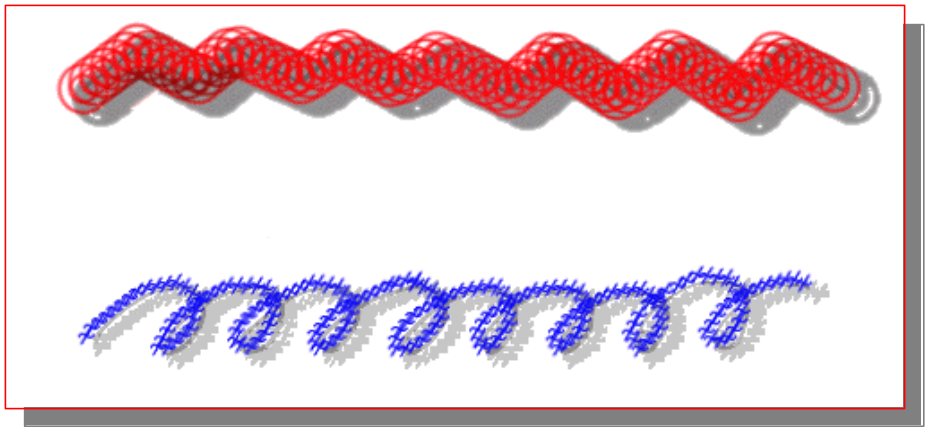
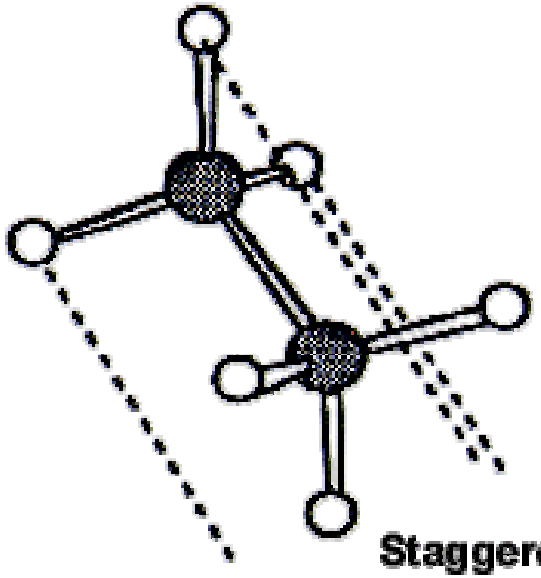
Conformations

