Cylinder

All the calculations below make heavily use of the fact that P[R2-R1] the two-point probability distribution of two vectors connecting two points being e.g. inside the cylinder, on the ends, on the hull, or .. can be stated as a convolution of two one-point correlation functions going from the center to R1 and from the centre to R2, where we choose the center of the cylinder as origo of our coordinate system. In Fourier space, the two-point probability distribution is just the product of the two one-point correlation functions. Although we have to take care of an additional average over the direction from which the q-vector hits the cylinder.

In[367]:=
```
$Assumptions := {R > 0, q > 0, L > 0, r > 0, θq > 0, θq ≤ π/2}
```

To integrate a cylinder we choose cylindrical coordinates putting the cylinder symmetry axis along the z axis . Again we can place the q vector anywhere in the upper xz plane due to rotational symmetry .

In[368]:=
```
Rvec := {r Cos[ϕ], r Sin[ϕ], z}
```

In[369]:=
```
qvec := {q Sin[θq], 0, q Cos[θq]}
```

In[370]:=
```
Rvec.qvec
```

Out[370]=

$$q\ z\ \text{Cos}[\theta q] + q\ r\ \text{Cos}[\phi]\ \text{Sin}[\theta q]$$

Normalization is the volume of the cylinder :

In[371]:=
```
Integrate[r, {r, 0, R}, {ϕ, -π, π}, {z, -L/2, L/2}]
```

Out[371]=

$$L\ \pi\ R^2$$

The form factor amplitude of all scatterers relative to the center (at the origin) is then for fixed q vector

In[372]:=
```
FFA = Integrate[Exp[I Rvec.qvec] r, {r, 0, R}, {ϕ, -π, π}, {z, -L/2, L/2}] / (L π R^2)
```

Out[372]=

$$\frac{4\ \text{BesselJ}[1,\ q\ R\ \text{Sin}[\theta q]]\ \text{Csc}[\theta q]\ \text{Sec}[\theta q]\ \text{Sin}[\frac{1}{2}\ L\ q\ \text{Cos}[\theta q]]}{L\ q^2\ R}$$

Doing the average over the direction of the q vector, since the cylinder is rotationally invariant . The integral can not be performed analytically.

In[373]:=
```
Fcylinder = Integrate[FFA^2 Sin[θq], {θq, 0, π/2}]
```

Out[373]=

$$\int_0^{\frac{\pi}{2}} \frac{16\ \text{BesselJ}[1,\ q\ R\ \text{Sin}[\theta q]]^2\ \text{Csc}[\theta q]\ \text{Sec}[\theta q]^2\ \text{Sin}[\frac{1}{2}\ L\ q\ \text{Cos}[\theta q]]^2}{L^2\ q^4\ R^2}\ d\theta q$$

Ref : G . Fournet, Bull . Soc . Fr . Mineral . Crist ., 74 (1951) 39 - 113.
To calculate the phase factor between the centre point and any point on the round hull of the

cyllinder, we differentiate. Note that we still need to perform the orientational average for all the expressions below.

In[374]:=
```
Psicenter2hull = D[FFA (L π R^2), R] / (L 2 π R) // FullSimplify
```

Out[374]=

$$\frac{2\,\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Sec}[\theta q]\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]}{L\,q}$$

In[375]:=
```
Psicenter2hull /. L → y / q /. R → x / q /. θq → t // CForm // Simplify
```

Out[375]//CForm=
```
(2*BesselJ(0,x*Sin(t))*Sec(t)*Sin((y*Cos(t))/2.))/y
```

In[376]:=
```
Psihull2hull = Psicenter2hull^2 // FullSimplify
```

Out[376]=

$$\frac{4\,\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]^2\,\text{Sec}[\theta q]^2\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2}{L^2\,q^2}$$

In[377]:=
```
Ahull = Psicenter2hull FFA // FullSimplify
```

Out[377]=

$$\frac{8\,\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Csc}[\theta q]\,\text{Sec}[\theta q]^2\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2}{L^2\,q^3\,R}$$

Phase factor from center to a point on the circular cross-section at z.

In[384]:=
```
Psicenter2endz[z_] =
  Integrate[Exp[I Rvec.qvec] r, {r, 0, R}, {ϕ, -π, π}] / (π R^2) // FunctionExpand
```

Out[384]=

$$\frac{2\,e^{i\,q\,z\,\text{Cos}[\theta q]}\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Csc}[\theta q]}{q\,R}$$

Phase factor from center to a point on one of the two circular cross-sections at L/2, -L/2.

In[385]:=
```
Psicenter2ends = (Psicenter2endz[L / 2] + Psicenter2endz[-L / 2]) / 2 // FullSimplify
```

Out[385]=

$$\text{Cos}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]\,\text{Hypergeometric0F1Regularized}\left[2,\ -\frac{1}{4}\,q^2\,R^2\,\text{Sin}[\theta q]^2\right]$$

In[386]:=
```
Psicenter2ends /. L → y / q /. R → x / q /. θq → t // CForm // Simplify
```

Out[386]//CForm=
```
Cos((y*Cos(t))/2.)*Hypergeometric0F1Regularized(2,-0.25*(Power(x,2)*Power(Sin(t),2)))
```

In[381]:=
```
Psiend2end = Psicenter2ends Psicenter2ends // FullSimplify
```

Out[381]=

$$\text{Cos}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2\,\text{Hypergeometric0F1Regularized}\left[2,\ -\frac{1}{4}\,q^2\,R^2\,\text{Sin}[\theta q]^2\right]^2$$

In[382]:=
```
Aends = Psicenter2ends FFA // FullSimplify
```

Out[382]=

$$\frac{4\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]^2\,\text{Csc}[\theta q]^2\,\text{Sec}[\theta q]\,\text{Sin}\left[L\,q\,\text{Cos}[\theta q]\right]}{L\,q^3\,R^2}$$

In[387]:=
```
Psiend2hull = Psicenter2ends Psicenter2hull // FullSimplify
```

Out[387]=

$$\frac{2\,\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Csc}[\theta q]\,\text{Sec}[\theta q]\,\text{Sin}\left[L\,q\,\text{Cos}[\theta q]\right]}{L\,q^2\,R}$$

In[388]:=
```
Psicenter2surface =
 (2 π R^2 Psicenter2ends + 2 π R L Psicenter2hull) / (2 π R L + 2 π R^2) // FullSimplify
```

Out[388]=

$$\frac{1}{q\,(L+R)}\,2\left(\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Cos}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]\,\text{Csc}[\theta q]+\right.$$
$$\left.\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Sec}[\theta q]\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]\right)$$

Comparing to sampled data and saving data for validation:

In[389]:=
```
PARENTDIR = Directory[]
```

Out[389]=

/home/zqex/source/SEB/Mathematica

In[441]:=
```
Clear[DIR1, DIR2, DIRO1, DIRO2]
DIR1 := PARENTDIR <> "/Sampled/SolidCylinder_R1.000000_L1.500000/"
DIR2 := PARENTDIR <> "/Sampled/SolidCylinder_R2.000000_L0.500000/"
DIRO1 := PARENTDIR <> "/../Examples/Validation/SolidCylinder_mathematica_R1_L1.5/"
DIRO2 := PARENTDIR <> "/../Examples/Validation/SolidCylinder_mathematica_R2_L0.5/"
CreateDirectory[DIRO1];
CreateDirectory[DIRO2];
```

CreateDirectory: /home/zqex/source/SEB/Examples/Validation/SolidCylinder_mathematica_R1_L1.5/ already exists.

CreateDirectory: /home/zqex/source/SEB/Examples/Validation/SolidCylinder_mathematica_R2_L0.5/ already exists.

