Thermodynamics & Statistical Physics

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http://physics.whu.edu.cn/shizi/jiaoshi/31.html

My Research:

- 发展物理模型，预测RNA分子三维结构及热力学；
- 发展统计力学理论，预测RNA、DNA结构折叠中的离子静电效应；
- 利用计算机模拟方法，理解和预测核酸分子折叠的机制；
- 发展聚电解质统计力学理论，定量预测高价离子溶液中聚电解质的结构性质；
- 软物质复杂系统的自组织和动力学。

http://physics.whu.edu.cn/shizi/jiaoshi/31.html

QQ群号：657054030

助　　教：　谭雅岚　（博士生；物理楼3-512）

Statistical Physics

Statistical → ensemble system

(many body, strong fluctuation→

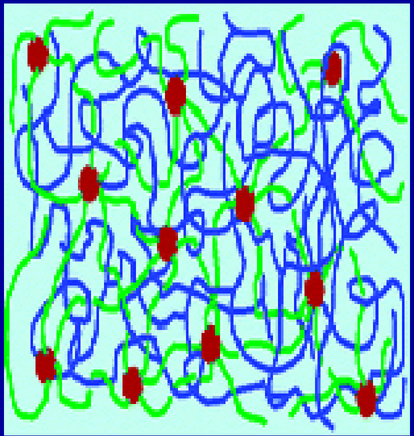
many possible micro-states)

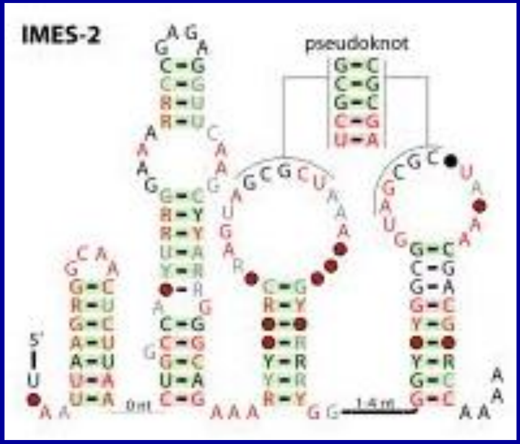
common properties

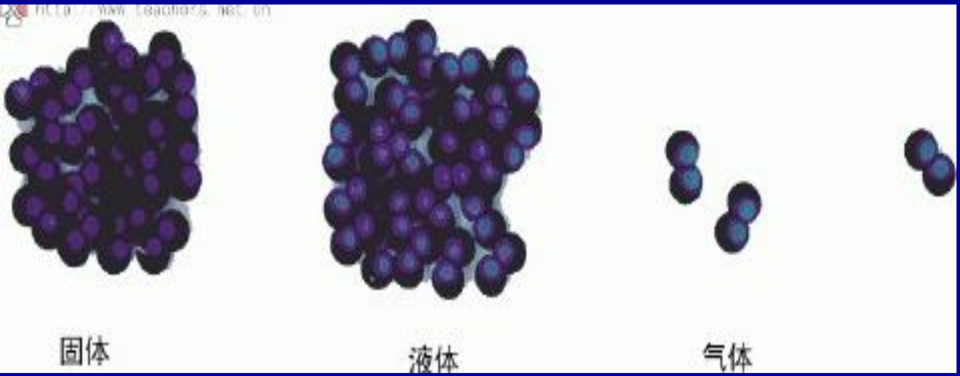
Liquid/solution, (bio) polymer (complex), gas, complex fluid, solid (crystal, ferromagnetism, glass)