Ordered

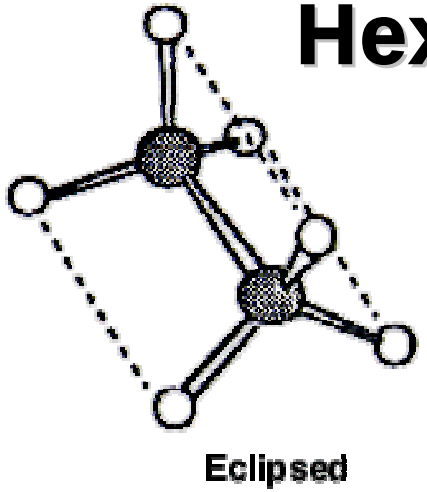


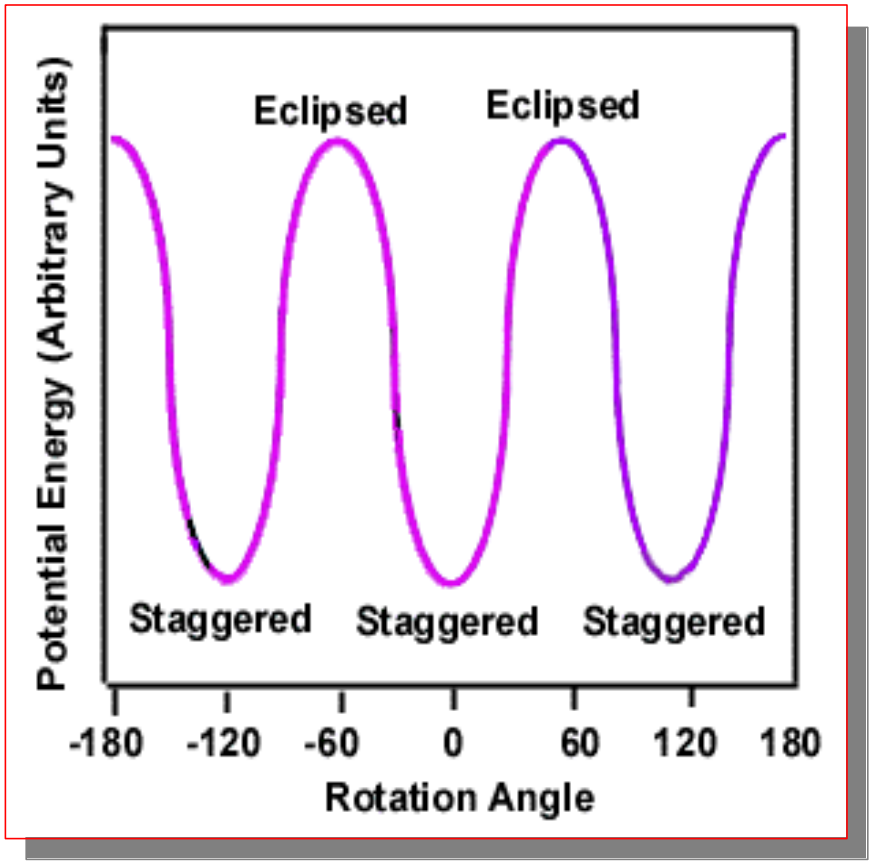
Disordered

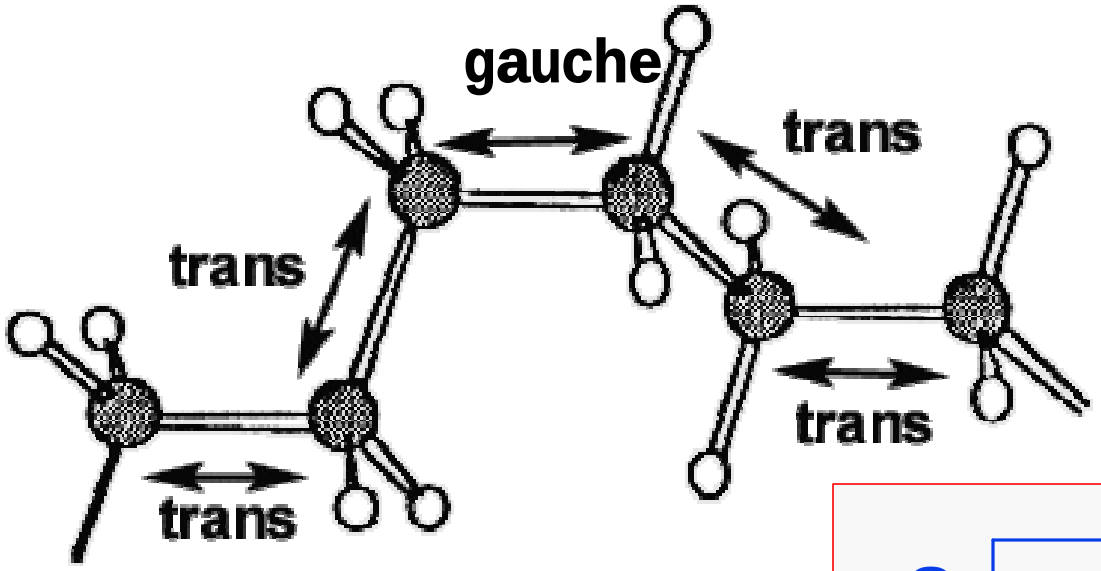
How Do Chains Fold?



