020404 Quiz 2 Properties

1) Calculate the radius of gyration for a rod of length L and radius R. The answer should be

\[ R_g^2 = \frac{R^2}{2} + \frac{L^2}{12} \]

This can be obtained by integration over a differential volume element, \( dV \sim rdrdl \), where the distance from the center of mass is given by \( R^2 = (r^2 + l^2) \). You will need to integrate from \( r = 0 \) to \( R \) and from \( l = 0 \) to \( L/2 \) since the distance from the center of mass to the end of the rod is \( L/2 \).

2) Give the Debye scattering function for a Gaussian polymer coil.
   - Show mathematically that the low-q limit is Guinier's law
   - and that the high-q limit is a mass-fractal scaling law.

3) For a polymer coil the step size \( b \) is related to a physical feature, the persistence length (or Kuhn step length = \( 2l_{\text{pc}} \)) that can be measured using rheology, dynamic light scattering or static neutron scattering. The persistence length is a size where chain scaling has a transition to linear scaling at high-q.
   - Sketch the neutron scattering curve for a Gaussian chain with persistence in a log I versus log q plot.
   - Plot the same curve on a Kratky plot, \( Iq^2 \) versus \( q \),
   - and on a modified Kratky plot, \( Iq \) versus \( q \).

4) How can the number of Kuhn units in a chain, \( N_K \), be determined from the first plot of question 3?
1) \[ R_g^2 = \sum \frac{(\text{density})(\text{volume})(\text{Position})^2}{\sum \text{(density)(volume)}} \]

Consider a differential volume element, dV, for a rod, dV ~ r dr dl, and the density is constant in the rod. The squared position from the center of mass is \((l^2 + r^2)\) so,

\[
R_g^2 = \frac{\int_0^L \int_0^R (r^2 + l^2) r dr dl}{\int_0^L \int_0^R r dr dl} = \frac{\int_0^L \left( \frac{Lr^3}{2} + \frac{L^3r}{24} \right) dr}{\int_0^L \frac{Lr}{2} dr} = \frac{\left( LR^4 \right)}{8} + \frac{L^3R^2}{48} = \frac{R^2}{2} + \frac{L^2}{12}
\]

2) **Extensions of the Debye Equation for an Ideal Polymer Coil.**

The Debye equation for polymer coils was given above,

\[ g(q)_{\text{Gaussian}} = \frac{2N}{Q^2} \left[ Q - 1 + \exp(-Q) \right] \]

where \(Q = (qR_g)^2\). At low-q this function extrapolates to \(N\) (expansion of \(\exp(-x)\) for small \(x\) is \(1 - x + x^2/2\)). At high-q the Debye function extrapolates to \(2N/(qR_g)^2\) (at high-q, \(\exp(-Q)\) goes to 0 and \(Q \gg 1\)). This high-q limit is a -2 slope power-law for intensity in \(q\), so a log I vs log q plot will be a line with slope -2. In general, weak slopes in log-log plots of this type reflect the negative of the mass-fractal dimension of the object. The cutoff between this power-law behavior and the constant intensity behavior at low-q is governed by \(R_g\).

3) 

4) \(R_g^2\) for the chain = \(N_K \cdot 2l_{\text{per}}^2/3\). The plot yields \(R_g\) and \(l_{\text{per}}\) so \(N_K\) can be determined. \(\pi/l_{\text{per}}\) is the intercept of the modified Kratky plot or can be obtained from \(R_g\) for the persistence transition using the function obtained in question 1.