1/22/10 Homework 2 Polymer Properties (Due 1/29/10 at 5 pm)

1) Demonstrate that the chain scaling for a random walk does not change with changes in the step length for a random walk simulation on a cubic lattice by varying the step length and comparing the Flory radius to the number of steps in your computer program from the last homework.

2) Polyelectrolytes often display large persistence lengths. Define the persistence length. Use the ISI web of knowledge (using a UC computer or a VPN connection to UC) to find a paper by Ermi and Amis from 1997 that in the second column of the first page describes the basic model for polyelectrolyte structural changes during increase in polymer concentration and changes in charge density. Give the number of citations that this paper has received.

3) Briefly explain in your own words the theory for polyelectrolyte persistence in the Ermi and Amis paper. You may want to consider a paper by Dobrynin, Rubenstein and Colby from 1995 in Macromolecules that gives a scaling theory for polyelectrolyte solutions. Include cartoons of the chain structure in your explanation.

4) In Paul Flory's second book *Statistical Mechanics of Chain Molecules*, published in 1969 p. 11, Flory presents the relationship:

$$C_\infty = \left(\frac{\langle R^2 \rangle_0}{nl^2} \right) = \frac{2l_p}{l_0} - 1$$

where n and l refer to Kuhn units (FJC model), l_p refers to the persistence length (Worm like chain model) and l_0 is the bond length. Derive this expression.

5) Dave Lohse presents the following expression in his review paper presented in class:

$$C_\infty = \frac{6m_0}{l_p l_0^2 \rho N_a}$$

where N_a is Avogadro's Number and m_0 is the molecular weight for the monomer and ρ is the polymer melt density. Derive this expression.

6) From 4 and 5 give an expression between p (or l_p) and l_K. Explain this relationship as best you can (your explanation may indicate that one of these numbers is not fundamental).

7) Derive an expression for the lateral size of a polymer chain in terms of the volume of a mer unit , v_0, and l_0. How is this value related to p or l_p?

8) Describe what the plateau modulus is and how it relates to the packing length.

9) Explain what the Ising model is and how it relates to a polymer chain and to calculation of thermal transitions. See notes, Strobl 3'rd edition p. 59 and a wikipedia or google search.

10) DNA displays polymer-like behavior on a micron scale so that the chain can be visualized using an optical microscope. Find in the literature an optical micrograph of a DNA chain and comment on which chain model it would best agree with. Describe from this micrograph what structural feature is associated with the persistence length. Consider the following Wikipedia web page http://en.wikipedia.org/wiki/Persistence_length in your discussion as well as pages 55 to 59 of Strobl 3'rd edition "*The Persistent Chain*".