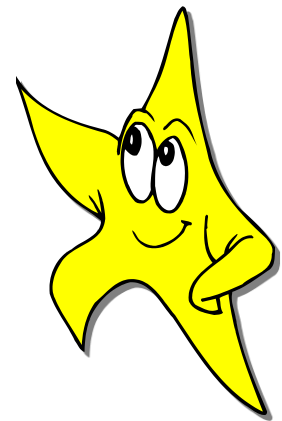


Lecture 4

Statistical thermodynamics: the concepts

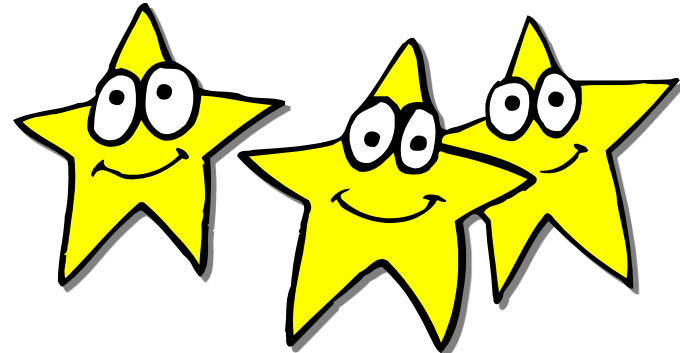


Dr. Sahar A. Fadlallah

23/11/2011

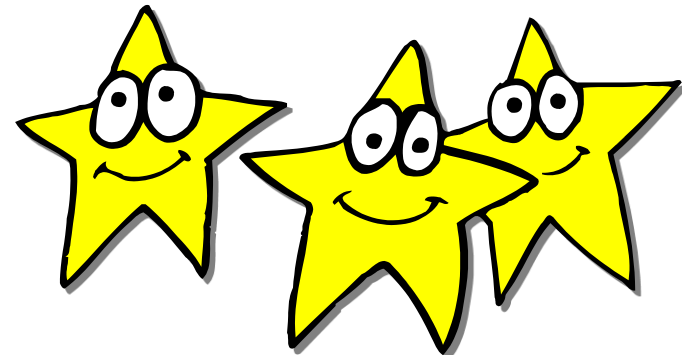
INTRODUCTION

- *Statistical Mechanics is the study of macroscopic phenomena from a microscopic point of view*
- *Statistical Mechanics helps us to understand, explain and predict macroscopic behavior of a collection of entities (e.g. molecules) given the microscopic behavior (e.g. inter-molecular interactions).*



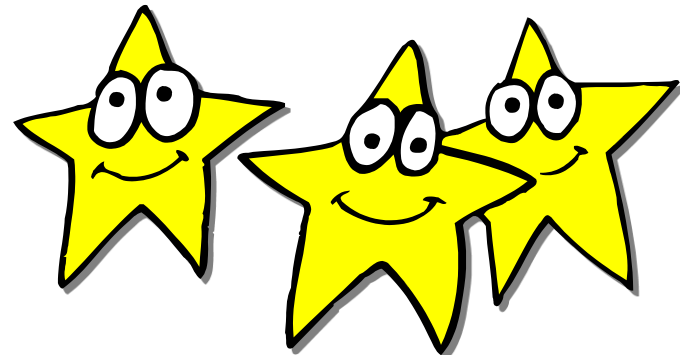
INTRODUCTION

- *The branch of statistical mechanics that deals with equilibrium thermodynamics behavior (e.g. pressure, entropy, free energy) is called Statistical thermodynamics.*
- *Only certain problems in statistical thermodynamics are exactly solvable (e.g. ideal gas).*
- Computer simulations provide exact numerical results for problems that are soluble by approximate methods or might be quite intractable.



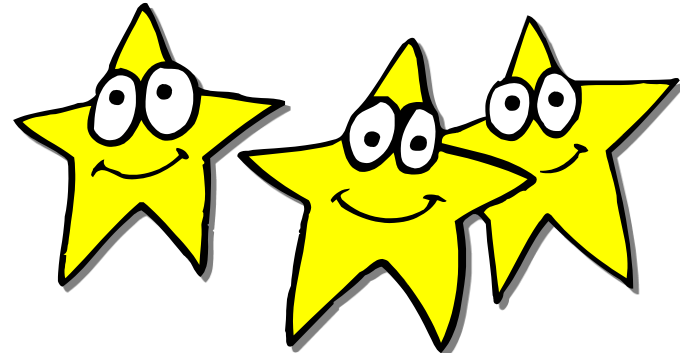
INTRODUCTION

- *We know that: Energy of atoms and molecules are confined to discrete values, these energies may be calculated, determined spectroscopically, and related to the sizes and shapes of molecules.*



INTRODUCTION

NEXT: is to show a knowledge of these permitted energy levels can be used to account for the behavior of matter in bulk.

