121024 Quiz 7 Polymer Properties

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

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

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

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

g) What is the intensity function (Fourier transform of this correlation function:

\[ I(q) = \frac{G\sin\left[(\Omega - 1)\arctan(\Omega\xi)\right]}{\xi^2 (1 + \xi^2 \gamma^2)^{1/2}} \]

when \( d_f = 1 \)?

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

\[ I(q)_{\text{OZ,Debye}} = \frac{2}{G} \left[ Q - 1 + \exp(-Q) \right] \]

where \( Q = qN_b/6 - q^2R_g^2 \)

c) Explain the origin of the Zimm plot.
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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, \( p(r) = \frac{K}{r} \exp \left( -\frac{r}{\xi} \right) \Rightarrow p(r) = K \left( 1 - \frac{1}{\xi} + \frac{r}{\xi^2} - \cdots \right) \) 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) \( p(r) = K \exp \left( -\frac{3r^2}{4R_g^2} \right) \Rightarrow p(r) = K \left( 1 - \frac{3r^2}{4R_g^2} + \cdots \right) \) there is no term linear in \( r \) so \( S/V \) is 0, there is no surface.

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

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

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

2) a, b) 

Ornstein-Zernike Function, Limits and Related Functions

<table>
<thead>
<tr>
<th>Ornstein-Zernike (Empirical)</th>
<th>Debye (Exact)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I(q) = -\frac{G}{q^2} )</td>
<td>( g(q) ) low limit</td>
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<tr>
<td>( I(q) = -\frac{G}{q^2} )</td>
<td>( 2\xi = R_g^2 )</td>
</tr>
<tr>
<td>( I(q) = -\frac{G}{q^2} )</td>
<td>( 3\xi = R_g^2 )</td>
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<tr>
<td>( I(q) ) - Gexp(-q\xi)</td>
<td>( I(q) ) - ( \frac{G}{q^2} ) - Gexp(-q\xi)</td>
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<tr>
<td>Zimm Plot</td>
<td>( g(q) = \frac{G}{q^2} )</td>
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<tr>
<td>Plot is linearized by ( G/\langle I(q) \rangle ) versus ( q^2 )</td>
<td>( G/\langle I(q) \rangle = 1 + \frac{qR_g^2}{3} )</td>
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<tr>
<td>Concentration part will be described later</td>
<td>( q = \frac{4\pi}{\lambda} \sin \left( \frac{\theta}{2} \right) )</td>
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