numba/jit calculation is 150 to 200 times faster.

5 Create list of modulation frequencies and charge densities

Set up arrays of modulation frequency ω_m and conductivity σ.

```
N_omega = 100
N_sigma = 50
```

```
omega_m = ureg.Quantity(
    np.logspace(
        start=np.log10(1e1),
        stop=np.log10(1e8),
        num=N_omega), 'Hz')
```

```
sigma = ureg.Quantity(
    np.logspace(
        start=np.log10(1e-9),
        stop=np.log10(1),
        num=N_sigma), 'S/m')
```

Assume a fixed mobility of $\mu = 10^{-8}\ \mathrm{m}^2/\mathrm{Vs}$, an ionic mobility.

```
mu = ureg.Quantity(1e-8, 'm^2/(V s)')
```

As we vary σ, we should vary the charge density ρ to keep the mobility constant.

```
rho = (sigma / (qe * mu)).to('1/m^3')
```

Get ready to run the simulations.

```
data = {}        # many simulations
data['01'] = {}  # the first simulation
```

Loop over conductivities, computing the BLDS spectrum and the friction.

```
%%time

# remember
sigma0 = sample1_jit.sigma
rho0 =  sample1_jit.rho

# set
for rho_, sigma_ in zip(rho, sigma):

    sample1_jit.rho = rho_.to('1/m^3').magnitude
    sample1_jit.sigma = sigma_.to('S/m').magnitude

    gamma = gamma_perpendicular_jit(theta1norm_jit, sample1_jit).to('pN s/m')
    f_BLDS = blds_perpendicular_jit(theta1norm_jit, sample1_jit, omega_m).to('Hz')

    data['01'][str(sigma_.to('S/m').magnitude)] = {
```

```
        'omega_m': omega_m,
        'f_BLDS': f_BLDS,
        'gamma': gamma,
        'sigma': ureg.Quantity(sample1_jit.sigma, 'S/m'),
        'd': ureg.Quantity(sample1_jit.cantilever.d, 'm'),
        'rho': ureg.Quantity(sample1_jit.rho, '1/m^3'),
        'LD': ureg.Quantity(sample1_jit.LD, 'm'),
        'omega_c': ureg.Quantity(sample1_jit.cantilever.omega_c, 'Hz'),
        'omega_0': (ureg.Quantity(sample1_jit.sigma, 'S/m')/epsilon0).to('Hz')}

# reset
sample1_jit.rho = rho0
sample1_jit.sigma = sigma0
```

```
CPU times: user 16.4 s, sys: 179 ms, total: 16.6 s
Wall time: 17.8 s
```

Explore the `data['01']` object. The keys are the conductivity in S/m, running from 10^{-9} to 1.

```
(list(data['01'].keys())[0],
 list(data['01'].keys())[-1])
```

```
('1e-09', '1.0')
```

The BLDS frequencies are given as a 100×3 array, with 100 being the number of modulation frequencies and 3 being the number of terms in Loring's sum.

```
data['01']['1e-09']['f_BLDS'].shape
```

```
(100, 3)
```

To get the BLDS frequency, sum up the three components. We do this by summing over the second dimension.

```
data['01']['1e-09']['f_BLDS'].sum(axis=1)[0]
```

