Solutions to

PS #5 due 10/21/02

A (2.22)

Start with Kramers' Theorem, $R_g^2 = \frac{b^2}{N}\langle N_1(N-N_1)\rangle$

For a f-arm star, $\langle N_1(N-N_1)\rangle = \frac{1}{(N/f)}\int_0^{N/f} N_1(N-N_1)\,dN_1$

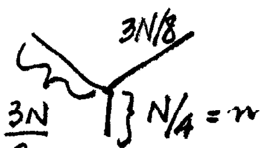
$$= \frac{N^2(3f-2)}{6f^2}$$

$$\therefore R_g^2 = \frac{b^2}{N}\cdot\frac{N^2(3f-2)}{6f^2} = \frac{Nb^2}{6}\left(\frac{3f-2}{f^2}\right)$$

which correctly reduces to $R_g^2 = \frac{Nb^2}{6}$ if $f=2$, linear chain case.

B. (2.23)

(i) $R_g^2 = \frac{b^2}{N}\langle N_1(N-N_1)\rangle = \frac{b^2}{N}\left\{\frac{1}{N}\int_0^{N/4} N_1(N-N_1)\,dN_1 + \frac{2}{N}\int_0^{\frac{3N}{8}} N_1(N-N_1)\,dN_1\right\}$



$$= \frac{b^2}{N}\left\{\left(\frac{N}{4}\right)^2\left(\frac{1}{2}-\frac{1}{12}\right) + \frac{2\cdot 9N^2}{64}\left(\frac{1}{2}-\frac{1}{8}\right)\right\} = Nb^2\left(\frac{101}{768}\right) = \frac{Nb^2}{6}\left(\frac{101}{128}\right)$$

$R_g^2/R_{g,linear}^2 = \frac{101}{128}$, $R_g/R_{g,linear} = 0.888$

(ii) If $b = 3\text{Å}$, $N = 10^3$, $R_g = \left(\frac{101}{768}\right)^{1/2} N^{1/2} b \cong 34.4\text{Å}$

(iii) Equal branch size, $R_g^2 = \frac{Nb^2}{6}\left(\frac{3\cdot 3-2}{3\cdot 3}\right) = \frac{Nb^2}{6}\left(\frac{7}{9}\right) =$

$f=3$ Smallest $R_g = \left(\frac{7N}{54}\right)^{1/2} b = 34.2\text{Å}$

Linear case, $R_g = \left(\frac{N}{6}\right)^{1/2} b = 38.7\text{Å}$

C (2.27)

$R = \left(\frac{5}{3}\right)^{1/2} R_g = 581\text{Å}$, Mass density $\rho = \frac{M}{\frac{4\pi}{3}R^3 N_{AV}} = \underline{\underline{5.25\cdot 10^{-2}\,g/cm^3}}$

D. (2.34) The solution is provided in Handout #8

$$L(\underline{s}) = \int_{-\infty}^{\infty} \mathbb{P}(\underline{R})\, e^{-\underline{R}\cdot\underline{s}}\, d\underline{R} = \int_0^{\infty} \mathbb{P}(\underline{R})\, 4\pi R^2 \left[\frac{\sinh(Rs)}{Rs}\right] dR$$

$$= \int_0^{\infty} \mathbb{P}(\underline{R}) \left(1 + \frac{R^2 s^2}{3!} + \frac{R^4 s^4}{5!} + \cdots\right) 4\pi R^2 dR$$

$$= 1 + \frac{\langle R^2\rangle s^2}{3!} + \frac{\langle R^4\rangle s^4}{5!} + \cdots$$

Also, $L(\underline{s}) = e^{\langle R^2\rangle s^2/6} = 1 + \dfrac{\langle R^2\rangle s^2}{6} + \dfrac{1}{2!}\left(\dfrac{\langle R^2\rangle}{6}\right)^2 s^4 + \dfrac{1}{3!}\left(\dfrac{\langle R^2\rangle}{6}\right)^3 s^6 + \cdots$

Comparison of the terms with the same s powers,

$$\frac{1}{3!}\langle R^2\rangle = \frac{\langle R^2\rangle}{6}$$

$$\frac{1}{5!}\langle R^4\rangle = \frac{1}{2!}\left(\frac{\langle R^2\rangle}{6}\right)^2, \quad \langle R^4\rangle = \frac{5!}{2!}\left(\frac{\langle R^2\rangle}{6}\right)^2$$

$$\frac{1}{7!}\langle R^6\rangle = \frac{1}{3!}\left(\frac{\langle R^2\rangle}{6}\right)^3, \quad \langle R^6\rangle = \frac{7!}{3!}\left(\frac{\langle R^2\rangle}{6}\right)^3$$

$$\vdots$$

$$\underline{\underline{\langle R^{2p}\rangle = \frac{(2p+1)!}{p!}\left(\frac{\langle R^2\rangle}{6}\right)^p}}$$

