001-SphereExample

March 21, 2017

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In [1]: from ScatterSim.NanoObjects import SphereNanoObject, PolydisperseNanoObject
        import numpy as np
        import matplotlib.pyplot as plt
        %matplotlib inline

In [2]: def form_factor_slices(smod, qmax):
            ''' Compute the xy, xz, and yz projections.

            '''
            q = np.linspace(-qmax, qmax,100)
            QROWS, QCOLS = np.meshgrid(q,q, indexing="ij")
            Q0 = QROWS*0
            P2_xy = smod.form_factor_squared(np.array([QCOLS, QROWS, Q0]))
            P2_yz = smod.form_factor_squared(np.array([Q0, QCOLS, QROWS]))
            P2_xz = smod.form_factor_squared(np.array([QROWS, QCOLS, Q0]))

            return P2_xy, P2_yz, P2_xz

        def show_qslices(F_xy, F_xz, F_yz, length, num=4, **kwargs):
            '''plot the xy, xz, and yz projections with length used from
                projections function, in figure num
            '''
            extent = 2*np.pi/length*np.array([-.5, .5, -.5, .5])
            plt.figure(num);plt.clf();
            plt.subplot(2,2,1)
            plt.title("x-y plane")
            plt.imshow(F_xy,extent=extent, **kwargs)
            plt.subplot(2,2,2)
            plt.title("x-z plane")
            plt.imshow(F_xz,extent=extent, **kwargs)
            plt.subplot(2,2,3)
            plt.title("y-z plane")
            plt.imshow(F_yz,extent=extent, **kwargs)


        def show_projections(V_xy, V_xz, V_yz, length, num=4):
            '''plot the xy, xz, and yz projections with length used from
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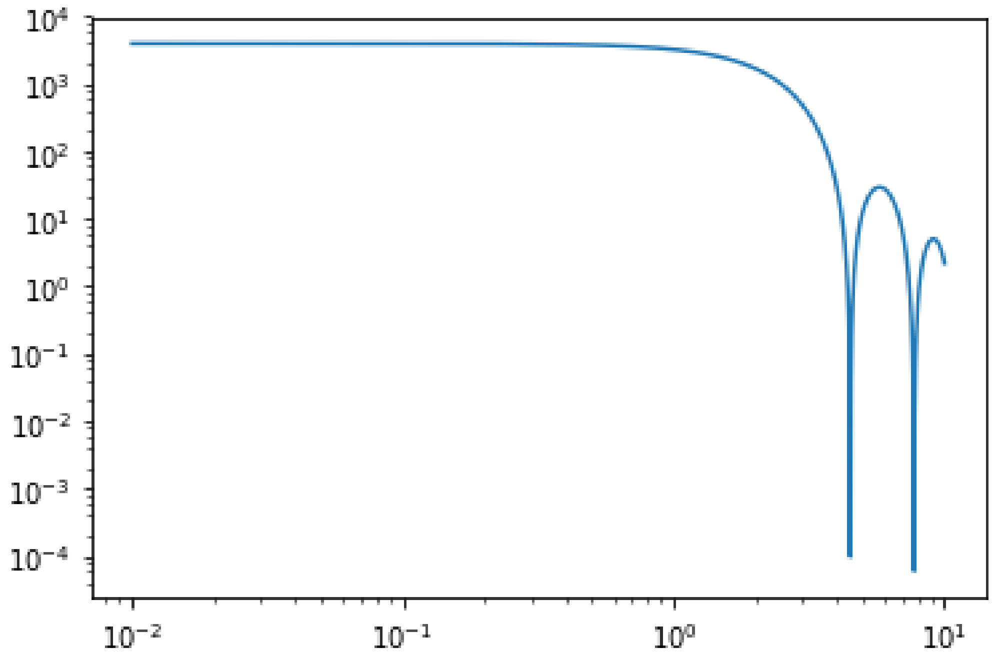
```
        projections function, in figure num
    '''
    extent = [-length/2, length/2., length/2., -length/2.]
    plt.figure(num);plt.clf();
    plt.subplot(2,2,1)
    plt.title("x-y plane")
    plt.imshow(V_xy,extent=extent)
    plt.subplot(2,2,2)
    plt.title("x-z plane")
    plt.imshow(V_xz,extent=extent)
    plt.subplot(2,2,3)
    plt.title("y-z plane")
    plt.imshow(V_yz,extent=extent)
```