-3.6261448167750916 hertz

From `Study 25`, a helper function to plot the BLDS spectra. Make sure to add up the three terms to get the total BLDS frequency shift.

```
def plotBLDS(data):

    rho = np.zeros(len(data))
    for index, key in enumerate(data.keys()):

        rho[index] = data[key]['rho'].to('1/cm^3').magnitude

    # colormap = plt.cm.jet
```

```
    colormap = plt.cm.magma_r
    color_list = [colormap(i) for i in np.linspace(0, 1, len(data))]

    normalized_colors = mcolors.LogNorm(vmin=min(rho), vmax=max(rho))
    scalar_mappable = cm.ScalarMappable(norm=normalized_colors, cmap=colormap)
    scalar_mappable.set_array(len(color_list))

    fig, ax = plt.subplots(figsize=(4.5, 3))
    for index, key in enumerate(data.keys()):

        with plt.style.context('seaborn-v0_8'):
            plt.semilogx(
                data[key]['omega_m'].to('Hz').magnitude,
                np.abs(data[key]['f_BLDS'].sum(axis=1).to('Hz').magnitude),
                '-',
                color=color_list[index])

    # color bar
    clb=plt.colorbar(scalar_mappable, ax=ax)
    clb.ax.set_title(r'$\rho \: [\mathrm{cm}^{-3}]$', fontsize=12)

    plt.ylabel('|$\Delta f_{\mathrm{BLDS}}$| [Hz]')
    plt.xlabel('mod. freq. $\omega_{\mathrm{m}}$ [rad/s]')
    plt.tight_layout()
    plt.show()

    return fig
```

Plot every 3rd BLDS spectrum.

```
data['01-short'] = {}
for key in list(data['01'].keys())[::3]:
    data['01-short'][key] = data['01'][key]

fig['01'] = plotBLDS(data['01-short'])
```

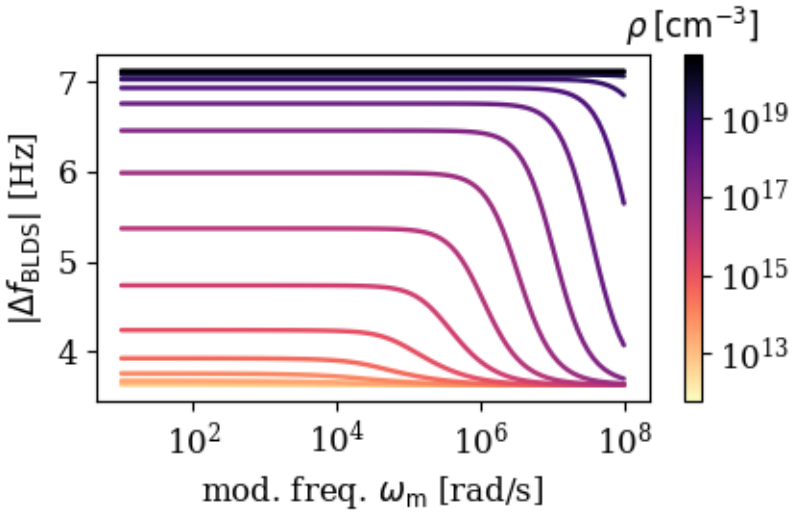


Figure 1: Broadband local dielectric spectrum of a semi-infinite semiconductor versus charge density.

I have rewritten the `BLDSlimits` function to return low-density and high-density limits for all three terms; see `BLDSzerohigh` and `BLDSzerolow` in `dissipation3`. I want to rewrite the plotting function below, `plotme`, to use these new function.

I think I can consense the code considerably by using `pandas` dataframes. Convert `data['01']` to a `pandas` dataframe and explore.

```
df = pandas.DataFrame.from_dict(data['01'])
df
```

	1e-09	1.5264179671752366e-09	2
omega_m	[10.0 hertz, 11.768119524349984 hertz, 13.8488...	[10.0 hertz, 11.768119524349984 hertz, 13.8488...	[
f_BLDS	[[-2.6979093482955756 hertz, -0.39730981074967...	[[-2.698090920476028 hertz, -0.397398186774877...	[
gamma	[42.51061503924813 piconewton * second / meter...	[42.519745468636685 piconewton * second / mete...	[
sigma	1e-09 siemens / meter	1.5264179671752366e-09 siemens / meter	2
d	3.8e-08 meter	3.8e-08 meter	3
rho	6.241509090043338e+17 / meter ** 3	9.527151617329711e+17 / meter ** 3	1
LD	1.5129390669059824e-06 meter	1.2245730647396677e-06 meter	9
omega_c	471238.89803846896 hertz	471238.89803846896 hertz	4
omega_0	112.94090673730192 hertz	172.39502927288035 hertz	2

