A. Plot the following for rod (R=L/2), Gaussian coil (R=Rg) and sphere(R=radius).
   1. P(q) vs. q^2R^2 for $0 \le q^2R^2 \le 30$
   2. $q^2R^2 \cdot P(q)$ vs. qR for $0 \le qR \le 10$
   3. P(q) vs. log(qR) for $10^{-3} \le qR \le 10$

B. Plot $[P(q) \,.\, q^4R^4]$ vs. qR for a sphere with radius R

C. 3.5

D. 3.6

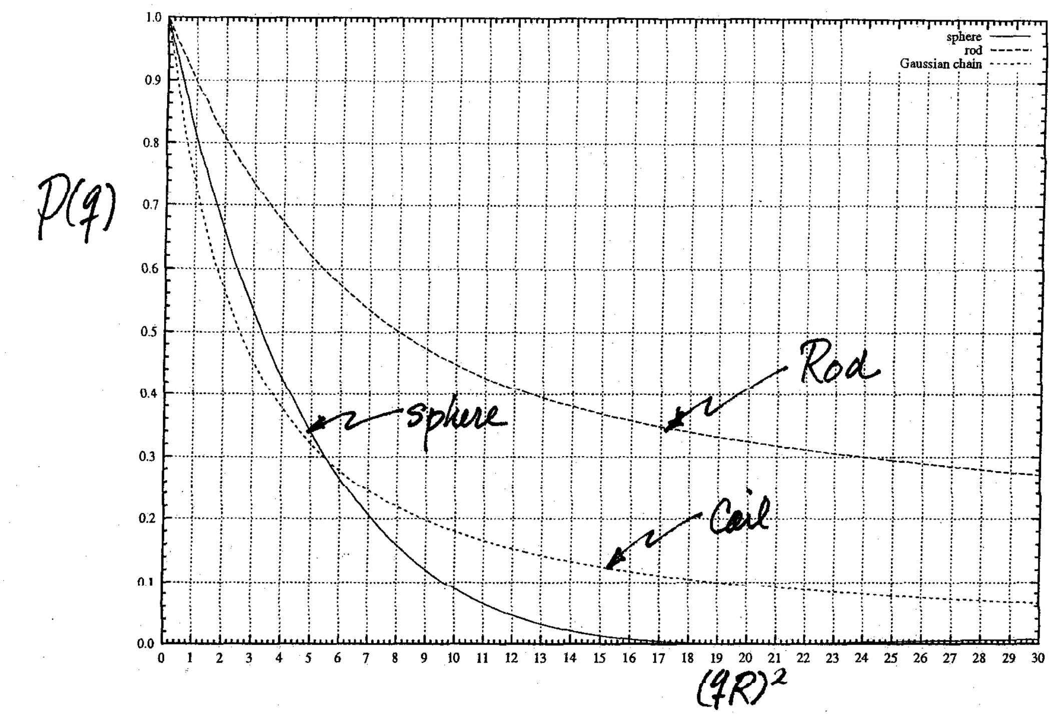
E. 3.7

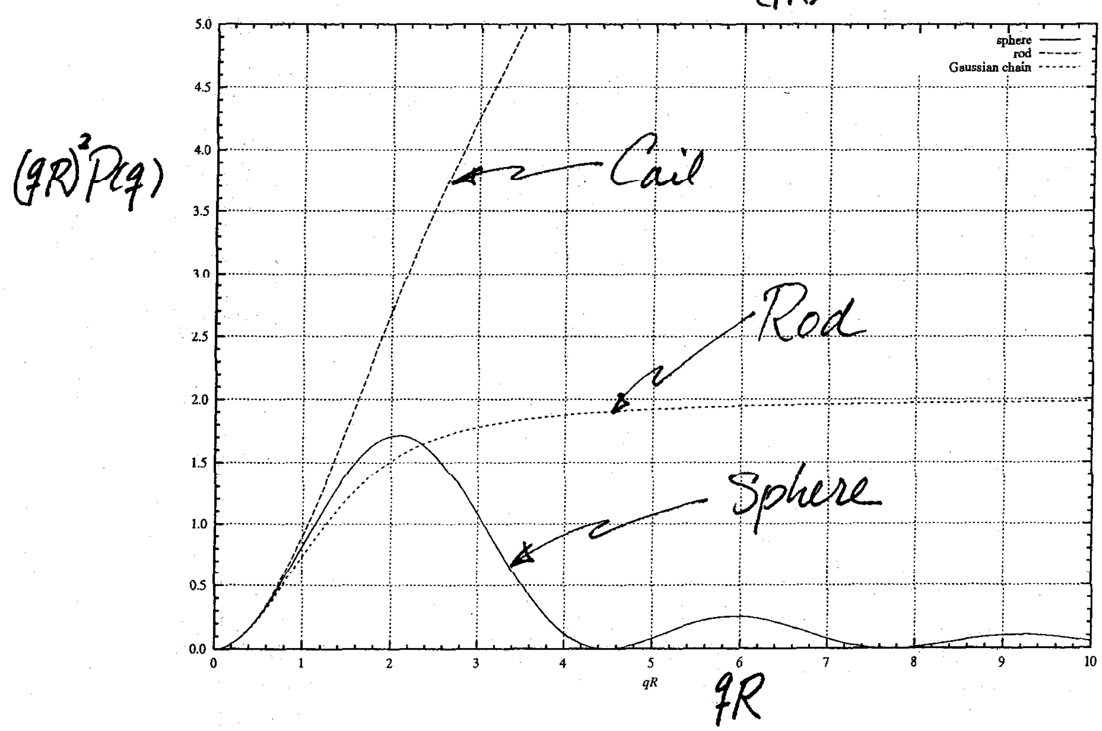
F. 3.8

G. 3.9

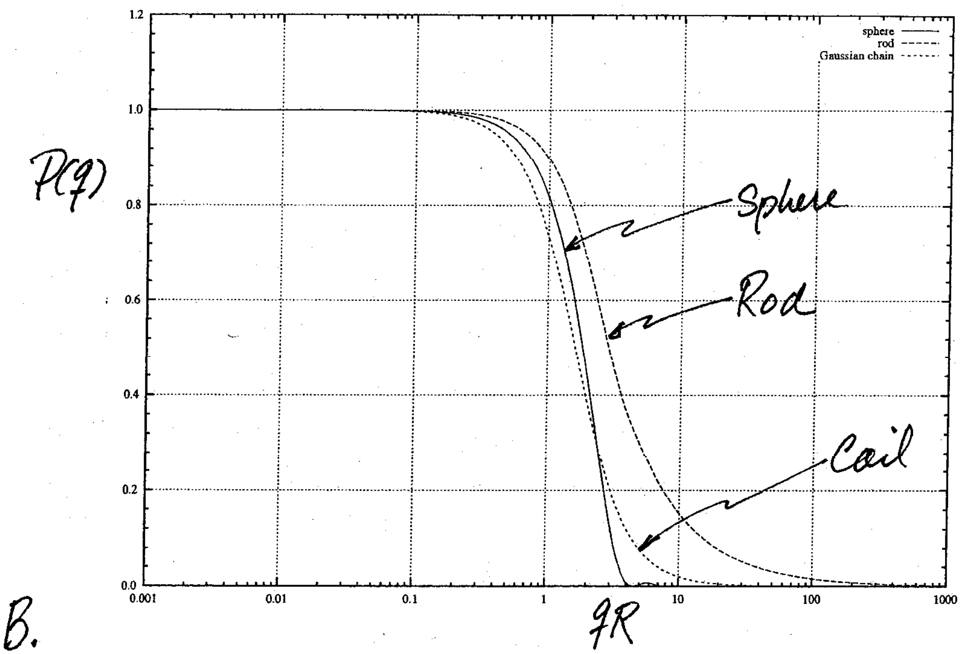
Solutions to PS #6 10/28/02

A



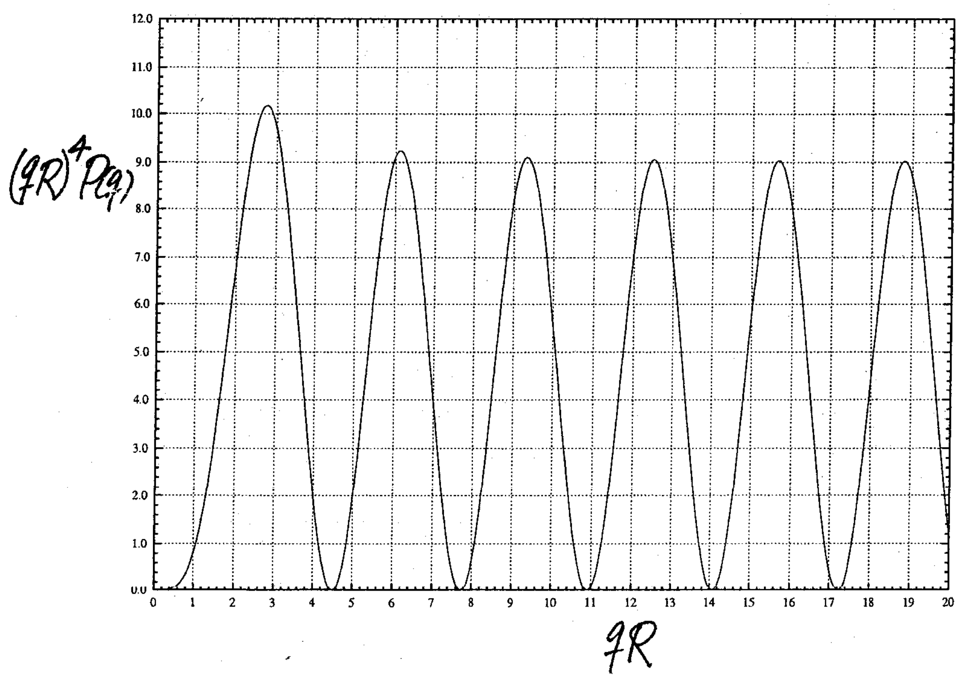


SPS 6/2



B.

The following is a plot of $q^4R^4P(q)$ versus qR for a solid sphere of radius R.



SPS 6/3

