Derivation of scattering contributions from a thin rigid rod.

In[73]:=
```
$Assumptions := {L > 0, Rg > 0, q > 0}
```

Rod model

We regard a rod of length L with a homogeneous scattering length along its contour.

Compared to a polymer, now the spatial distance and the contour distance between two scatterers is exactly the same. However, we have to remember that the rod can be orientated in all directions.

Lets now calculate all the relevant mean - square distance measures explicitly

Lets assume the rod has coordinates (-L/2,0,0) to (+L/2,0,0) hence we can describe it by (x,0,0) making square distances one dimensional.
The averaged square distance from one end to any internal point is:

In[73]:= $<[R-R(end1)]^2> =$

$$\frac{1}{L}\int_{-L/2}^{+L/2}\left(x-\left(-\frac{L}{2}\right)\right)^2 dx$$

Out[∘]= $$\frac{L^2}{3}$$

In[73]:= $<[R-R(end2)]^2> =$

In[∘]:= $$\frac{1}{L}\int_{-L/2}^{+L/2}\left(x-\left(+\frac{L}{2}\right)\right)^2 dx$$

Out[∘]= $$\frac{L^2}{3}$$

In[73]:= $<[R-Rmid]^2>$

In[∘]:= $$\frac{1}{L}\int_{-L/2}^{+L/2}(x)^2\, dx$$

Out[∘]= $$\frac{L^2}{12}$$

The averaged distance between a pair of points along the chain, here I divide by two since x1,x2 and x2,x1 gives the same distance twice which provides the radius of gyration:

In[73]:= $<[Ri-Rj]^2> = \ (\text{unique } i,j)$

In[∘]:= $$\frac{1}{2\,L^2}\int_{-L/2}^{+L/2}\int_{-L/2}^{+L/2}(x2-x1)^2\,dx1\,dx2$$

Out[∘]= $$\frac{L^2}{12}$$

In[73]:= <[Ri-Rj]^2> = (any i,j)

In[∘]:= $$\frac{1}{L^2}\int_{-L/2}^{+L/2}\int_{-L/2}^{+L/2}(x2-x1)^2\,dx1\,dx2$$

Out[∘]= $$\frac{L^2}{6}$$

Scattering Form Factor

Using the Debye formula, we can calculate the scattering contribution between any two scatterers along the rod, the Debye formula takes care of the orientational average:

In[∘]:= $$\frac{1}{L^2}\int_{-L/2}^{+L/2}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx1\,dx2$$

Out[∘]= $$\frac{2\left(-1+\text{Cos}[L\,q]+L\,q\,\text{SinIntegral}[L\,q]\right)}{L^2\,q^2}$$

It seems that x = q L is a good dimensionless variable .

In[75]:= $$F=\frac{1}{L^2}\int_{-L/2}^{+L/2}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx1\,dx2\ /.\ q\to x/L$$

Out[75]= $$\frac{2\left(-1+\text{Cos}[x]+x\,\text{SinIntegral}[x]\right)}{x^2}$$

SinIntegral[z]) = Si(z) = $\int_0^z \sin(t)/t\,dt$.

Reference for this form factor: T. Neugebauer, Ann. Phys. (Leipzig) 42, 509 (1943). P. I. Teixeira, D. J. Read, and T. C. B. McLeish, J. Chem. Phys. 126,
074901 (2007).

Form factor amplitude relative to ends

In[77]:= $$\text{Aend1}=\frac{1}{L}\int_{-L/2}^{+L/2}\frac{\text{Sin}\left[q\left(x+\frac{L}{2}\right)\right]}{q\left(x+\frac{L}{2}\right)}\,dx\ /.\ q\to x/L$$

Out[77]= $$\frac{\text{SinIntegral}[x]}{x}$$

In[78]:= Aend2 = $\frac{1}{L}\int_{-L/2}^{+L/2}\frac{\text{Sin}\left[q\left(x-\frac{L}{2}\right)\right]}{q\left(x-\frac{L}{2}\right)}\,dx$ /. q → x / L

Out[78]= $\frac{\text{SinIntegral}[x]}{x}$

Due to symmetry, these gives the same result, which is not that obvious given the two expressions above, but e.g. Taylor expanding shows the they match term-by-term as expected.

Reference : “A formalism for scattering of complex composite structures. II. Distributed reference points.” C . Svaneborg and J . S . Pedersen J . Chem . Phys . 136, 154907 (2012) DOI : http://dx.-doi.org/10.1063/1.3701737

Phase factor between the ends

In[81]:= Psiend1end2 = $\frac{\text{Sin}[q\,L]}{q\,L}$ /. q → x / L // Simplify

Out[81]= $\frac{\text{Sin}[x]}{x}$

Scattering terms involving a mIddle reference point.