We want to exract the data in the rows, as numbers without units, for plotting. Read the `rho` row and convert it to a numpy array. Loop over the elements of the array, specify the element's units, and get the magnitude of the resulting element. Convert the result list to a numpy array. Print out every 10th element of the resulting arrray.

```
np.array([a.to('1/m^3').magnitude for a in df.loc['rho'].to_numpy()])[0:-1:10]
```

```
array([6.24150909e+17, 4.28572501e+19, 2.94278813e+21, 2.02066207e+23,
       1.38748528e+25])
```

Some of the rows return an array of arrays. Run one of these, `omega_m`, through the same procedure. Now we get an array of arrays, stripped of their units.

```
np.array([a.to('Hz').magnitude for a in df.loc['omega_m'].to_numpy()])[0][0:-1:10]
```

```
array([1.00000000e+01, 5.09413801e+01, 2.59502421e+02, 1.32194115e+03,
       6.73415066e+03, 3.43046929e+04, 1.74752840e+05, 8.90215085e+05,
       4.53487851e+06, 2.31012970e+07])
```

Generalize this procedure, simultaneously looping of all the rows and specifying each of their units.

```
adict = {}
keys = ['omega_m', 'f_BLDS', 'gamma', 'sigma', 'd', 'rho', 'LD', 'omega_c', 'omega_0']
units = ['Hz', 'Hz', 'pN s/m', 'S/m', 'm', '1/m^3', 'm', 'Hz', 'Hz']

for key, unit in zip(keys, units):
    adict[key] = np.array([a.to(unit).magnitude for a in df.loc[key].to_numpy()])
```

Check that the above does what we expect. Look at the shape of the resulting arrays. We have 50 columns, one for each charge density. For the spectra, we have 100 frequencies. Then, for the calculated signals, `f_BLDS` and `gamma`, we have three components, one from each or Loring's terms.

```
adict['rho'].shape
```

```
(50,)
```

```
adict['omega_m'].shape
```

```
(50, 100)
```

```
adict['f_BLDS'].shape
```

```
(50, 100, 3)
```

```
adict['gamma'].shape
```

```
(50, 3)
```

Check out the new code computing the limiting cases.

```
BLDSzerohigh(sample1, np.logspace(-1,1,5)).shape
```

```
(5, 3)
```

```
BLDSzerolow(sample1, np.logspace(-1,1,5)).shape
```

```
(5, 3)
```

Check out the new code for computing the linear approximation to the K_2 term.

```
x_sub, BLDSapprox = BLDSapproxK2(sample1, np.logspace(-3,3,100))
(x_sub.shape, BLDSapprox.shape)
```

```
((60,), (60,))
```

```
(x_sub.min(), x_sub.max())
```

```
(0.001, 3.7649358067924674)
```

Check out the new code for computing the $\gamma_\perp$ (a) $\rho \to 0$ limit and (b) linear ρ expansion.

```
xR = adict['omega_0']/(sample1.epsilon_s.real.magnitude * adict['omega_c'])
g_low, g_approx = gamma_perpendicular_approx(sample1, xR)
(g_low.shape, g_approx.shape)
```

```
((50, 3), (50, 3))
```

Now rewrite the `Study 26` code.

```
def plotme(data, sample):

    df = pandas.DataFrame.from_dict(data)

    keys =  ['omega_m', 'f_BLDS', 'gamma',  'sigma', 'd', 'rho',   'LD', 'omega_c', 'omega_0']
    units = ['Hz',      'Hz',     'pN s/m', 'S/m',   'm', '1/m^3', 'm',  'Hz',      'Hz']

    adict = {}
    for key, unit in zip(keys, units):
        adict[key] = np.array([a.to(unit).magnitude for a in df.loc[key].to_numpy()])

    # (Left hand plot)
    # Make the x-axis the unitless ratio of the height to Debye length squared,
    # which is proportional to charge density.

    xL = (adict['d']/adict['LD'])**2
    rho0L = (adict['rho']/xL)[0]

    # Define functions to convert from xL to rho and back again

    def fwdL(xL):
        return xL*rho0L

    def revL(rho):
        return rho/rho0L
```