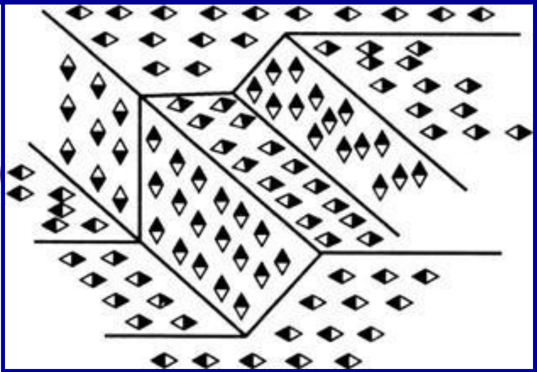
Statistical Physics

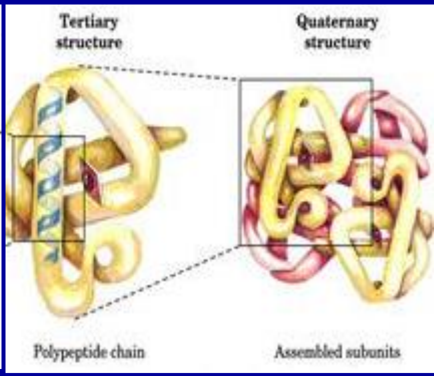
Liquid/solution, (bio) polymer (complex), gas, complex fluid, solid (crystal, ferromagnetism, glass)