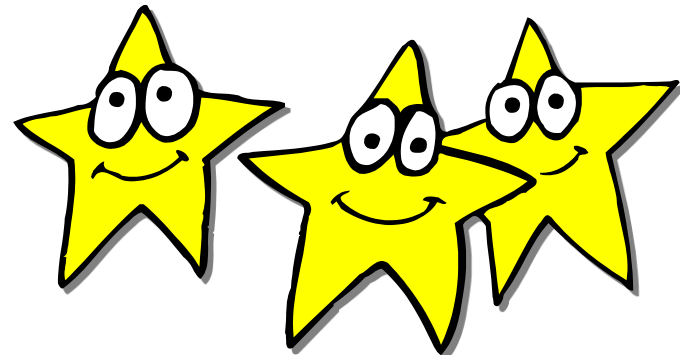


INTRODUCTION

Quantum mechanics deals with the detailed arrangement and motion of molecules.

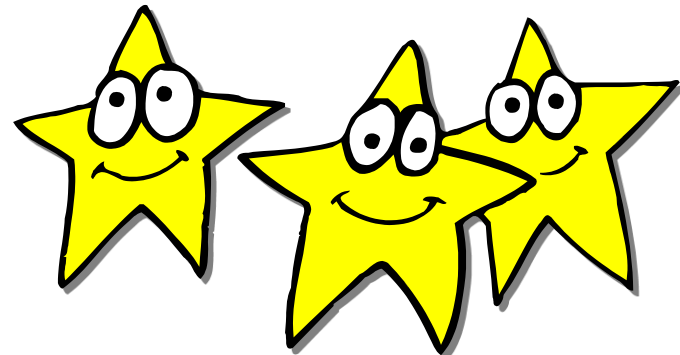
Thermodynamics deals with their average behavior.

Example: pressure



INTRODUCTION

Statistical thermodynamics: is based on the principle that thermodynamics observables are averages of molecular properties, and it sets up a scheme for calculating these averages.

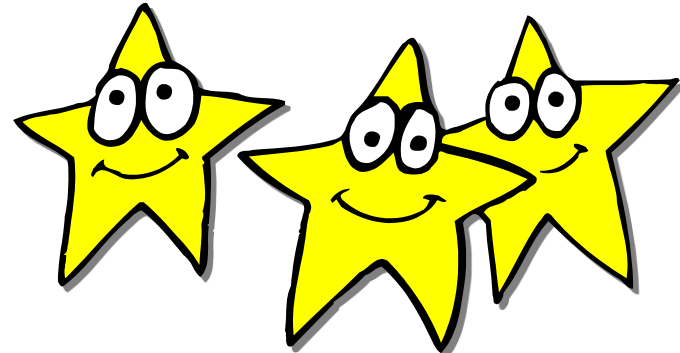


Statistical Thermodynamics: In 3 stages

First: derivation of the Boltzmann distribution for independent molecules

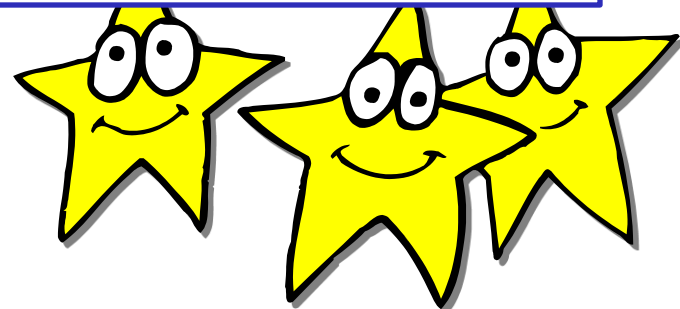
Second: The arguments are elaborated a little in order to accommodate systems composed of interacting molecules.

Third: the presentation is turned round and the basis of the subject is examined from an entirely different perspective.



AIM

Is to show how all the functions of thermodynamics- both those arising from the first law, such as the internal energy, the enthalpy, and the pressure, and those based on the second law, such as the entropy, the Gibbs function, and equilibrium constants- can be calculated on the basis of structural information about the molecules involved.



Molecular energy levels and Boltzmann distribution