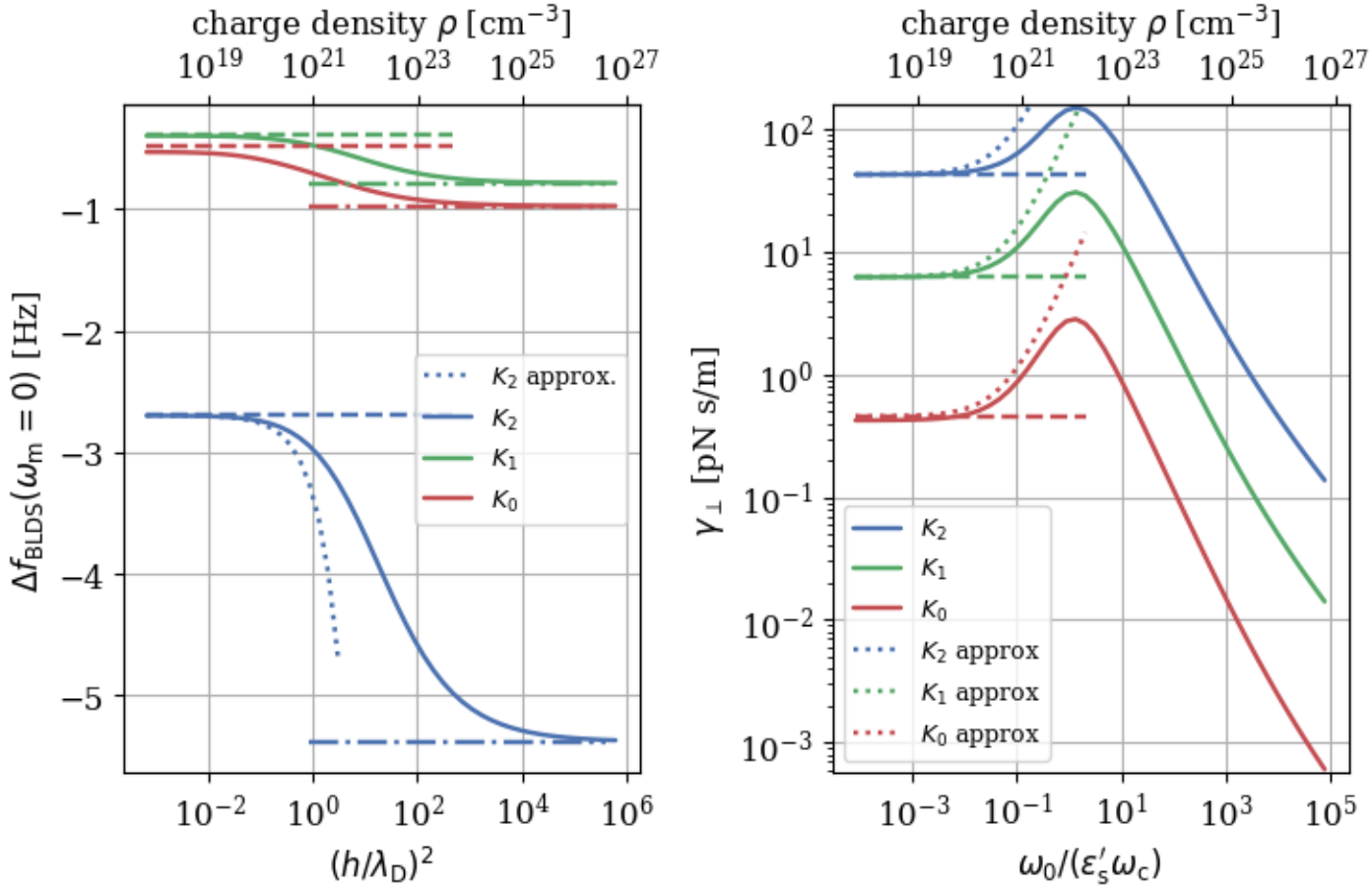
```
# (Right hand plot)
# Make the x-axis the unitless ratio of omega_0 to omega_c, which
# is proportional to conductivity and therefore charge density

xR = adict['omega_0']/(sample.epsilon_s.real.magnitude * adict['omega_c'])
rho0R = (adict['rho']/xR)[0]

# Define functions to convert from xR to rho and back again

def fwdR(xR):
    return xR*rho0R

def revR(rho):
    return rho/rho0R

# Now make the nice plot

fig, ax = plt.subplots(1, 2, figsize=(7.5, 5))

ax2L = ax[0].secondary_xaxis("top", functions=(fwdL,revL))
ax2R = ax[1].secondary_xaxis("top", functions=(fwdR,revR))

# xL_sub, BLDS_sub = BLDSapprox(sample, xL)

with plt.style.context('seaborn-v0_8'):

    # get current color cycle

    colors = plt.rcParams['axes.prop_cycle'].by_key()['color']
    color_cycle = cycler.cycler('color', colors[0:3])
    ax[0].set_prop_cycle(color_cycle)
    ax[1].set_prop_cycle(color_cycle)

    # approximation for zero-freq BLDS, K2 term

    x_sub, BLDSapprox = BLDSapproxK2(sample1, xL)
    ax[0].semilogx(
        x_sub,
        BLDSapprox,
        ':',
        color=colors[0],
        label=['$K_2$ approx.'])

    # exact calculations

    ax[0].semilogx(
        xL,
        adict['f_BLDS'][:,0,:],
```

```
        '-',
        label=['$K_2$','$K_1$','$K_0$'])

    ax[1].loglog(
        xR,
        adict['gamma'],
        '-',
        label=['$K_2$','$K_1$','$K_0$'])

    # limiting cases

    nL_part = int(2*len(xL)/3)

    ax[0].semilogx(