In[448]:=
```
SaveFunction[func_, filename_, NN_, qmin_, qmax_] := Module[{}, Export[filename,
    {#, N[func[#]]} & /@ Table[10^(Log[10, qmax / qmin] * i / NN + Log[10, qmin]), {i, 0, NN}]]]
SetAttributes[SaveFunction, HoldAll]
```

In[450]:=
```
Clear[qvec, qq]
qvec[qmin_, qmax_, NN_] :=
 Table[10^(Log[10, qmax / qmin] * i / NN + Log[10, qmin]), {i, 0, NN}]
qq := qvec[0.8, 50, 500] // N
```

Form factor :

In[489]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = FFA^2
FILE = "FF.q";
OFILE = "F.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π/2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π/2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} &/@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} &/@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} &/@ qq, {#, Abs[Func2[#]]} &/@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

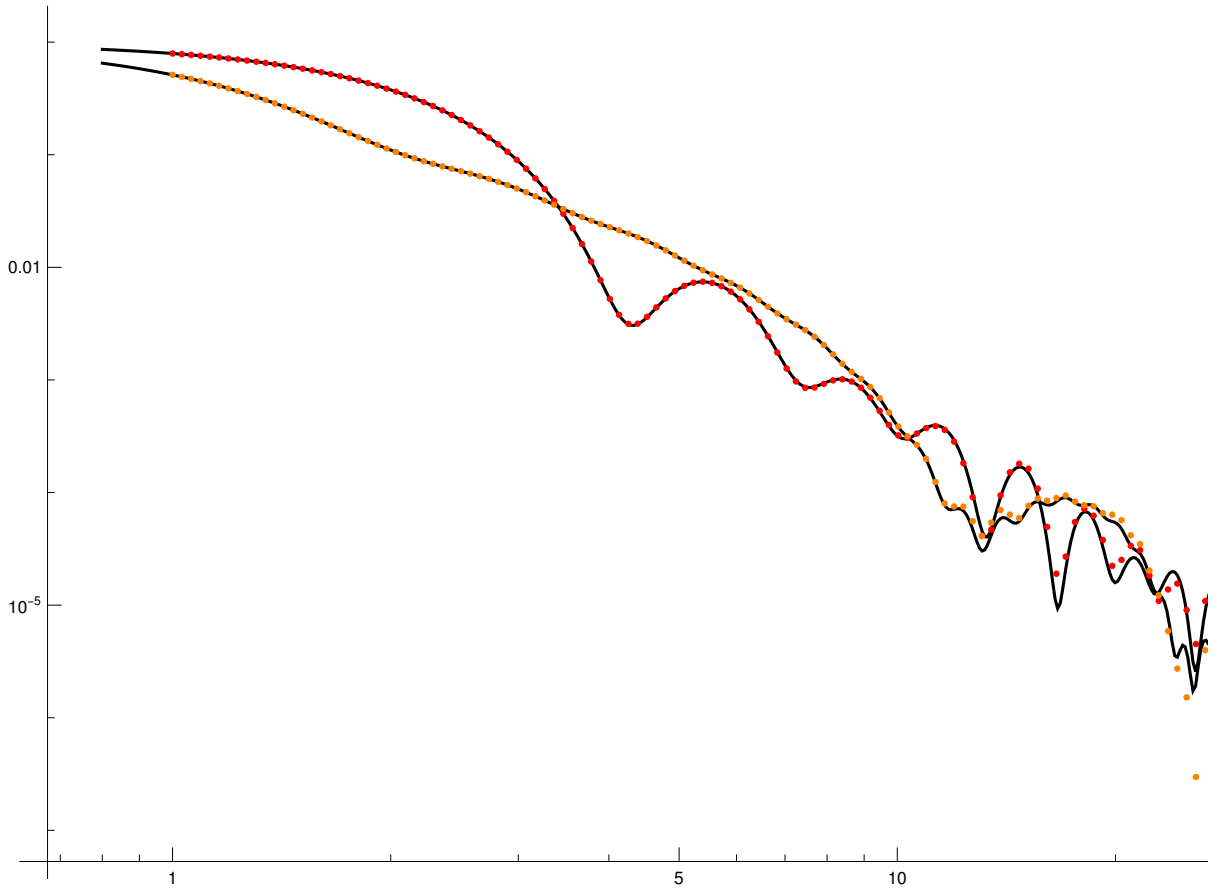
Out[490]=

$$\frac{16\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]^2\,\text{Csc}[\theta q]^2\,\text{Sec}[\theta q]^2\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2}{L^2\,q^4\,R^2}$$

Out[493]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/F.dat
```

Out[500]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 Rg2/3, Rg2] // Simplify
```

Out[•]=
$$\left\{\left\{Rg2 \to \frac{1}{12}\left(L^2 + 6\,R^2\right)\right\}\right\}$$

In[•]:=
```
Term[q] /. L → y/q /. R → x/q /. θq → t // CForm
```

Out[•]//CForm=
```
(16*Power(BesselJ(1,x*Sin(t)),2)*Power(Csc(t),2)*Power(Sec(t),2)*Power(Sin((y*Cos(t))/2.),2))/
   (Power(x,2)*Power(y,2))
```

Form factor Amplitude relative to center:

In[501]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = FFA
FILE = "FFA_center.q";
OFILE = "FFA_center.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

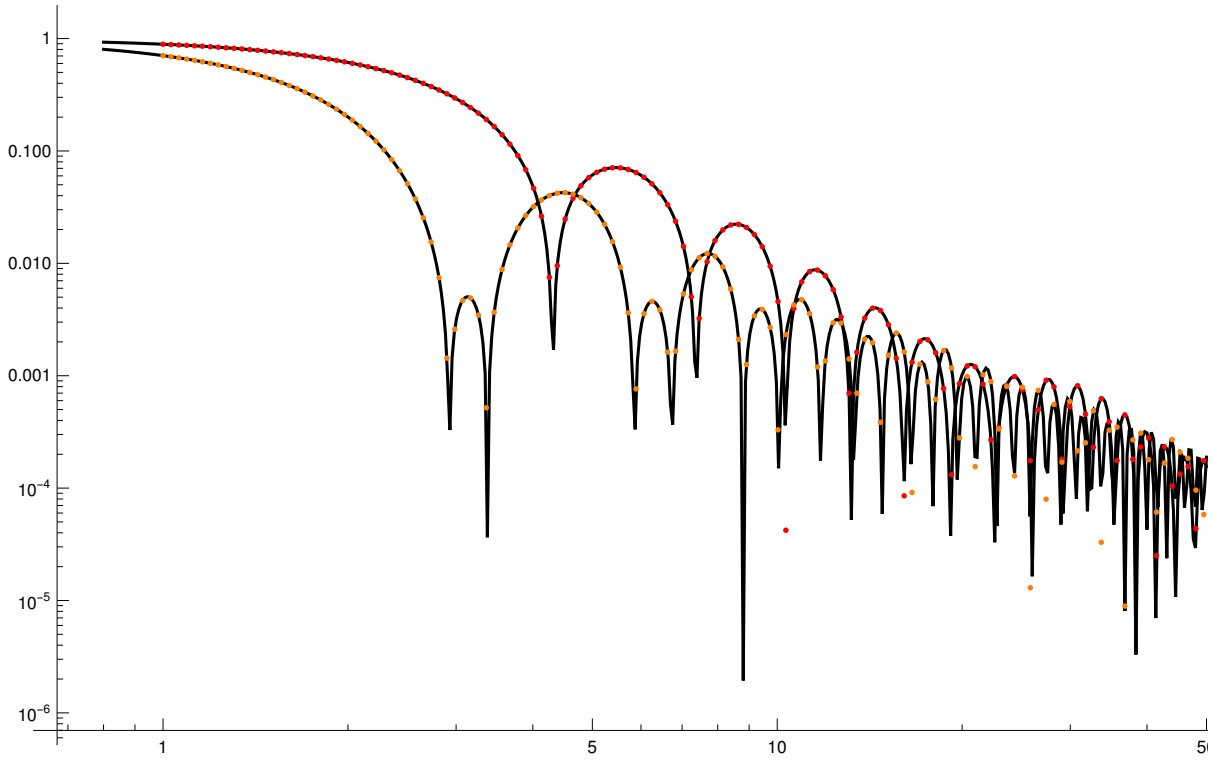
Out[502]=

$$\frac{4\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\,\text{Csc}[\theta q]\,\text{Sec}[\theta q]\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]}{L\,q^2\,R}$$