Hexane

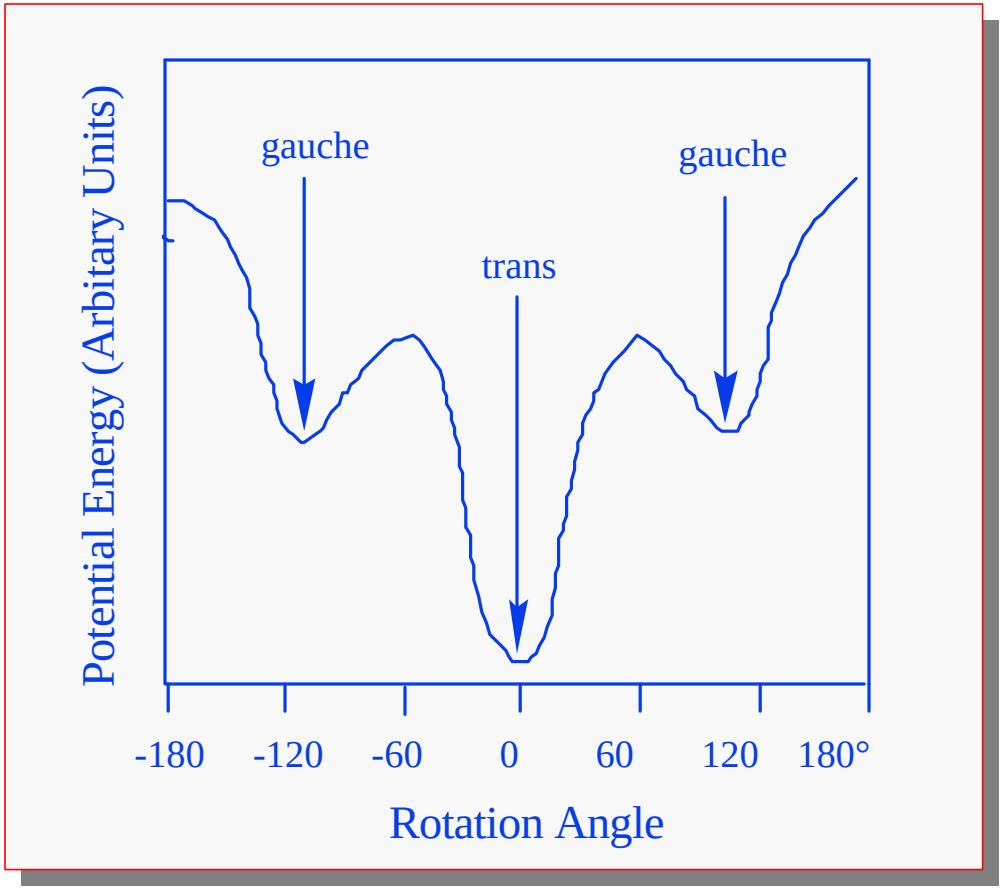






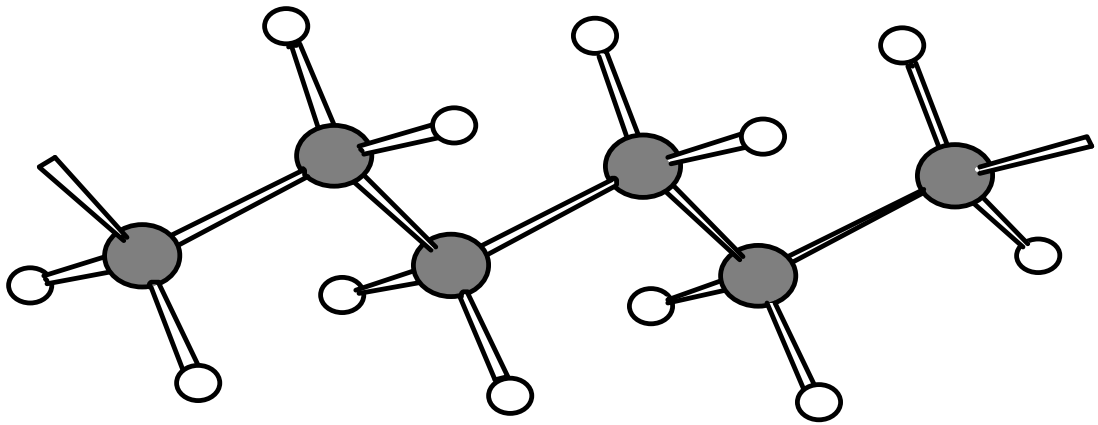
How Do Chains Fold?