Assuming we place a reference point at the middle of the rod at (0, 0, 0) we get the following form factor amplitude, and phase factor .

In[85]:= Amiddle = $\frac{1}{L}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,(x-0)]}{q\,(x-0)}\,dx$ /. q → x / L

Out[85]= $\frac{2\,\text{SinIntegral}\left[\frac{x}{2}\right]}{x}$

In[90]:= Psimiddle2end = $\frac{\text{Sin}\left[q\,\frac{L}{2}\right]}{q\,\frac{L}{2}}$ /. q → x / L // Simplify

Out[90]= $\frac{2\,\text{Sin}\left[\frac{x}{2}\right]}{x}$

Contour distributed reference points :

We need to calculate the scattering between a reference point at x1 uniformly distributed in [-L/2,+L/2] and a scatterer at x2 uniformly distributed in [-L/2,+L/2] :

In[96]:=
$$\text{Acontour} = \frac{1}{L^2}\int_{-L/2}^{+L/2}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx1\,dx2\ /.\ q\to x/L\ //\ \text{Simplify}$$

Out[96]=
$$\frac{2\left(-1+\text{Cos}[x]+x\,\text{SinIntegral}[x]\right)}{x^2}$$

To calculate the average phase factor between the end x1=-L/2 and a uniformly distributed reference point at x2:

In[∘]:=
$$\text{Psiend1contour} = \frac{1}{L}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx2\ /.\ x1\to -\frac{L}{2}\ /.\ q\to x\Big/L$$

Out[∘]=
$$\frac{\text{SinIntegral}[x]}{x}$$

In[∘]:=
$$\text{Psiend2contour} = \frac{1}{L}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx1\ /.\ x2\to \frac{L}{2}\ /.\ q\to x\Big/L$$

Out[∘]=
$$\frac{1}{8\,x}\Bigg(2\,\text{CosIntegral}[x]\,\text{Sin}[x]+2\,\text{Log}[4]\,\text{Sin}[x]-2\,\text{Log}[x]\,\text{Sin}[x]+6\,\text{SinIntegral}[x]-$$
$$2\,\text{Cos}[x]\,\text{SinIntegral}[x]-\sqrt{\pi}\,x\,\text{Cos}\left[\frac{x}{2}\right]\text{Hypergeometric0F1Regularized}^{(1,0)}\left[\frac{3}{2},-\frac{x^2}{16}\right]\Bigg)$$

Again an ugly expression, which is identical to Psi_end1contour.
To calculate the phase factor between x1 and x2 uniformly distributed along the rod, we get the form factor again:

In[∘]:=
$$\text{Psicontour2contour} = \frac{1}{L^2}\int_{-L/2}^{+L/2}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx1\,dx2\ /.\ q\to x/L\ //\ \text{Simplify}$$