Out[505]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/FFA_center.dat
```

Out[512]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π / 2}], q] == 1 - q^2 sR2 / 6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{1}{12}\left(L^2 + 6\,R^2\right)\right\}\right\}$$

In[•]:=
```
Term[q] /. L → y / q /. R → x / q /. θq → t // CForm // Simplify
```

Out[•]//CForm=
```
(4*BesselJ(1,x*Sin(t))*Csc(t)*Sec(t)*Sin((y*Cos(t))/2.))/(x*y)
```

Form factor Amplitude relative to hull:

In[513]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = FFA Psicenter2hull
FILE = "FFA_hull.q";
OFILE = "FFA_hull.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

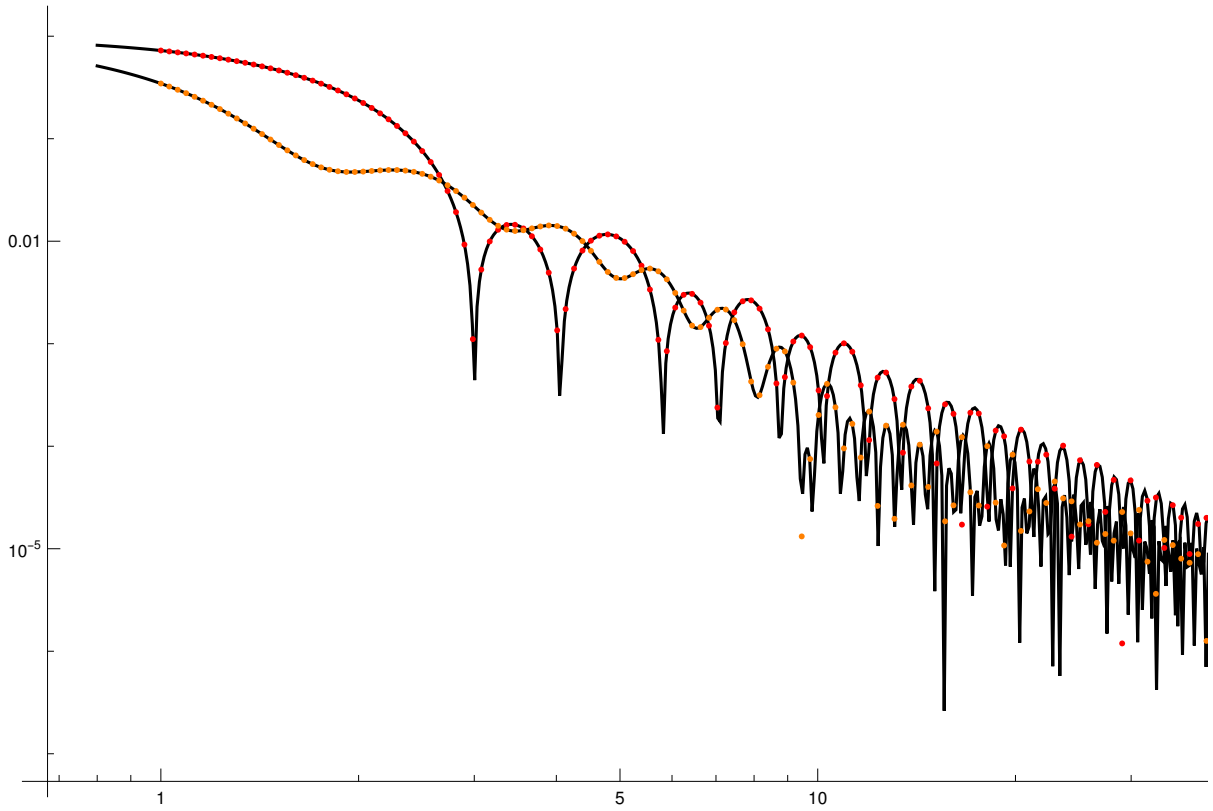
Out[514]=

$$\frac{8\,\text{BesselJ}[0,\,q\,R\,\text{Sin}[\theta q]]\,\text{BesselJ}[1,\,q\,R\,\text{Sin}[\theta q]]\,\text{Csc}[\theta q]\,\text{Sec}[\theta q]^2\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2}{L^2\,q^3\,R}$$

Out[517]=

/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica_R1_L1.5/FFA_hull.dat

Out[524]=



Form factor Amplitude relative to ends:

In[525]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = FFA Psicenter2ends
FILE = "FFA_end.q";
OFILE = "FFA_ends.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

Out[526]=

$$\frac{1}{L\,q^2\,R}\,4\,\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\text{Cos}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]\text{Csc}[\theta q]$$

$$\text{Hypergeometric0F1Regularized}\left[2,\ -\frac{1}{4}\,q^2\,R^2\,\text{Sin}[\theta q]^2\right]\text{Sec}[\theta q]\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]$$

Out[529]=

/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica_R1_L1.5/FFA_ends.dat

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.5708}. NIntegrate obtained –0.0000228683 and 5.2906138947513324`*^–11 for the integral and error estimates.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.5708}. NIntegrate obtained –0.0000187586 and 3.851348749496803`*^–11 for the integral and error estimates.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.5708}. NIntegrate obtained -5.75476×10^{-6} and 3.5488245233260163`*^–11 for the integral and error estimates.

General: Further output of NIntegrate::ncvb will be suppressed during this calculation.

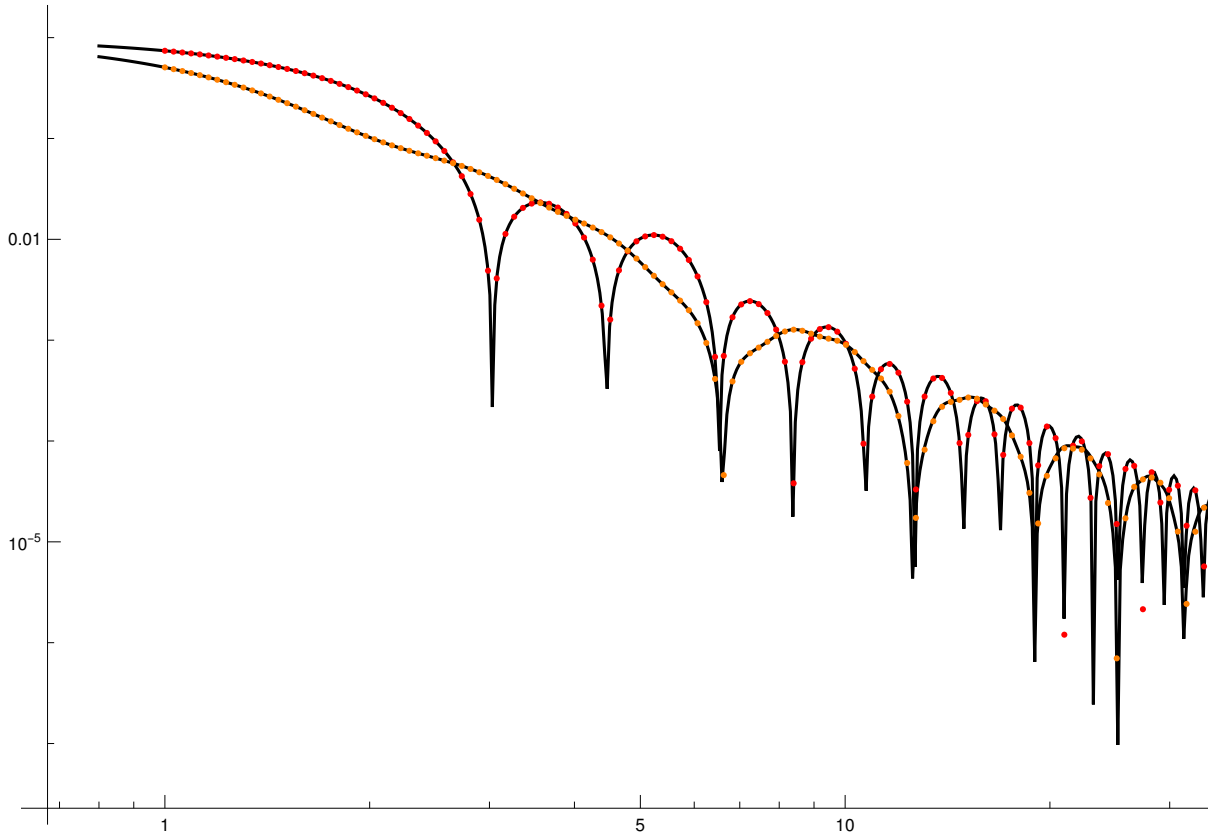
NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.5708}. NIntegrate obtained 1.0923657159717094`*^–6 and 1.666312123316506`*^–11 for the integral and error estimates.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.5708}. NIntegrate obtained –0.0000103871 and 3.555180065076667`*^–11 for the integral and error estimates.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.5708}. NIntegrate obtained –0.0000130573 and 5.1783999230986764`*^–11 for the integral and error estimates.

General: Further output of NIntegrate::ncvb will be suppressed during this calculation.

Out[536]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 sR2/6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^2}{3} + R^2\right\}\right\}$$

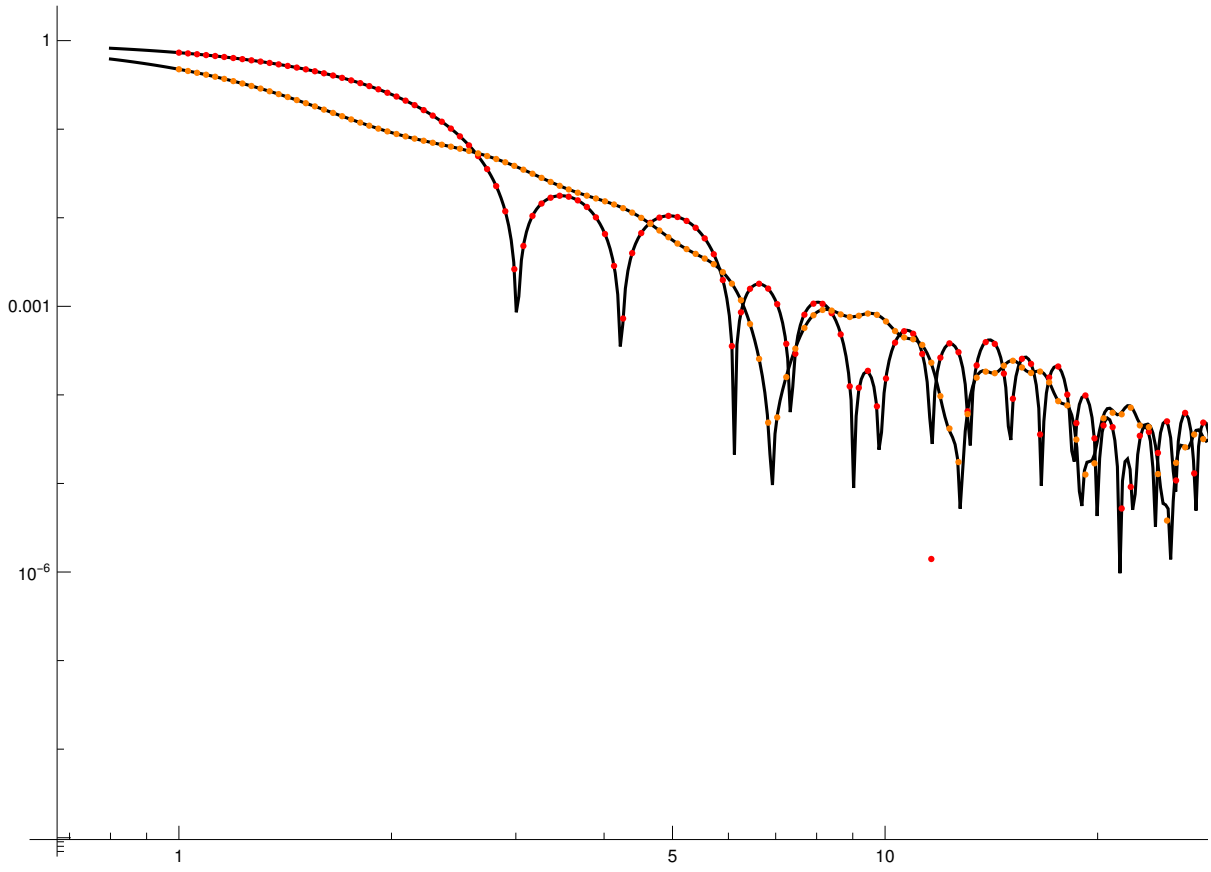
Form factor amplitude relative to surface:

In[537]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = FFA Psicenter2surface
FILE = "FFA_surface.q";
OFILE = "FFA_surface.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π/2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π/2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} &/@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} &/@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} &/@ qq, {#, Abs[Func2[#]]} &/@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

Out[538]=
$$\frac{1}{L\, q^3\, R\, (L+R)}\, 8\, \text{BesselJ}\left[1,\, q\, R\, \text{Sin}[\theta q]\right] \text{Csc}[\theta q]\, \text{Sec}[\theta q]$$
$$\text{Sin}\left[\frac{1}{2}\, L\, q\, \text{Cos}[\theta q]\right]\left(\text{BesselJ}\left[1,\, q\, R\, \text{Sin}[\theta q]\right] \text{Cos}\left[\frac{1}{2}\, L\, q\, \text{Cos}[\theta q]\right] \text{Csc}[\theta q] + \right.$$
$$\left. \text{BesselJ}\left[0,\, q\, R\, \text{Sin}[\theta q]\right] \text{Sec}[\theta q]\, \text{Sin}\left[\frac{1}{2}\, L\, q\, \text{Cos}[\theta q]\right]\right)$$

Out[541]=
```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/FFA_surface.dat
```

Out[548]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 sR2/6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^3 + 2\,L^2\,R + 9\,L\,R^2 + 6\,R^3}{6\,(L + R)}\right\}\right\}$$

Phase factor center to end:

In[549]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = Psicenter2ends // FullSimplify
FILE = "PF_center_end.q";
OFILE = "PF_center2ends.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

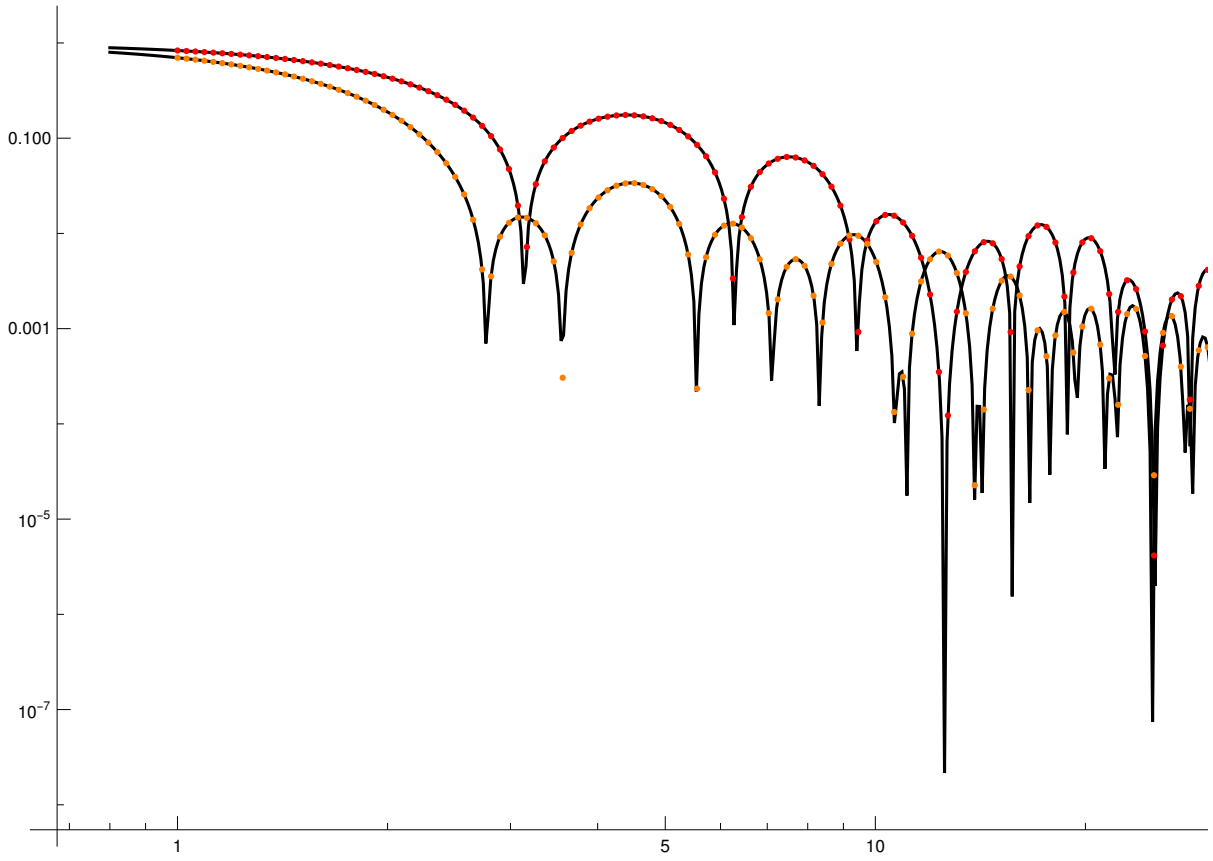
Out[550]=

$$\text{Cos}\left[\frac{1}{2}\ \text{L}\ \text{q}\ \text{Cos}[\theta\text{q}]\right]\ \text{Hypergeometric0F1Regularized}\left[2,\ -\frac{1}{4}\ \text{q}^2\ \text{R}^2\ \text{Sin}[\theta\text{q}]^2\right]$$

Out[553]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_center2ends.dat
```