Polyethylene



Interesting Questions

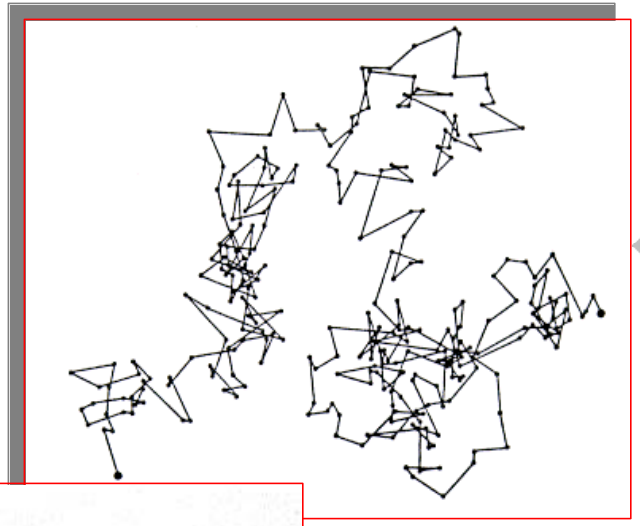
- ***Why Doesn't the Chain Just Sit in its Minimum Energy Conformation?***
  - ***e.g. polyethylene***



- ***What is the Effect of Thermal Motion ?***

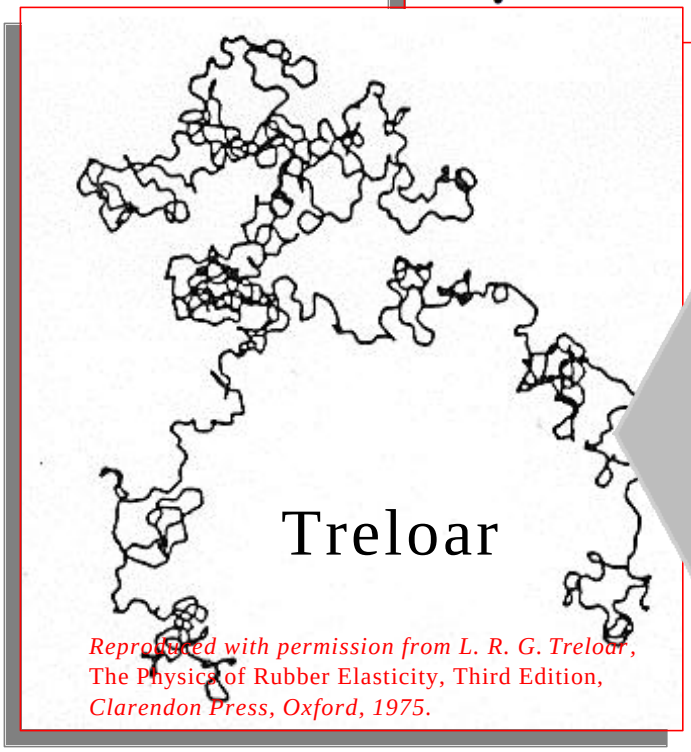
- ***How Many Shapes or Conformations are Available to a Chain ?***