Out[∘]=
$$\frac{2\left(-1+\text{Cos}[x]+x\,\text{SinIntegral}[x]\right)}{x^2}$$

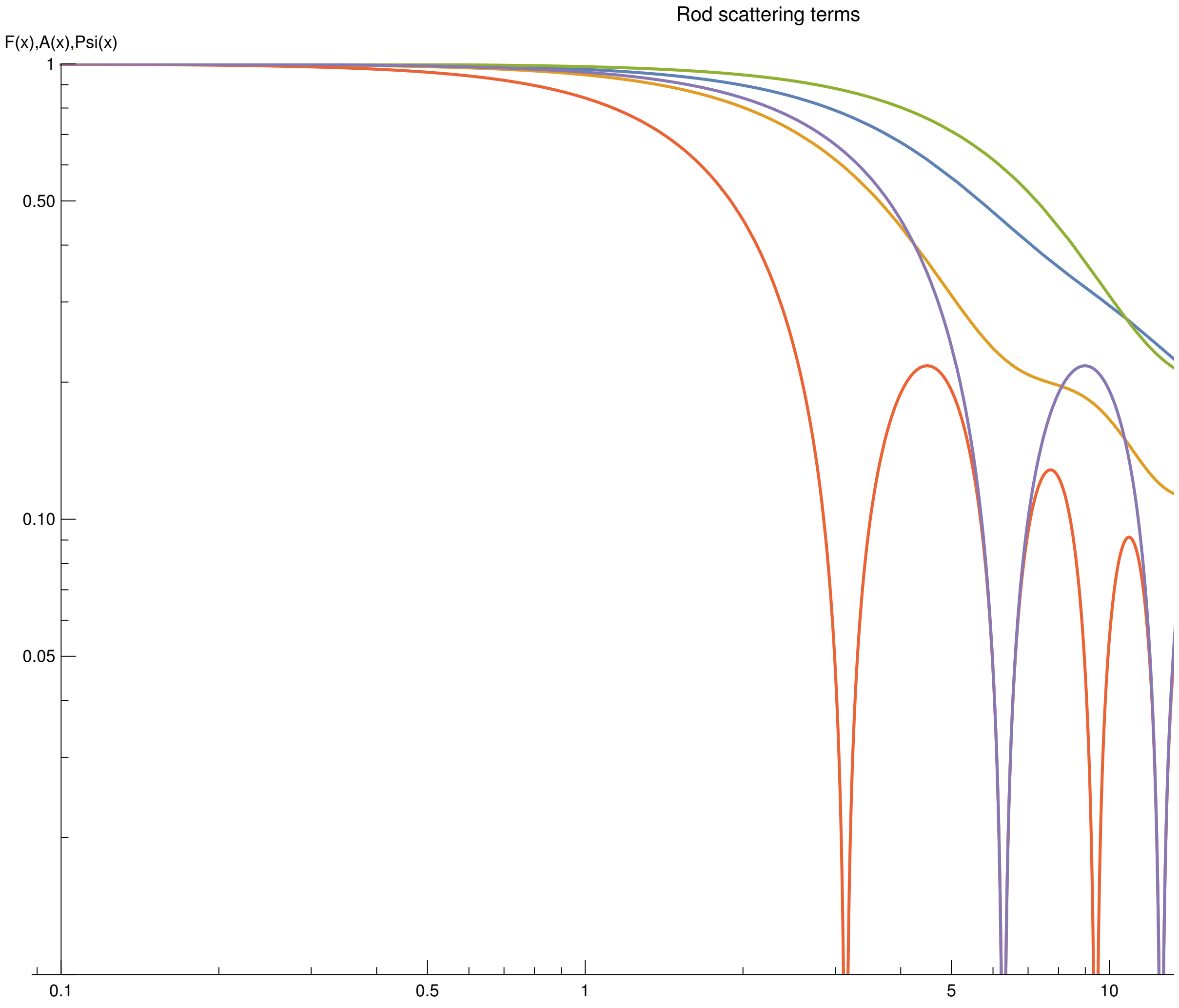
The final missing expression is the average phase factor between a random along the contour (x1 in [-L/2, L/2]) and the middle point x2 = 0 :

In[97]:=
$$\text{Psicontour2middle} = \frac{1}{L}\int_{-L/2}^{+L/2}\frac{\text{Sin}[q\,\text{Abs}[x2-x1]]}{q\,\text{Abs}[x2-x1]}\,dx1\ /.\ x2\to 0\ /.\ q\to x\Big/L$$

Out[97]=
$$\frac{2\,\text{SinIntegral}\left[\frac{x}{2}\right]}{x}$$

In[∘]:=
```
LogLogPlot[{F, Aend1, Amiddle, Abs[Psiend1end2], Abs[Psimiddle2end]}, {x, 0.1, 50},
 PlotLabel → "Rod scattering terms", AxesLabel → {"x", "F(x),A(x),Psi(x)"},
 PlotLegends → {"F", "Aend1", "Amiddle", "|Psiend2end2|", "|Psimiddle2end|"},
 PlotRange → {0.01, 1}]
```

Out[∘]=



Guinier - expansions

Above we derived the mean - square distances explicitly. Here we show how to obtain these from a Guinier expansion of the various scattering terms.

The Guinier expansion of F is
$1 - q^2\ \mathrm{Rg}^2 / 3 + O(q^4)$

In[∘]:=
```
Series[F /. x → q L, {q, 0, 3}]
```

Out[∘]= $1 - \frac{L^2\, q^2}{36} + O[q]^4$

Hence to isolate the radius of gyration in the series:

In[∘]:=
$$\frac{3\left(1-\text{Normal}\left[\text{Series}\left[F\ /.\ x\to q\,L,\ \{q,\ 0,\ 3\}\right]\right]\right)}{q^2}$$

Out[∘]=
$$\frac{L^2}{12}$$

This works as expected.

The Guinier expansion of A and Psi are : $1 - q^2 < \text{distance}^2 > / 6 + O(q^4)$.