Out[560]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π / 2}], q] == 1 - q^2 sR2 / 6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{1}{4}\left(L^2 + 2\,R^2\right)\right\}\right\}$$

Phase factor center to hull:

In[561]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = Psicenter2hull // FullSimplify
FILE = "PF_center_hull.q";
OFILE = "PF_center2hull.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

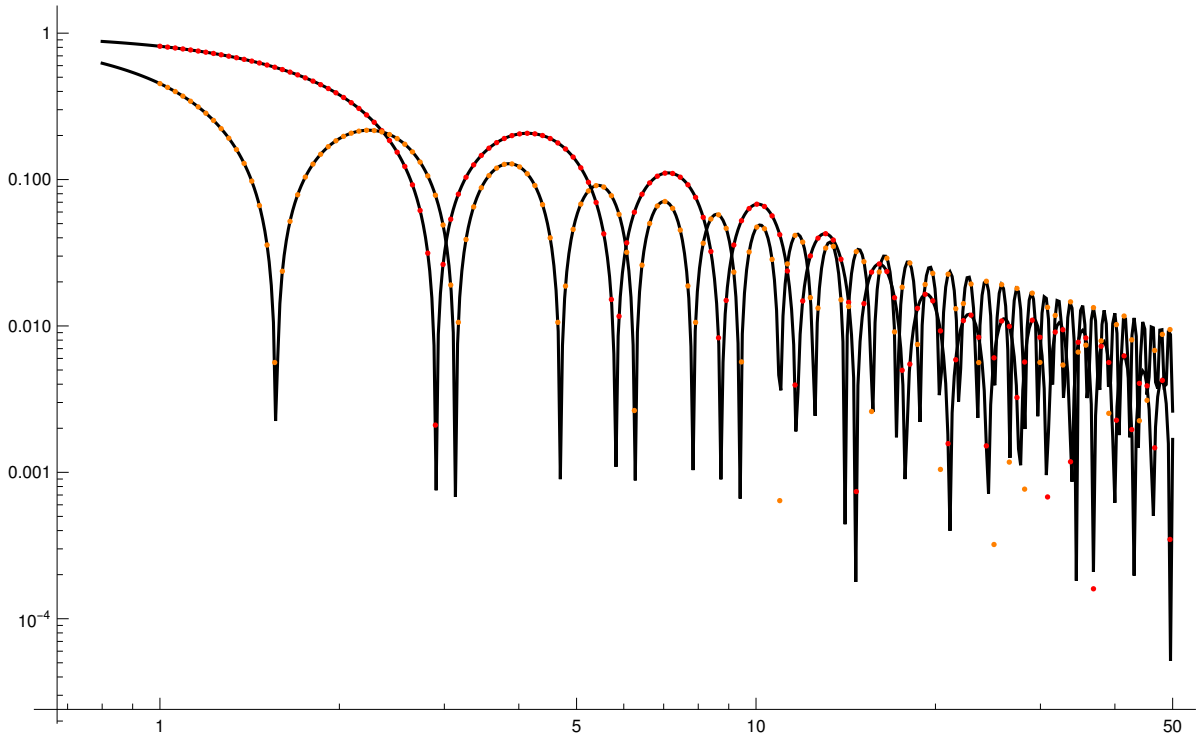
Out[562]=

$$\frac{2\,\text{BesselJ}[0,\ q\,R\,\text{Sin}[\theta q]]\,\text{Sec}[\theta q]\,\text{Sin}[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]]}{L\,q}$$

Out[565]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_center2hull.dat
```

Out[572]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π / 2}], q] == 1 - q^2 sR2 / 6,
  sR2] // Simplify
```

Out[•]=
$$\left\{\left\{\text{sR2} \to \frac{L^2}{12} + R^2\right\}\right\}$$

Phase factor center to surface:

In[573]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] =  Psicenter2surface // FullSimplify
FILE = "PF_center_surface.q";
OFILE = "PF_center2surface.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

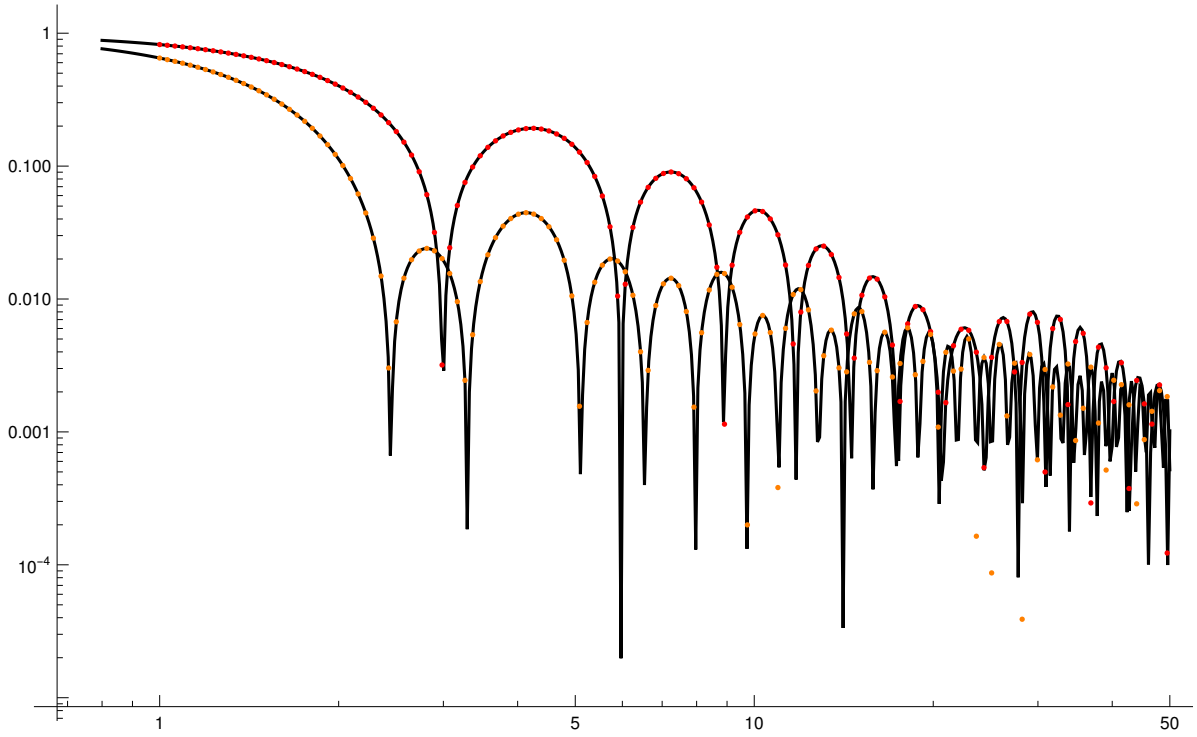
Out[574]=

$$\frac{1}{q\,(L+R)}\,2\left(\text{BesselJ}\left[1,\ q\,R\,\text{Sin}[\theta q]\right]\text{Cos}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]\text{Csc}[\theta q]+\right.$$
$$\left.\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]\text{Sec}[\theta q]\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]\right)$$