Random Flights



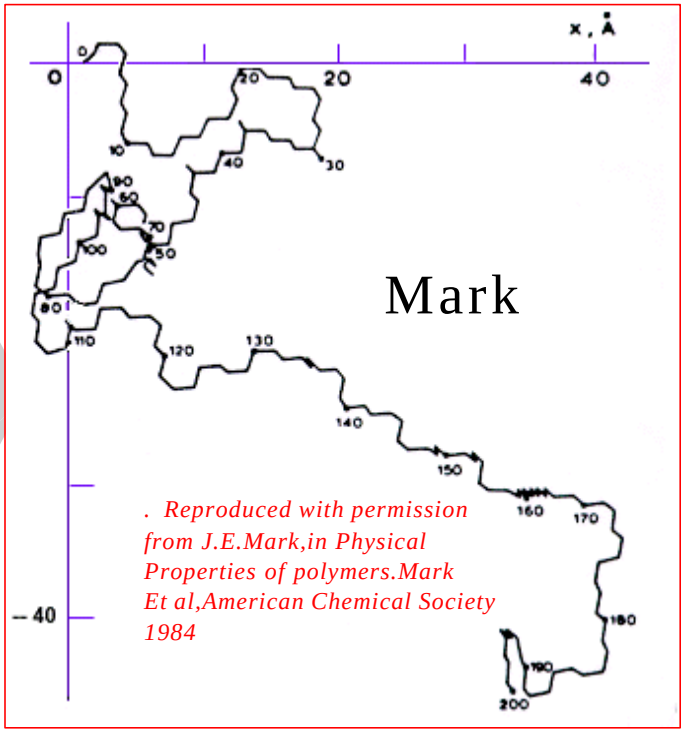
. *Reproduced with permission from J. Perrin,* Atoms, *English translation by D. L. Hammick, Constable and Company, London, 1916.*

Brownian Motion



Reproduced with permission from L. R. G. Treloar, The Physics of Rubber Elasticity, Third Edition, *Clarendon Press, Oxford, 1975.*

Polymer Chains



. *Reproduced with permission from J.E.Mark,in Physical Properties of polymers.Mark Et al,American Chemical Society 1984*

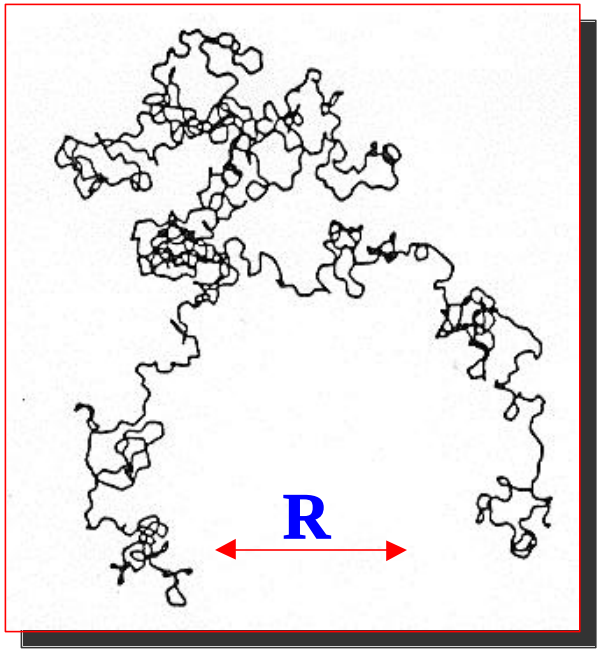
Random Flight....