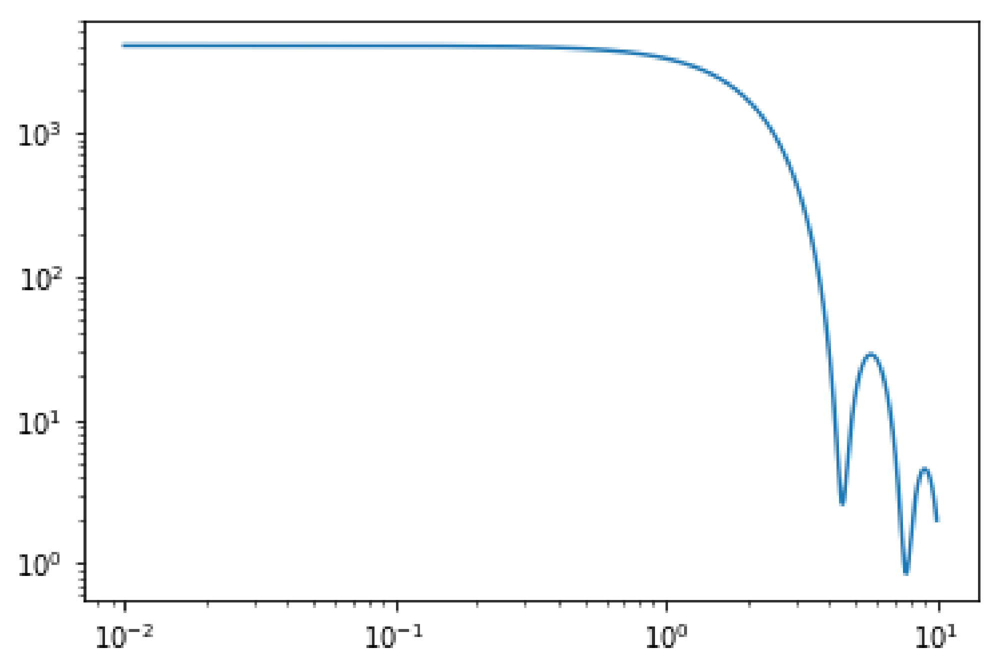
In [3]:
```
# Definining a sphere is simple
pargs_sphere = {'radius' : 1}
sphere = SphereNanoObject(pargs_sphere)

# You can also define a NanoObject with a stochastic parameter
# in this case, we'll make a polydisperse sphere
# The varied parameter will be the radius
pargs_polysphere = dict(radius= 1, sigma_R=.04) # (alternate way of defining dictionarie
# Just give the object the class you're interested in, and tell it what the parameter it
# is you're varying
# The parameter is assumed to be sampled from a Gaussian distribution of mean 'argname'
# and standard deviation (sigma) 'sigma_R'
polysphere = PolydisperseNanoObject(SphereNanoObject, pargs_polysphere, argname='radius'



# Now choose a q domain for the plotting. The units of q will be the inverse of units yo
# as parameters to the object. For example, we used nanometers, so q will be in inverse
q = np.linspace(0, 10, 1000)

# finally, calculate
sq_sphere = sphere.form_factor_squared_isotropic(q)
# The polydisperse sphere should take roughly 21 times longer. This is because
# by default it computes the form factors of spheres of radii from 21 points in the dist
# You can change this, and even change the distribution by reading more into the code
# of NanoObjects.PolydisperseNanoObject
sq_polysphere = polysphere.form_factor_squared_isotropic(q)
```

In [4]:
```
# plot using your favorite plotting library
plt.figure(0);
plt.clf()
plt.loglog(q, sq_sphere)
```

```
# even with a small polydispersity (4%), polydisperse sphere scattering looks much diffe
plt.figure(1);
plt.clf()
plt.loglog(q, sq_polysphere)
```

Out[4]: [<matplotlib.lines.Line2D at 0x7f9c7aaa88d0>]





```
In [5]: # For any object, you can compute the form factor or projection. See functions
        # above on how to do it.
        # P2 means |P|^2 (form factor squared)
        qmax = 10
        P2_xy, P2_yz, P2_xz = form_factor_slices(sphere, qmax)
        rmax = 1.5
        V_xy, V_yz, V_xz = sphere.projections(rmax)
```