Out[577]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_center2surface.dat
```

Out[584]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 sR2/6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^3 + 3\,L^2\,R + 12\,L\,R^2 + 6\,R^3}{12\,(L+R)}\right\}\right\}$$

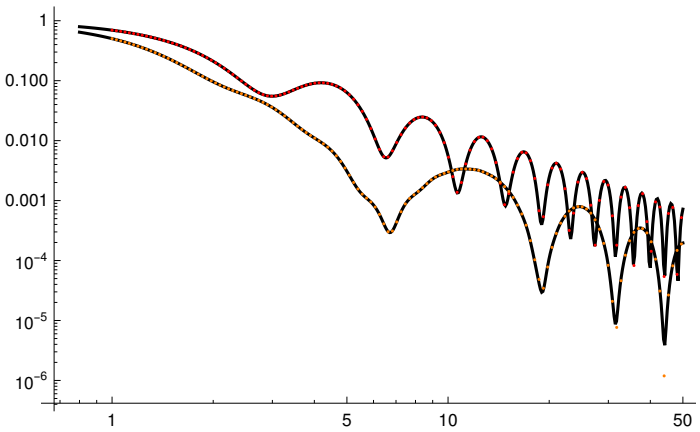
Phase factor end to end:

In[585]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = Psicenter2ends Psicenter2ends // FullSimplify
FILE = "PF_end_end.q";
OFILE = "PF_end2end.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π/2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π/2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} &/@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} &/@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} &/@ qq, {#, Abs[Func2[#]]} &/@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

Out[586]=
$$\text{Cos}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2\,\text{Hypergeometric0F1Regularized}\left[2, -\frac{1}{4}\,q^2\,R^2\,\text{Sin}[\theta q]^2\right]^2$$

Out[589]=
```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_end2end.dat
```

Out[596]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π / 2}], q] == 1 - q^2 sR2 / 6,
  sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^2}{2} + R^2\right\}\right\}$$

Phase factor end to hull:

In[597]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = Psicenter2ends Psicenter2hull // FullSimplify
FILE = "PF_end_hull.q";
OFILE = "PF_end2hull.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

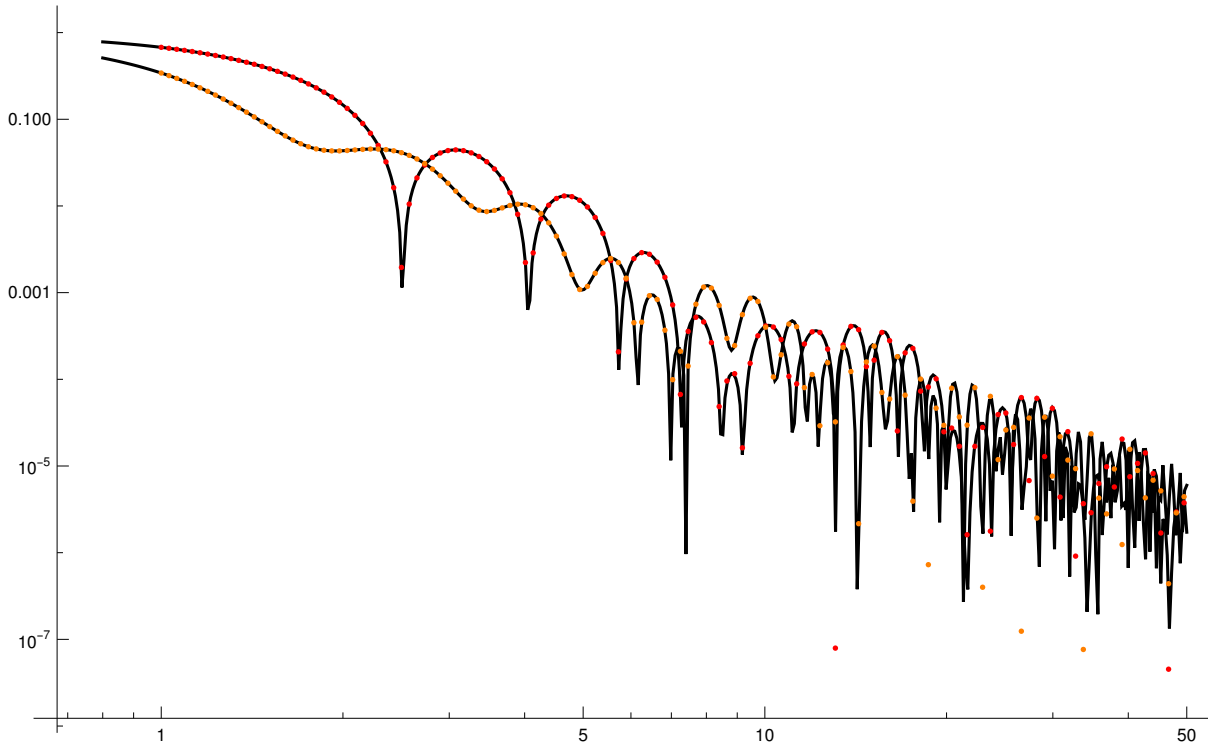
Out[598]=

$$\frac{2\,\text{BesselJ}[0,\, q\,R\,\text{Sin}[\theta q]]\,\text{BesselJ}[1,\, q\,R\,\text{Sin}[\theta q]]\,\text{Csc}[\theta q]\,\text{Sec}[\theta q]\,\text{Sin}[L\,q\,\text{Cos}[\theta q]]}{L\,q^2\,R}$$

Out[601]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_end2hull.dat
```

Out[608]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 sR2/6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{1}{6}\left(2\,L^2 + 9\,R^2\right)\right\}\right\}$$

Phase factor end to surface:

In[609]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = Psicenter2ends Psicenter2surface // FullSimplify
FILE = "PF_end_surface.q";
OFILE = "PF_end2surface.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π/2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π/2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]], Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]], Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {#, Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

Out[610]=
$$\frac{1}{q\,(L+R)}\,2\,\mathrm{Cos}\left[\frac{1}{2}\,L\,q\,\mathrm{Cos}[\theta q]\right]^2\,\mathrm{Hypergeometric0F1Regularized}\left[2,\,-\frac{1}{4}\,q^2\,R^2\,\mathrm{Sin}[\theta q]^2\right]$$
$$\left(\mathrm{BesselJ}\left[1,\,q\,R\,\mathrm{Sin}[\theta q]\right]\mathrm{Csc}[\theta q] + \mathrm{BesselJ}\left[0,\,q\,R\,\mathrm{Sin}[\theta q]\right]\mathrm{Sec}[\theta q]\,\mathrm{Tan}\left[\frac{1}{2}\,L\,q\,\mathrm{Cos}[\theta q]\right]\right)$$

Out[613]=
```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica_R1_L1.5/PF_end2surface.dat
```

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {0.0337476}. NIntegrate obtained 1.1947407972251158`*^-6 and 9.629865048311607`*^-6 for the integral and error estimates.

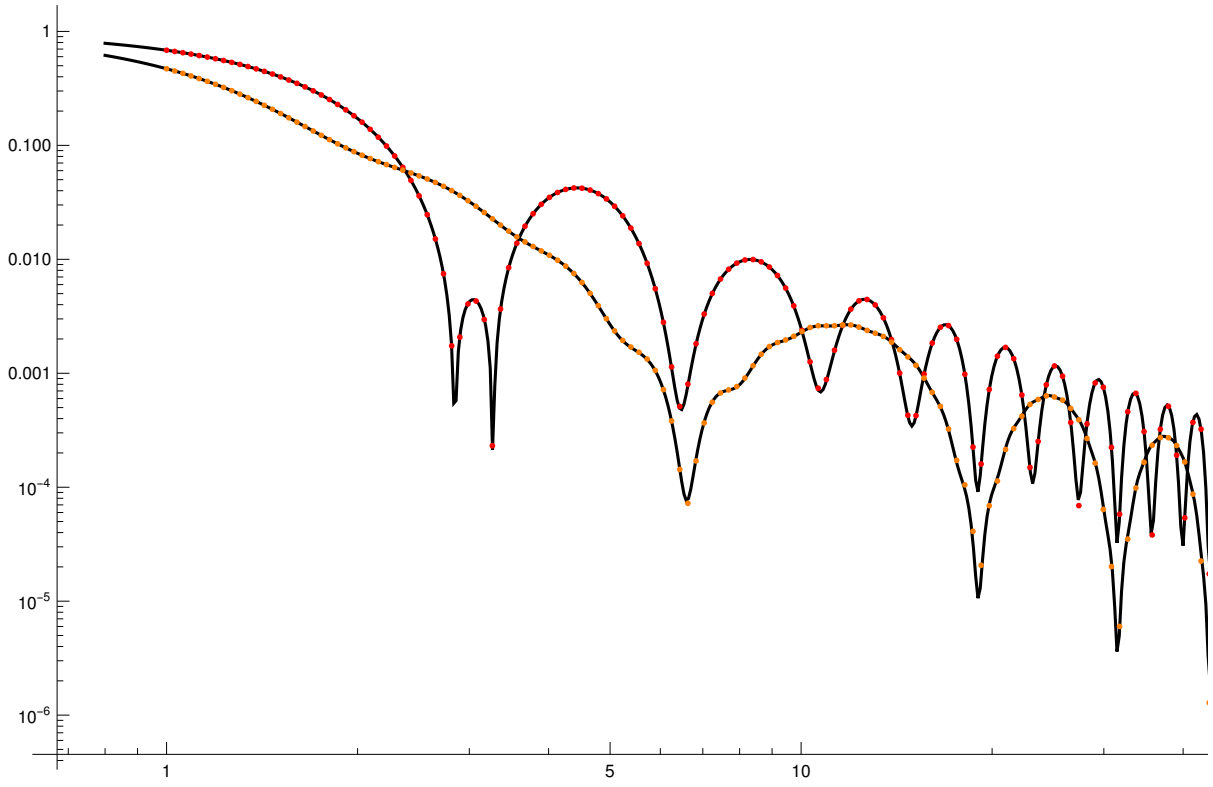
NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {0.929592}. NIntegrate obtained 3.6176816724577075`*^-6 and 8.837226804645919`*^-12 for the integral and error estimates.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.37445}. NIntegrate obtained 4.968403240887053`*^-6 and 3.499046183021942`*^-11 for the integral and error estimates.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in θq near {θq} = {1.37445}. NIntegrate obtained 0.000012224443959643234` and 2.3287321117609453`*^-11 for the integral and error estimates.

