121024 Quiz 7 Polymer Properties

1) Correlation functions have certain basic features. The correlation function for a structure at small distances "r" follows:

$$p(r) = 1 - \frac{S}{4V} r + \cdots \qquad (1)$$

where S is the surface area and V is the volume.

Further, $V = 4\pi \int_0^{\infty} p(r) r^2 \, dr$ (2).

a) What is S/V for the Debye-Bueche correlation function, $p(r) = K \exp\left(-\frac{r}{\xi}\right)$

(Use the exponential expansion at low values of the argument.)

b) What is S/V for the Ornstein-Zernike correlation function?

c) What are the units of K for the DB structure based on your answer to a) and the function itself?

d) What is S/V for the transform of Guinier's Law, $p(r) = K \exp\left(-\frac{3r^2}{4R_g^2}\right)$? Is this consistent with the idea of a particle with no surface?

e) Using equation 2 and $\int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2) dx = \frac{\pi^{1/2}}{2\alpha^{3/2}}$, calculate the volume for the Guinier correlation function?

f) The Sinha function has a related correlation function, $p(r) = \frac{K}{r^{3-d_f}} \exp\left(-\frac{r}{\xi}\right)$. Show that this function describes both the DB and OZ functions.

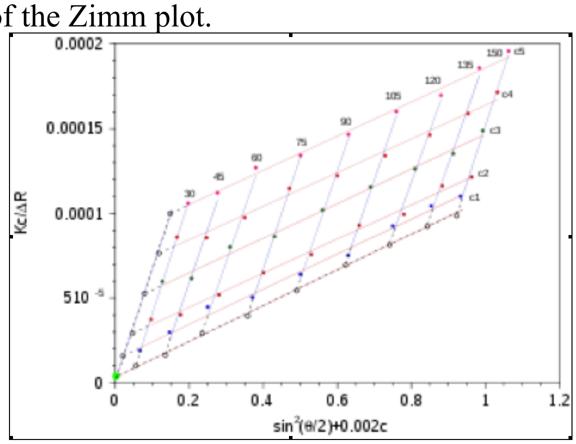
g) What is the intensity function (Fourier transform of this correlation function: $I(q) = \frac{G \sin\left[(d_f - 1)\arctan(q\xi)\right]}{q\xi \left(1 + q^2\xi^2\right)^{(d_f-1)/2}}$) when $d_f = 1$?

2) a,b) Show that the OZ and Debye functions have incompatible limits at low and high q.

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

Debye: where $Q = q^2 N b^2/6 = q^2 R_g^2$

c) Explain the origin of the Zimm plot.



ANSWERS: 121024 Quiz 7 Polymer Properties

1) a) $p(r) = K\exp\left(-\frac{r}{\xi}\right)$ at small r can be expanded as $p(r) = K\left(1 - \frac{r}{\xi} + \cdots\right)$ so $\frac{\xi}{K} = \frac{4V}{S}$, 6V/S is called the Sauter Mean diameter or equivalent spherical diameter.

b) Following the same expansion, $p(r) = \frac{K}{r}\exp\left(-\frac{r}{\xi}\right)$ => $p(r) = K\left(\frac{1}{r} - \frac{1}{\xi} + \frac{r}{\xi^2} - \cdots\right)$ so

$\frac{\xi^2}{K} = \frac{4V}{S}$.

c) K is unitless from the function itself since p(r) is a probability (no units). From the answer to "a)" K is also unitless.

d) $p(r) = K\exp\left(-\frac{3r^2}{4R_g^2}\right) \Rightarrow K\left(1 - \frac{3r^2}{4R_g^2} + \cdots\right)$ there is no term linear in r so S/V is is 0, there is no surface.

e) $\alpha = \frac{3}{4R_g^2}$ and the integral is ½ of the integral from -∞ to ∞ so $V = K\frac{2\pi^{1/2}R_g^3}{3^{3/2}}$.

f) For $d_f = 3$ the function correlation function is the DB function and for $d_f = 2$ the crrelation function is the OZ function.

g) The intensity function is 0 for all 1 for $d_f = 1$ since $(d_f\text{-}1)$ in the numerator is 0 and sin(0) = 0. This means that the function doesn't work for all fractal objects.

2) a, b) , c)