C(3.5) Let the chain dimension at the interface of air/water be R_{2D}

$$A = A_{int} + A_{ext} = kT\left(a\frac{N^2}{R_{2D}^2} + \frac{R_{2D}^2}{R_o^2}\right) \quad \text{where } R_o^2 = b^2N$$

$$\left(\frac{\partial A}{\partial R_{2D}}\right)_{T,V} = kT\left(-2a\frac{N^2}{R_{2D}^3} + \frac{2R_{2D}}{Nb^2}\right)$$

$$\frac{aN^2}{R_{2D}^3} = \frac{R_{2D}}{Nb^2}, \quad R_{2D}^4 = a\,b^2N^3$$

$$R_{2D} = a^{1/4}\,b^{1/2}\,N^{3/4}$$

For $N=10^3$, $b=3\mathring{A}$, $a=7.2\mathring{A}^2$, $v=21.6\mathring{A}^3$

$$R_{2D} = (7.2\mathring{A}^2)^{1/4}(3\mathring{A})^{1/2}(10^3)^{3/4} \cong 1.64\cdot 1.73\cdot 1.78\cdot 10^2 \cong 5.04\cdot 10^2\mathring{A}$$

$$R_F = v^{1/5}\,b^{2/5}\,N^{3/5} \Longleftarrow A = kT\left(v\frac{N^2}{R^3} + \frac{R^2}{Nb^2}\right)$$

$$= (21.6\mathring{A}^3)^{1/5}(3\mathring{A})^{2/5}\cdot(10^3)^{3/5} \cong 1.8\cdot 10^2\mathring{A}$$

D(3.6) Let $R_g \cong R_{o,b} = bN^{1/4}$, Randomly branched chain

$$A = kT\left(v\frac{N^2}{R_b^3} + \frac{3}{2}\frac{R_b^2}{R_{o,b}^2}\right)$$

$$3v\frac{N^2}{R_b^4} \approx 3\frac{R_b}{b^2N^{1/2}}, \quad R_b^5 \approx v\,b^2N^{5/2}$$

$R_b \cong (21.6\mathring{A}^3)^{1/5}(3\mathring{A})^{2/5}(10^3)^{5/2} \cong 90\mathring{A}$ (randomly branched chain in good solvent)

$R_F \approx v^{1/2}b^{2/5}N^{3/5} \cong 1.8\cdot 10^2\mathring{A}$ (linear, good solvent)