In[73]:= <[R−Rend]^2>

In[∘]:=
$$\frac{6\left(1-\text{Normal}\left[\text{Series}\left[\frac{\text{SinIntegral}[x]}{x}\ /.\ x\to q\,L,\ \{q,\ 0,\ 3\}\right]\right]\right)}{q^2}$$

Out[∘]=
$$\frac{L^2}{3}$$

In[73]:= <[R−Rmid]^2>

In[∘]:=
$$\frac{6\left(1-\text{Normal}\left[\text{Series}\left[\frac{2\,\text{SinIntegral}\left[\frac{x}{2}\right]}{x}\ /.\ x\to q\,L,\ \{q,\ 0,\ 3\}\right]\right]\right)}{q^2}$$

Out[∘]=
$$\frac{L^2}{12}$$

In[73]:= <[Rend−Rmid]^2>

In[∘]:=
$$\frac{6\left(1-\text{Normal}\left[\text{Series}\left[\frac{2\,\text{Sin}\left[\frac{x}{2}\right]}{x}\ /.\ x\to q\,L,\ \{q,\ 0,\ 3\}\right]\right]\right)}{q^2}$$

Out[∘]=
$$\frac{L^2}{4}$$

In[73]:= <[Ri−Rj]^2>

In[∘]:=
$$\frac{1}{q^2}\,6\left(1-\text{Normal}\left[\text{Series}\left[\frac{2\left(-1+\text{Cos}[x]+x\,\text{SinIntegral}[x]\right)}{x^2}\ /.\ x\to q\,L,\ \{q,\ 0,\ 3\}\right]\right]\right)$$

Out[∘]=
$$\frac{L^2}{6}$$

In[∘]:= Series[SinIntegral[x] / x, {x, 0, 6}]

Out[∘]=
$$1-\frac{x^2}{18}+\frac{x^4}{600}-\frac{x^6}{35\,280}+O[x]^7$$

In[∘]:=
```
D[SinIntegral[x]/x, x]
```

Out[∘]=
$$\frac{\text{Sinc}[x]}{x}-\frac{\text{SinIntegral}[x]}{x^2}$$

In[∘]:=
```
Series[D[SinIntegral[x]/x, x], {x, 0, 6}]
```

Out[∘]=
$$-\frac{x}{9}+\frac{x^3}{150}-\frac{x^5}{5880}+O[x]^7$$

Save example data to file for Validation :

In[∘]:=
```
SaveFunction[func_, filename_, NN_, qmin_, qmax_] :=
 Module[{}, Export[filename, {#, N[func /. q → #]} & /@
    Table[10^(Log[10, qmax / qmin] * i / NN + Log[10, qmin]), {i, 0, NN}]]]
```

In[∘]:=
```
SaveFunction[F /. x → q L /. L → 1 ,
 "/home/zqex/source/SEB/source/Validation/ThinRod_mathematica/F.dat", 200, 0.01, 20]
SaveFunction[Aend1 /. x → q L /. L → 1 ,
 "/home/zqex/source/SEB/source/Validation/ThinRod_mathematica/A_end.dat",
 200, 0.01, 20]
SaveFunction[Amiddle /. x → q L /. L → 1 ,
 "/home/zqex/source/SEB/source/Validation/ThinRod_mathematica/A_middle.dat",
 200, 0.01, 20]
SaveFunction[Psiend1end2 /. x → q L /. L → 1 ,
 "/home/zqex/source/SEB/source/Validation/ThinRod_mathematica/Psi_end2end.dat",
 200, 0.01, 20]
SaveFunction[Psimiddle2end /. x → q L /. L → 1 ,
 "/home/zqex/source/SEB/source/Validation/ThinRod_mathematica/Psi_end2middle.dat",
 200, 0.01, 20]
SaveFunction[Psicontour2middle /. x → q L /. L → 1 ,
 "/home/zqex/source/SEB/source/Validation/ThinRod_mathematica/Psi_contour2middle.dat
   ", 200, 0.01, 20]
```

Out[∘]= /home/zqex/source/SEB/source/Validation/ThinRod_mathematica/F.dat

Out[∘]= /home/zqex/source/SEB/source/Validation/ThinRod_mathematica/A_end.dat

Out[∘]= /home/zqex/source/SEB/source/Validation/ThinRod_mathematica/A_middle.dat

Out[∘]= /home/zqex/source/SEB/source/Validation/ThinRod_mathematica/Psi_end2end.dat

Out[∘]= /home/zqex/source/SEB/source/Validation/ThinRod_mathematica/Psi_end2middle.dat

Out[∘]= /home/zqex/source/SEB/source/Validation/ThinRod_mathematica/Psi_contour2middle.dat