A polymer sample will Contain *billions and billions* of Chains:

Hence, we will need two things:

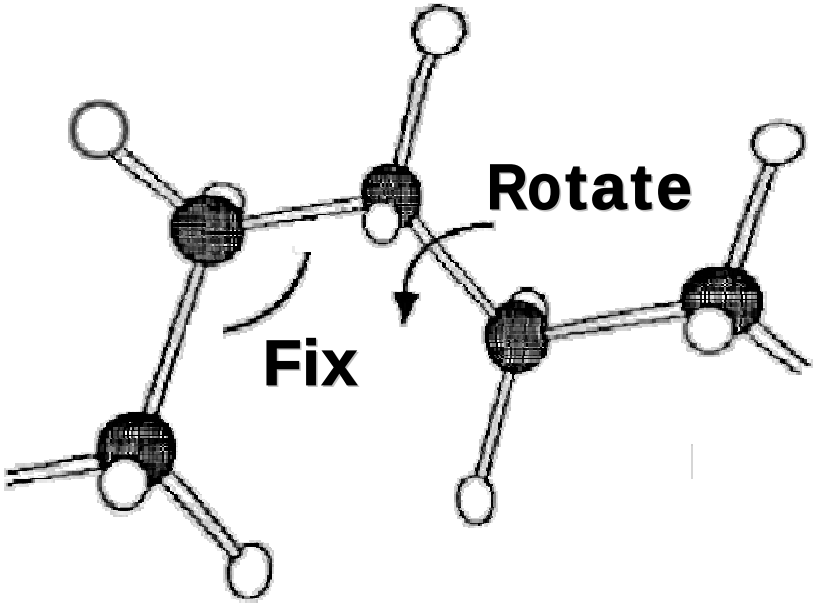
1. **Description of the Distribution of the End-to-End Distance (R)**

2. **Some measure of the average Value of the End-to-End Distance**



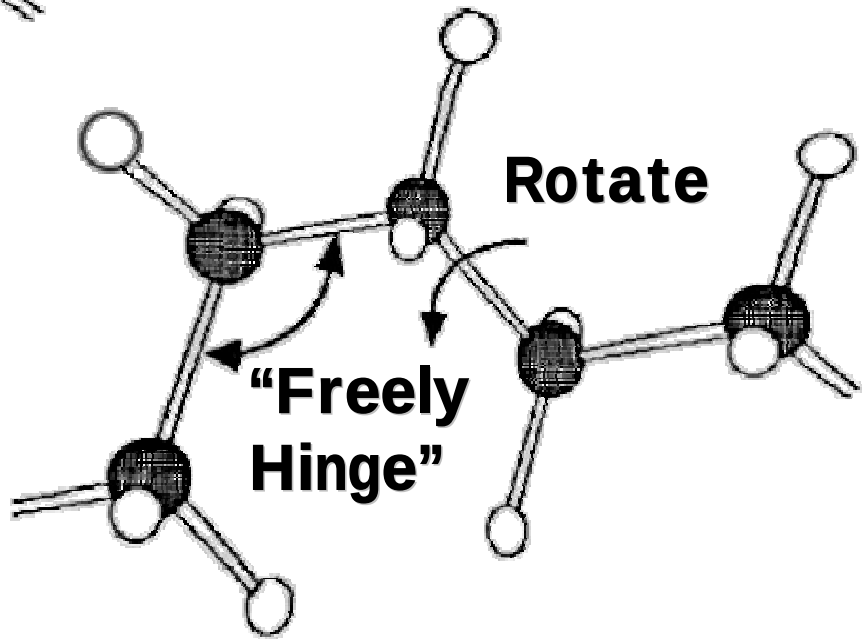
Reproduced with permission from L. R. G. Treloar, The Physics of Rubber Elasticity, Third Edition, *Clarendon Press, Oxford, 1975.*

Bond Angles & Rotations



What We Will Assume and Still Get the Right Answer . . .

The Way It Really Is . . . More or Less



1-Dimensional Random Walk

Q: ***What is the average distance traveled from the Phyrst for drunken walks of N steps? (Assume each step is 1 unit in length).***

WALK	R
1	+ 30
2	+ 50
3	- 40
4	- 50
5	+ 40
6	- 30
.	.
.	.