        xL[0:nL_part],
        BLDSzerolow(sample1, xL)[0:nL_part,:],
        '--')

    ax[0].semilogx(
        xL[-nL_part:-1],
        BLDSzerohigh(sample1, xL)[-nL_part:-1,:],
        '-.')

    nR_part = int(len(xR)/2)

    g_low, g_approx = gamma_perpendicular_approx(sample1, xR)

    ax[1].loglog(
        xR[0:nR_part],
        g_low[0:nR_part,:],
        '--')

    ax[1].loglog(
        xR[0:nR_part],
        g_approx[0:nR_part,:],
        ':',
        label=['$K_2$ approx','$K_1$ approx','$K_0$ approx'])

ax[0].set_xlabel(r'$(h / \lambda_{\mathrm{D}})^2$')
ax[0].set_ylabel(r'$\Delta f_{\mathrm{BLDS}}(\omega_{\mathrm{m}}=0)$ [Hz]')
ax[0].legend(fontsize=9)
ax[0].grid()
ax[1].grid()

ax[1].set_xlabel(r'$\omega_0/(\epsilon_{\mathrm{s}}^{\prime} \omega_{\mathrm{c}})$')
ax[1].set_ylabel(r'$\gamma_{\perp}$ [pN s/m]')
ax[1].legend(fontsize=9)
ax[1].set_ylim(
```

```
        [0.95 * adict['gamma'].min(),
         1.05 * adict['gamma'].max()])

    ax2L.set_xlabel(r'charge density $\rho$ [cm$^{-3}$]')
    ax2R.set_xlabel(r'charge density $\rho$ [cm$^{-3}$]')

    plt.tight_layout()
    plt.show()

    return fig
```

Pass sample parameters via `sample1`, where the parameters have units, not via `sample1_jit`, there the parameters don't have units.

```
fig['02'] = plotme(data['01'], sample1)
```



6 Save all figures

```
if 1:
    for num in fig.keys():
```

```
figname = THIS + "Fig-" + num
fig[num].savefig(figname + '.png', dpi=300)
fig[num].savefig(figname + '.pdf')
```