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 ~ 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 = $2l_{per}$) 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?

Answers: 020404 Quiz 2 Properties

1)

$$R_g^2 = \frac{\sum (density)(volume)(Position)^2}{\sum (density)(volume)}$$

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

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

2)

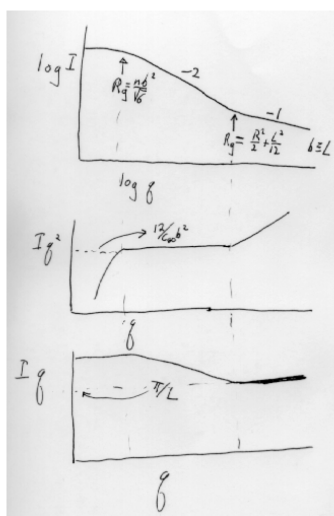
Extensions of the Debye Equation for an Ideal Polymer Coil.

The Debye equation for polymer coils was given above,

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

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 >>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^2_g for the chain = $N_K\, 2l_{per}^2/3$. The plot yields R_g and l_{per} so N_K can be determined. π/l_{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.