$R_o = bN^{1/2} \cong 3\mathring{A}\,10^{3/2} \cong 95\mathring{A}$ (linear, θ-solvent)

E(3.7) Randomly branched chain in good solvent,

The overlap volume fraction, $\phi_b^* \frac{Nb^3}{R_b^3}$

$$= \frac{Nb^3}{v^{3/5} b^{6/5} N^{3/2}}$$

$$R_b \approx v^{1/5} b^{2/5} N^{1/2}$$

$$\underline{\underline{= v^{-3/5} b^{9/5} N^{-1/2}}}$$

$$\phi_b^* \cong (21.5 Å^3)^{-3/5} \cdot (3 Å)^{9/5} (10^3)^{-1/2}$$

$$\cong 0.036$$

$$\phi_{linear}^* = \frac{Nb^3}{R_F^3} = \frac{Nb^3}{v^{3/5} b^{6/5} N^{9/5}} \cong 0.0046$$

$$\phi_{\theta,linear}^* = \frac{Nb^3}{(bN^{1/2})^3} = N^{-1/2} = 0.032$$

F. (3.8) Randomly branched chain on A/W

$$A = kT\left(a \frac{N^2}{R_{2D,b}^2} + \frac{R_{2D,b}^2}{R_{0,b}^2}\right)$$

$$R_{0,b} = bN^{1/4}$$

(i) $R_{2D,b} = a^{1/4} b^{1/2} N^{5/8}$

(ii) $R_{2D,b} = (7.2 Å^2)^{1/4} (3 Å)^{1/2} (10^3)^{5/8} \cong 210 Å$

(iii) $\sigma_{2D,b}^* \approx \frac{N}{R_{2D,b}^2} \approx \frac{N}{a^{1/2} b N^{5/4}} \approx \frac{1}{a^{1/2} b N^{1/4}} \cong 0.02$ Kuhn segments/$Å^2$

(iv) $\sigma_{2D,b}^* \cong 1.78 \cdot 0.02 \cong 0.04$ segments/$Å^2$

G.(3.9) SPS6/5

(i) Linear chain at $T=\theta$, $b=4\text{Å}$, $N=400$

$$A_{int} \approx kTR^3\left[v\left(\frac{N}{R^3}\right)^2 + w\left(\frac{N}{R^3}\right)^3 + \dots\right]$$

$$v \approx \left(1-\frac{\theta}{T}\right)b^3$$

$$w \approx b^6$$

$$A \approx kT\left(\frac{R_\theta^2}{b^2N} + w\frac{N^3}{R_\theta^6}\right), \quad R_\theta \approx (b^2w)^{1/8}N^{1/2}$$

$\approx bN^{1/2}$ (ideal) $\leftarrow$ if $w \approx b^6$

(ii) If $v > w\dfrac{N}{R^3} \approx \dfrac{w}{b^3\sqrt{N}} \approx \dfrac{b^3}{\sqrt{N}}$

$R \approx b\sqrt{N}$ $\qquad \approx 3.2\text{Å}^3$

(iii) $1-\dfrac{\theta}{T} > \dfrac{1}{\sqrt{N}}$, $\quad T > \dfrac{\theta}{1-\frac{1}{\sqrt{N}}} \approx 316K = 43°C$

(iv) $R_F \approx v^{1/5}b^{2/5}N^{3/5}$, $b=4\text{Å}$, $N=400$

at $T=60°c$, $\quad v \approx b^3\left(1-\dfrac{\theta}{T}\right) \approx 64\text{Å}^3\left(1-\dfrac{300}{333}\right)$

$$\approx 6\text{Å}^3$$

$R_F = 6^{1/5}\,4^{2/5}\,400^{3/5}$, $\quad R_F \approx \underline{\underline{90\text{Å}}}$

(v) $\phi^* \approx \dfrac{Nb^3}{R_F^3} \triangleq \dfrac{400\cdot 4^3}{(90\text{Å})^3} \triangleq 3.4\cdot 10^{-2}$

(vi) $g_T \approx \dfrac{b^6}{v^2} \approx \dfrac{(4\text{Å})^6}{(6\text{Å}^3)^2} \triangleq \underline{\underline{114}}$