Intuitive Answer

$$\langle R \rangle = 0$$

- **Distance Traveled Regardless of Direction**
- **Answer:**
  - **Determine R for a Whole Bunch of Walks**
  - **Determine $\langle R^2 \rangle$**
  - **Calculate $\langle R^2 \rangle^{0.5}$**

Feyman's Method

For a Walk of One Step: $\langle R^2_1 \rangle = 1$

For the Nth Step:

$$R_N = R_{N-1} + 1$$
$$R_N = R_{N-1} - 1$$

Square:

$$R^2_N = R^2_{N-1} + 2R_{N-1} + 1$$
$$R^2_N = R^2_{N-1} - 2R_{N-1} + 1$$

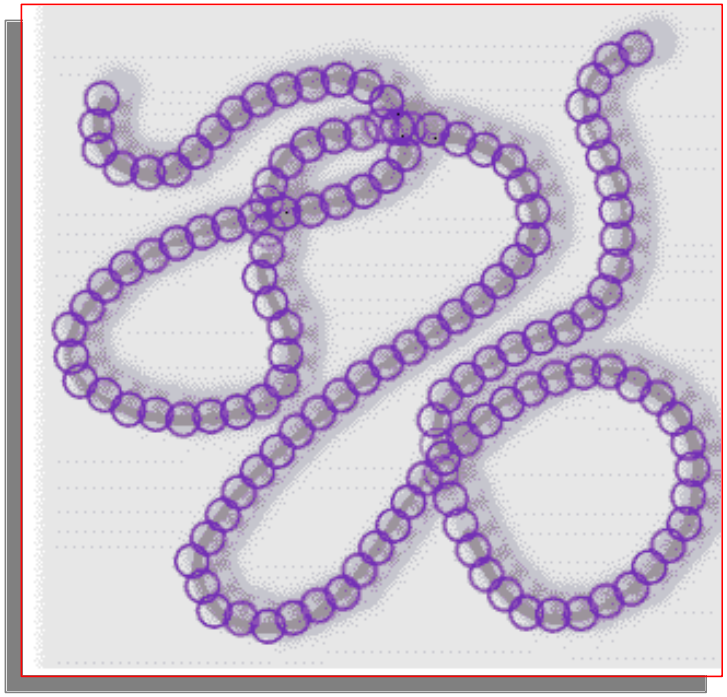
Average of Squares: $\langle R^2_N \rangle = \langle R^2_{N-1} \rangle + 1$

Recalling: $\langle R^2_1 \rangle = 1$

Then:

$$\langle R^2_2 \rangle = \langle R^2_1 \rangle + 1 = 2$$
$$\langle R^2_3 \rangle = 3 \text{ etc.}$$
$$\langle R^2_N \rangle = N$$

Polymer Chain - - - *end-to-end distance*

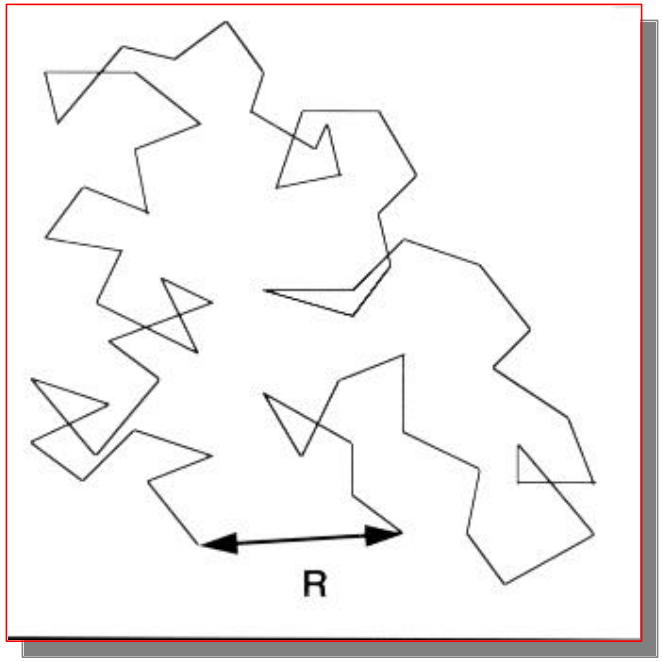


$$\langle R^2 \rangle = N l^2$$

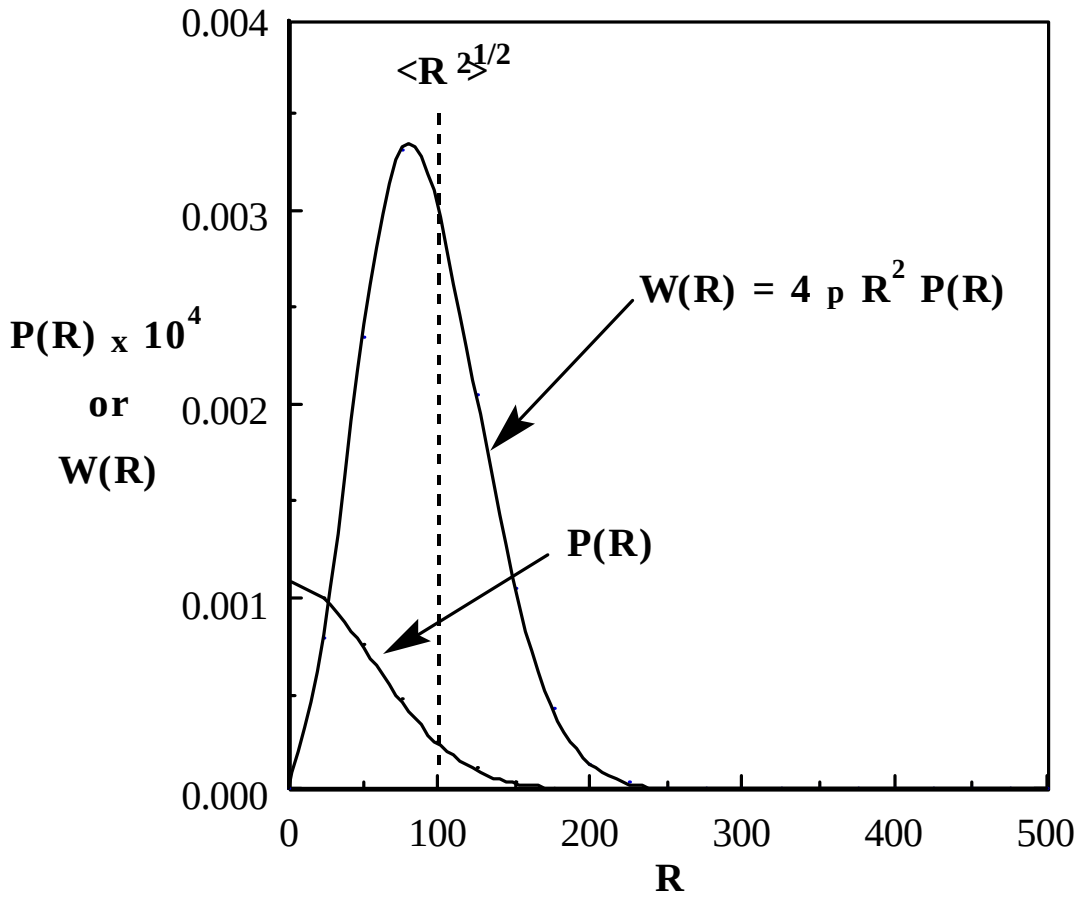
$$\langle R^2 \rangle^{0.5} = N^{0.5} l$$

If N = 10,000, l = 1;

$$\langle R^2 \rangle^{0.5} = 100 \text{ ! ! !}$$



Distribution of End-to-End Distances



- *If a chain in its most probable state is stretched, then it enters a less probable state*
- *An entropic driving force to return the chain to its most probable state is created*

Crucial Points

- *We have figured out a way to Describe a collection of random Chains*
- *A qualitative understanding of Rubber elasticity immediatly follows*
- *A pathway to more rigorous and quantitative work is opened up*