E. (2.40)

$$f_x = eE = \underbrace{\frac{3kT}{Nb^2}}_{\text{entropy spring const}} R_x, \quad eE = 1.6\cdot 10^{-19}\,C \cdot 10^4 \frac{V}{cm} = 1.6\cdot 10^{-19}\cdot 10^6 \frac{CV}{m}$$

$$\boxed{R_x = f_x \cdot \frac{Nb^2}{3kT}} \qquad = 1.6\cdot 10^{-13}\, J/m$$

$$kT(300K) = 4.14\cdot 10^{-21}\,J, \quad R_{x,0} = \langle R_{x,0}^2\rangle^{1/2} = \left(\tfrac{1}{3}Nb^2\right)^{1/2} = b\sqrt{\frac{N}{3}}$$

$$\langle R^2\rangle = \langle R_{x,0}^2\rangle + \langle R_{y,0}^2\rangle + \langle R_{z,0}^2\rangle = 3\langle R_{x,0}^2\rangle$$

$$R_x / \langle R_{x,0}^2\rangle^{1/2} = \frac{eENb^2}{3kT} \Big/ b\sqrt{\frac{N}{3}}$$

$$= \frac{eEb\sqrt{N}}{\sqrt{3}\,kT} = \frac{1.6\cdot 10^{-13}\frac{J}{m}\cdot 0.6\cdot 10^{-9}\,m \cdot 10^2}{\sqrt{3}\cdot 4.14\cdot 10^{-21}\,J} \cong 1.34$$

$b = 6 Å, N = 10^4$

34% extension over $\langle R_{x,0}^2\rangle^{1/2}$

F(2.41)

(i) $f_x = \frac{(Ze)^2}{\varepsilon R^2} = \frac{3kT}{Nb^2} R_x^3, \quad R_x^3 = \frac{Z^2 e^2 N b^2}{3\varepsilon kT}$

$$R_x = \left(\frac{Z^2 e^2 N b^2}{3kT\varepsilon}\right)^{1/3} = \left(\frac{Z^2 N b^2 l_B}{3}\right)^{1/3}$$

$$l_B \equiv \frac{e^2}{\varepsilon kT} \cong 7\text{Å} \text{ (water at 298K)}$$

Bjerrum length

(ii) $$\frac{R_x}{R_{x,0}} = \frac{(Z^2 N b^2 l_B/3)^{1/3}}{(N^{1/2} b/\sqrt{3})}$$

$$= \frac{(Z^2 N b^2 l_B/3)^{1/3}}{(N^{3/2} b^3/3^{3/2})^{1/3}} = \left(\frac{Z^2 l_B \sqrt{3}}{\sqrt{N}\cdot b}\right)^{1/3} = \left(\frac{10^2 \cdot 7\text{Å} \cdot \sqrt{3}}{10 \cdot 3\text{Å}}\right)^{1/3}$$

$= 3.43$, a substantial deformation!

G(2.44), Form factor for solid sphere with a radius R

$$P(q) = \left|\frac{1}{N}\sum_i e^{i q \cdot R_i}\right|^2 \approx \left[\frac{\int_0^R \frac{\sin qR_i}{qR_i} 4\pi R_i^2 \, dR_i}{\int_0^R 4\pi R_i \, dR_i}\right]^2$$

Eq.(2.143)

$$P(q) = \left[\frac{3}{(qR)^3}(\sin qR - qR\cos qR)\right]^2$$

solid sphere

H(2.45) P(q) for a rod with length L

$$P(q) = \frac{1}{N^2}\sum_i \sum_j \left\langle \frac{\sin q h_{ij}}{q h_{ij}} \right\rangle \qquad \text{Eq. (2.143)}$$

For rod, $h_{ij} = b|j-i|$, $b \leq h_{ij} \leq (N-1)b$

$$P(q) = \frac{2}{N^2}\sum_{j=2}^{N}\sum_{i=1}^{j-1} \frac{\sin qb(j-i)}{qb(j-i)}, \quad j-i \equiv k$$

$$= \frac{2}{N^2}\sum_{k=1}^{N-1}(N-k)k\left(\frac{\sin qbk}{qbk}\right)$$

$$= \frac{2b^2}{L^2}\sum_k (N-k)k\left(\frac{\sin qbk}{qbk}\right) = \frac{2}{L^2}\sum_k (Nb-kb)kb \cdot \times\left(\frac{\sin qbk}{qbk}\right)$$

$L = bN$

$$= \frac{2}{L^2}\int_0^L (L-y)\frac{\sin qy}{qy}dy = \frac{2}{L^2}\int_0^L L\frac{\sin qy}{qy}dy - \frac{2}{L^2}\frac{1}{q}\int_0^L(\sin qy)\,dy$$

$$= \frac{2}{qL}\int_0^{qL}\frac{\sin x}{x}dx - \frac{2}{q^2L^2}\cdot 2\sin^2\left(\frac{qL}{2}\right)$$

$$P(q) = \frac{2}{qL}\int_0^{qL}\frac{\sin x}{x}dx - \left[\frac{\sin(qL/2)}{(qL/2)}\right]^2$$

(Rod)