General: Further output of NIntegrate::ncvb will be suppressed during this calculation.

Out[620]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 sR2/6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{2\,L^3 + 3\,L^2\,R + 9\,L\,R^2 + 6\,R^3}{6\,(L+R)}\right\}\right\}$$

Phase hull end to hull:

In[621]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] = Psicenter2hull^2 // FullSimplify
FILE = "PF_hull_hull.q";
OFILE = "PF_hull2hull.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π/2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π/2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]], Abs[#[[2]]]} &/@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]], Abs[#[[2]]]} &/@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {#, Abs[Func1[#]]} &/@ qq, {#, Abs[Func2[#]]} &/@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

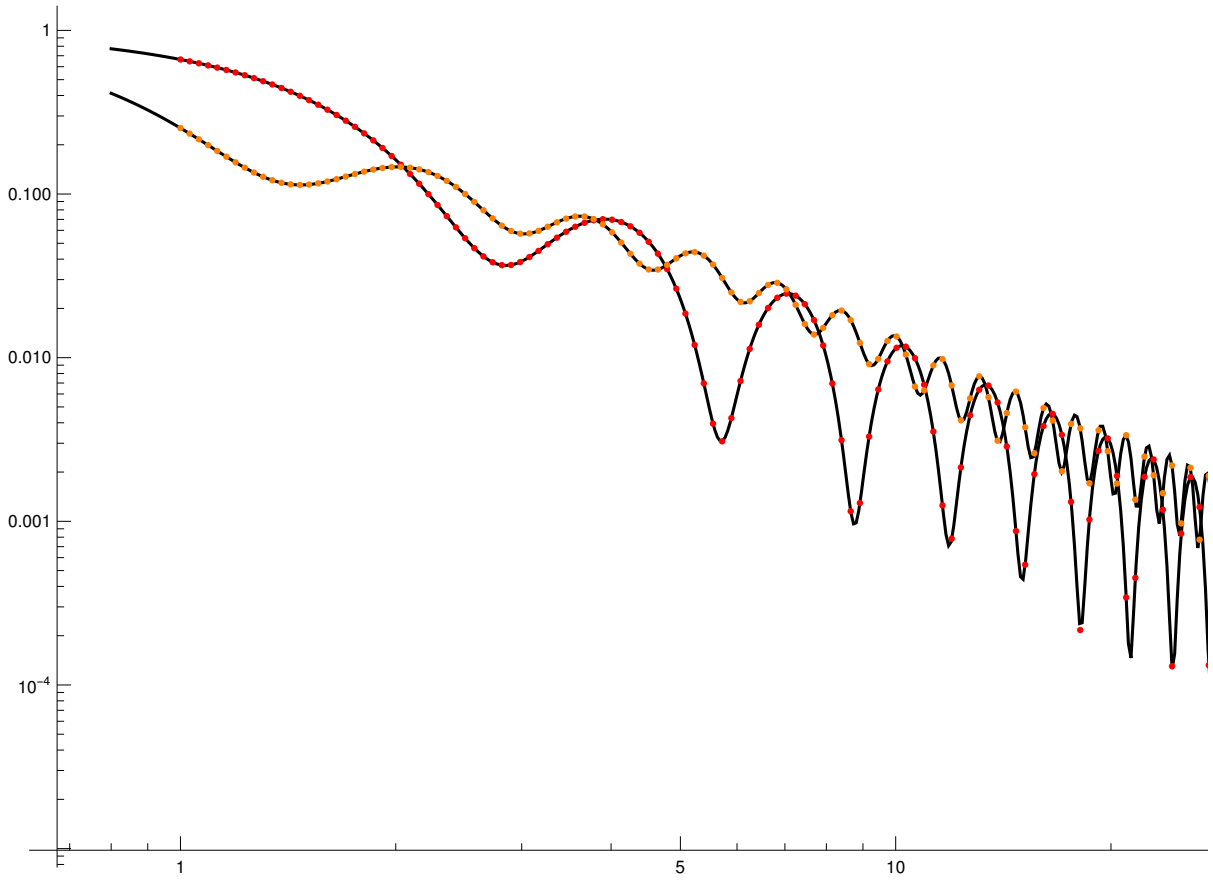
Out[622]=

$$\frac{4\,\text{BesselJ}\left[0,\ q\,R\,\text{Sin}[\theta q]\right]^2\,\text{Sec}[\theta q]^2\,\text{Sin}\left[\frac{1}{2}\,L\,q\,\text{Cos}[\theta q]\right]^2}{L^2\,q^2}$$

Out[625]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_hull2hull.dat
```

Out[632]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π / 2}], q] == 1 - q^2 sR2 / 6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^2}{6} + 2\,R^2\right\}\right\}$$

Phase hull end to surface:

In[633]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] =  Psicenter2hull Psicenter2surface // FullSimplify
FILE = "PF_hull_surface.q";
OFILE = "PF_hull2surface.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

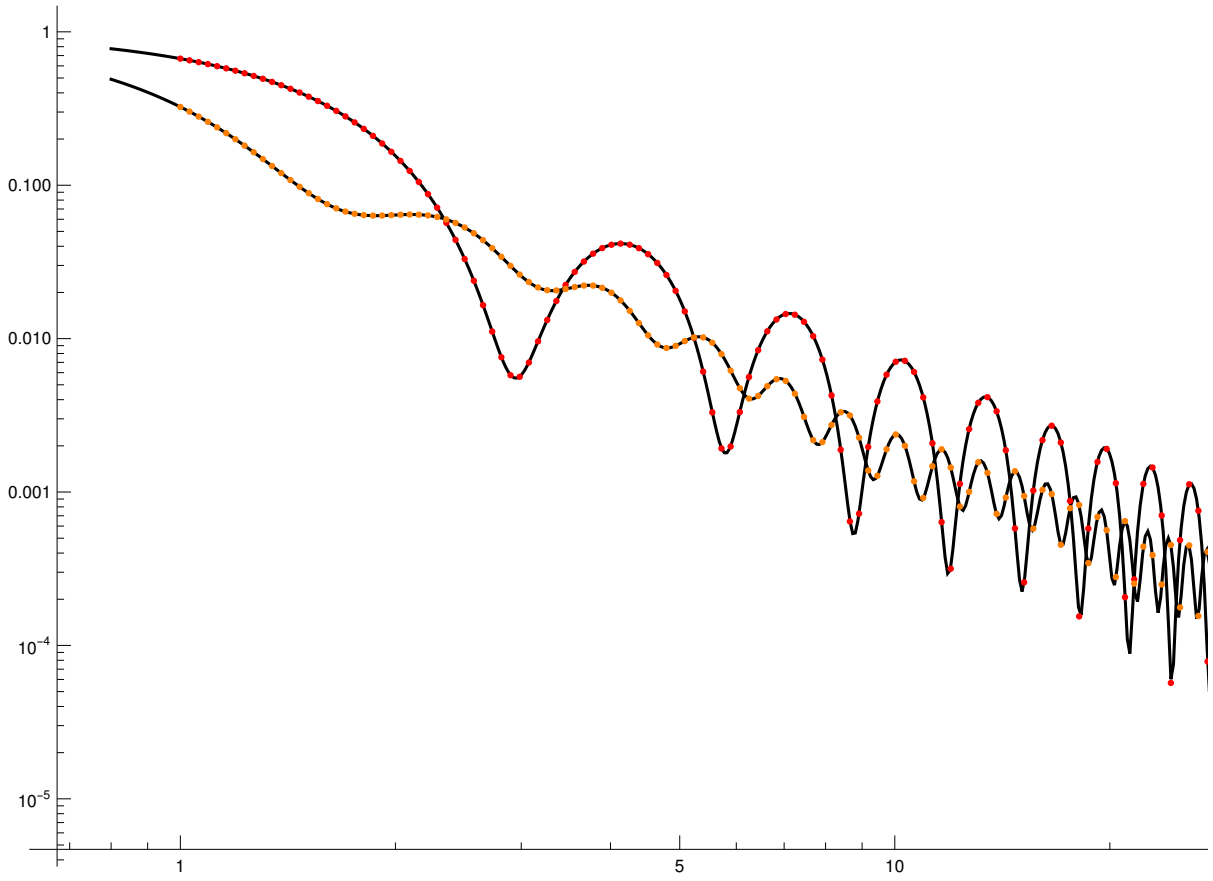
Out[634]=

$$\frac{1}{L\,q^2\,(L+R)}\,2\,\text{BesselJ}[0,\,q\,R\,\text{Sin}[\theta q]]\,\text{Sec}[\theta q]$$
$$\left(-\text{BesselJ}[0,\,q\,R\,\text{Sin}[\theta q]]\left(-1+\text{Cos}[L\,q\,\text{Cos}[\theta q]]\right)\text{Sec}[\theta q]+\right.$$
$$\left.\text{BesselJ}[1,\,q\,R\,\text{Sin}[\theta q]]\,\text{Csc}[\theta q]\,\text{Sin}[L\,q\,\text{Cos}[\theta q]]\right)$$

Out[637]=