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In [6]: # remember this is a 3D Object. We can look at projections of the object in real space
        # or slices of the scattering in Fourier (reciprocal) space
```

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In [7]: show_projections(V_xy, V_yz, V_xz, rmax, 3)
```

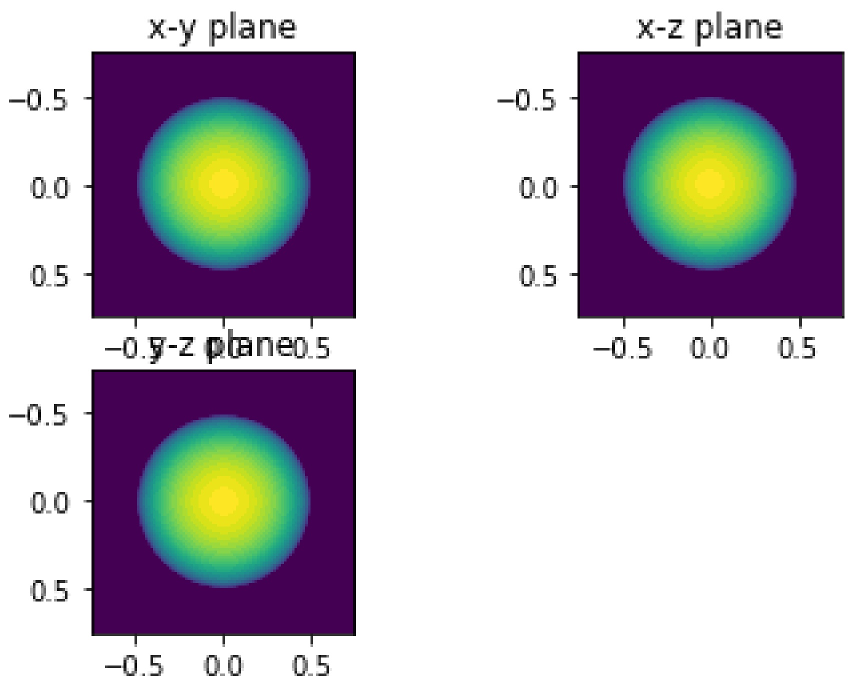


```
In [8]: # Showing the form factor
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In [9]: show_qslices(P2_xy, P2_yz, P2_xz, qmax, 2, vmin=0, vmax=6e1)
```

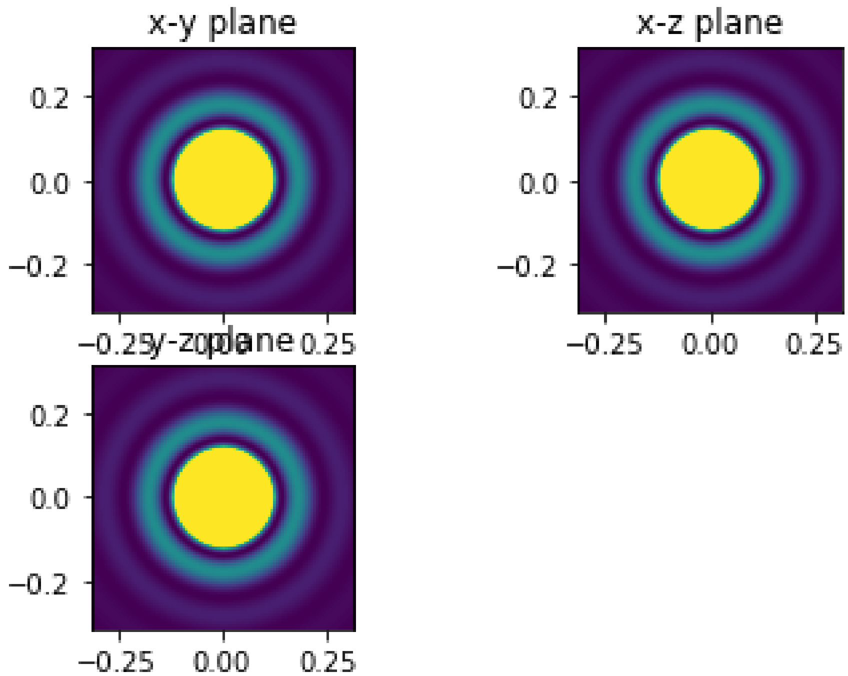

In [ ]: