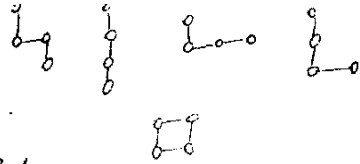


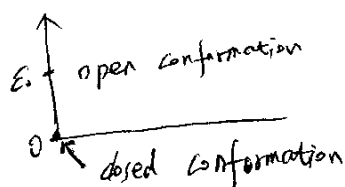
Course 565/665 Lecturer prof. Cavagnero
 Day 3.25.04 Date 9:55 am
 Notes Taken By J. Hong Total Number of Pages

ch. 10 Boltzmann Distribution

(ex) 8.2 (book) 4 beaded polymer 

4 open conformations, 1 closed form.

can do same calculation as in ex-8.1.



probability of each conformation
to exist, given their individual
energies?

$\left\{ \begin{array}{l} p_i \text{ is to be normalized} \\ \text{average energy is known.} \end{array} \right.$

$$E_{\text{TOT}} = E_{\text{internal total}} + E_{\text{interaction total}}$$

a system of N particles

$$E_{\text{internal total}} = E_{\text{rot}} + E_{\text{vibr}} + E_{\text{conf}} + \dots$$

↑
focus on it

Course 565/665 Lecturer prof. Cavagnaro
Day 3-25-04 Date 9:55 am
Notes Taken By J. Hong Total Number of Pages

$$E_{\text{interaction}} \cong \sum_{i,j} \epsilon_{ij} \quad \text{with } i \neq j$$

Consider only pairwise interactions.

E_j generic term for energies.

ϵ_j energies that assume no interaction energy is present.

Probability distribution for different ϵ states.

T, V, N constant.

recall. $\frac{S}{k} = - \sum_{j=1}^t P_j \ln P_j$ j : energy levels

$$dS = -k \sum (1 + \ln P_j) dP_j \quad \dots \dots \dots \textcircled{1}$$

$$U = \langle E \rangle = \sum_{j=1}^t P_j E_j$$

macroscopic quantity $\quad \quad \quad$ microscopic energy.

$$dU = d\langle E \rangle = \sum_{j=1}^t (E_j dP_j + P_j dE_j)$$

more or less, E_j does not depend on T.

but P_j depends on T.

DO NOT USE PENCIL ***** DO NOT STAPLE

Submit a COPY of these notes to the GenChem Office

Course 565/665 Lecturer prof. cavagnero
Day 3-25-04 Date _____
Notes Taken By J. Hong Total Number of Pages _____

Note: u and $\langle E \rangle$ depend on T .

$$dE_j = \left(\frac{\partial E_j}{\partial V} \right) dV + \left(\frac{\partial E_j}{\partial N} \right) dN = 0 \quad (\text{at const } N, V)$$

$$\text{so } du = d\langle E \rangle = \sum_{j=1}^I E_j dp_j$$

$$\text{recall. } du = \delta q + \delta w = \delta q \quad (\text{at const. } V) \\ \text{no other work}$$

3 of 6