```
/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica
  _R1_L1.5/PF_hull2surface.dat
```

Out[644]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π / 2}], q] == 1 - q^2 sR2 / 6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^3 + 2\,L^2\,R + 12\,L\,R^2 + 9\,R^3}{6\,(L + R)}\right\}\right\}$$

Phase factor surface to surface:

In[645]:=
```
Clear[Term, Func1, Func2, DATA1, DATA2, OFILE, DATA1, DATA2]
Term[q_] =  Psicenter2surface Psicenter2surface // FullSimplify
FILE = "PF_surface_surface.q";
OFILE = "PF_surface2surface.dat";
DIRO1 <> OFILE
Func1[q_] := NIntegrate[Term[q] Sin[θq] /. R → 1 /. L → 1.5, {θq, 0, π / 2}]
Func2[q_] := NIntegrate[Term[q] Sin[θq] /. R → 2 /. L → 0.5, {θq, 0, π / 2}]
SaveFunction[Func1, DIRO1 <> OFILE, 200, 0.01, 50];
SaveFunction[Func2, DIRO2 <> OFILE, 200, 0.01, 50];
DATA1 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR1 <> FILE, "Table"], 1];
DATA2 = {#[[1]] , Abs[#[[2]]]} & /@ Delete[Import[DIR2 <> FILE, "Table"], 1];
ListLogLogPlot[{DATA1, DATA2, {# , Abs[Func1[#]]} & /@ qq, {#, Abs[Func2[#]]} & /@ qq},
 PlotStyle → {{Red, Thick}, {Orange, Thick}, Black, Black},
 Joined → {False, False, True, True}]
```

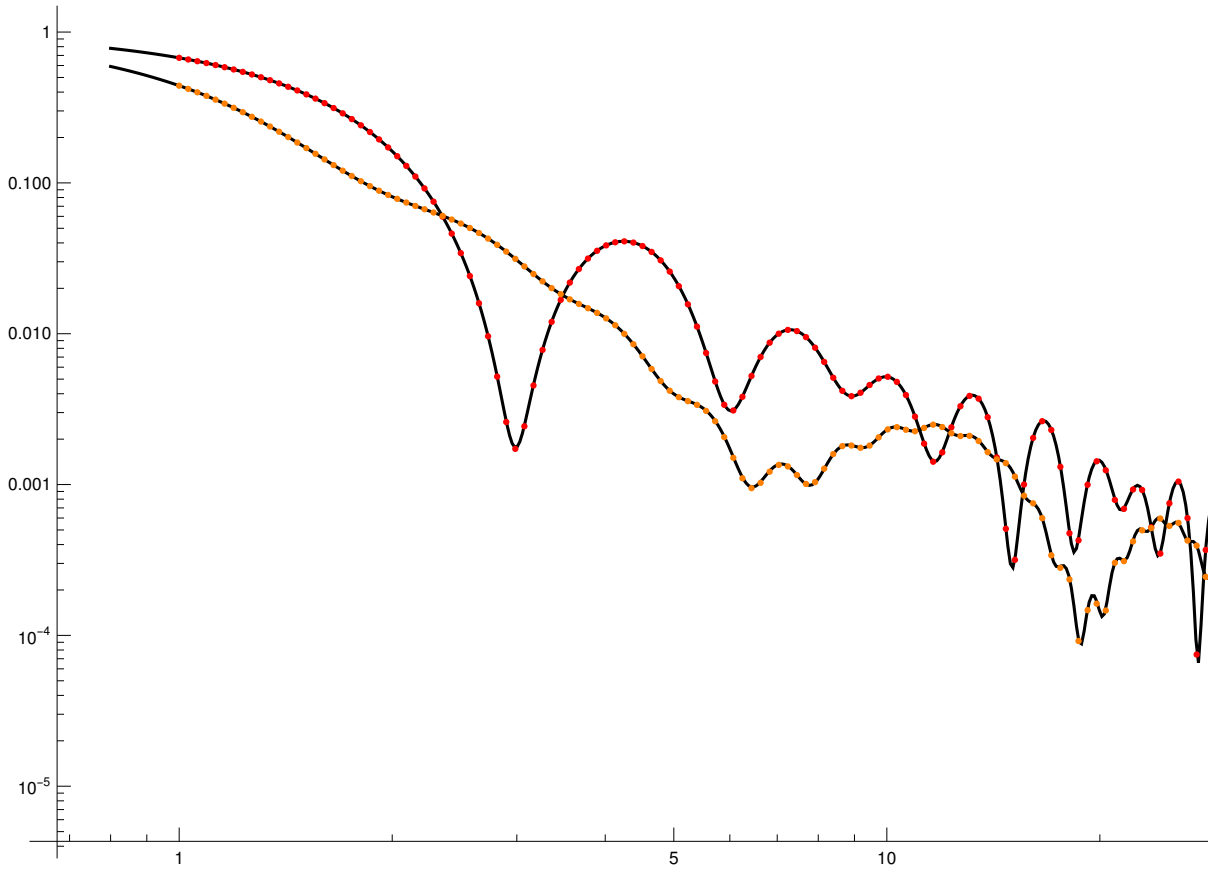
Out[646]=

$$\frac{1}{q^2 (L+R)^2} 4 \left(\text{BesselJ}\left[1, q R \text{Sin}[\theta q]\right] \text{Cos}\left[\frac{1}{2} L q \text{Cos}[\theta q]\right] \text{Csc}[\theta q] + \text{BesselJ}\left[0, q R \text{Sin}[\theta q]\right] \text{Sec}[\theta q] \text{Sin}\left[\frac{1}{2} L q \text{Cos}[\theta q]\right] \right)^2$$

Out[649]=

/home/zqex/source/SEB/Mathematica/../Examples/Validation/SolidCylinder_mathematica_R1_L1.5/PF_surface2surface.dat

Out[656]=



In[•]:=
```
Solve[Collect[Integrate[Series[Term[q], {q, 0, 3}] Sin[θq], {θq, 0, π/2}], q] == 1 - q^2 sR2/6, sR2] // Simplify
```

Out[•]=
$$\left\{\left\{sR2 \to \frac{L^3 + 3\,L^2\,R + 12\,L\,R^2 + 6\,R^3}{6\,(L + R)}\right\}\right\}$$