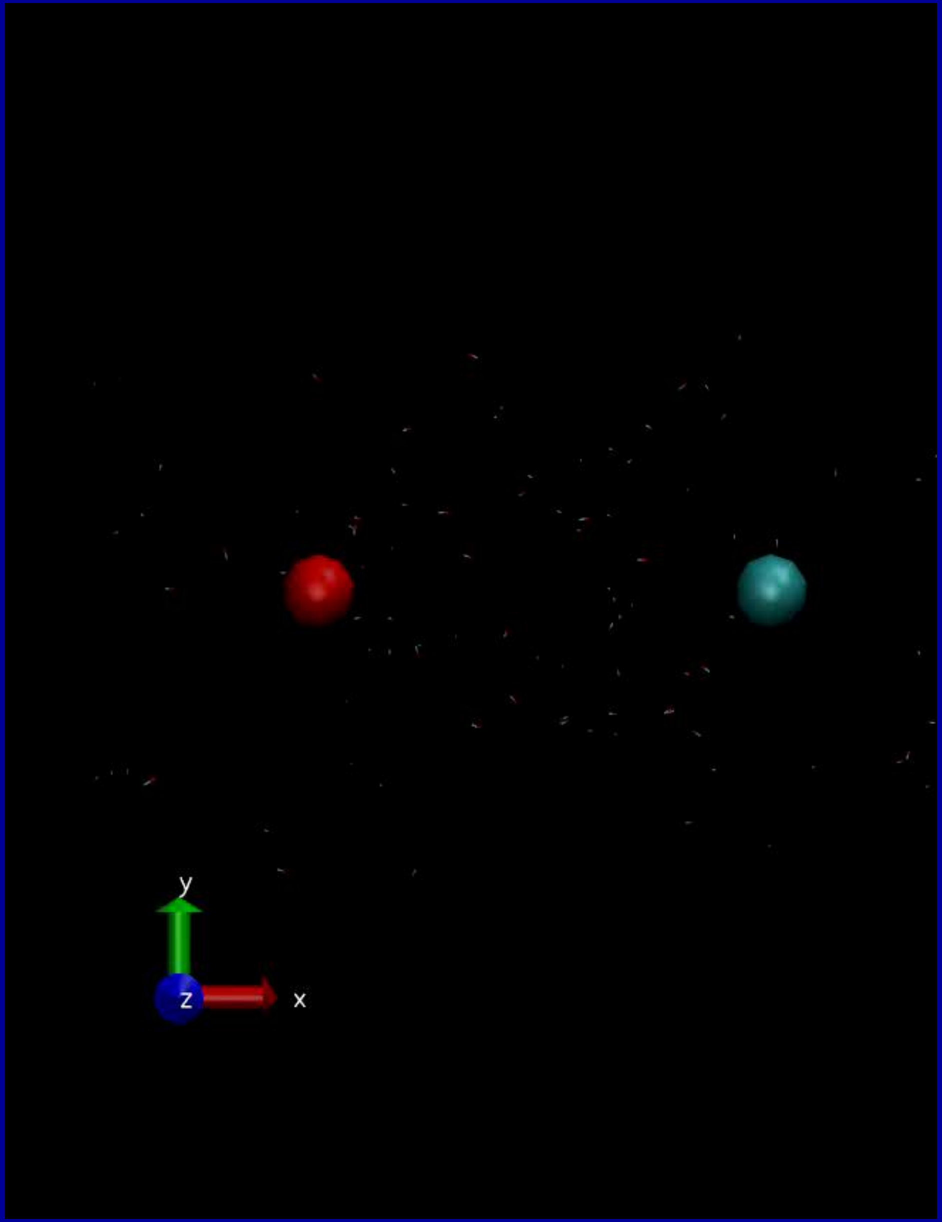




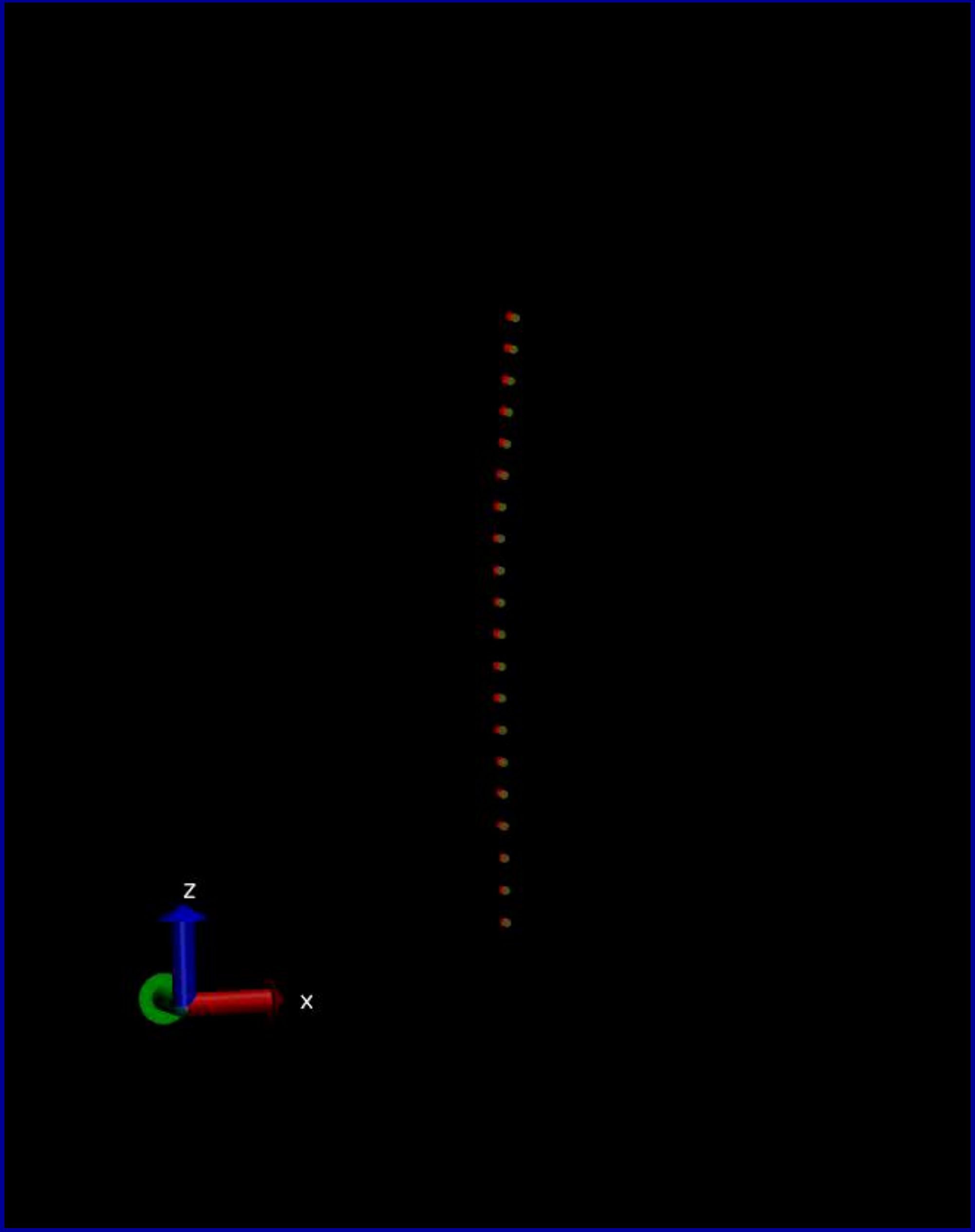




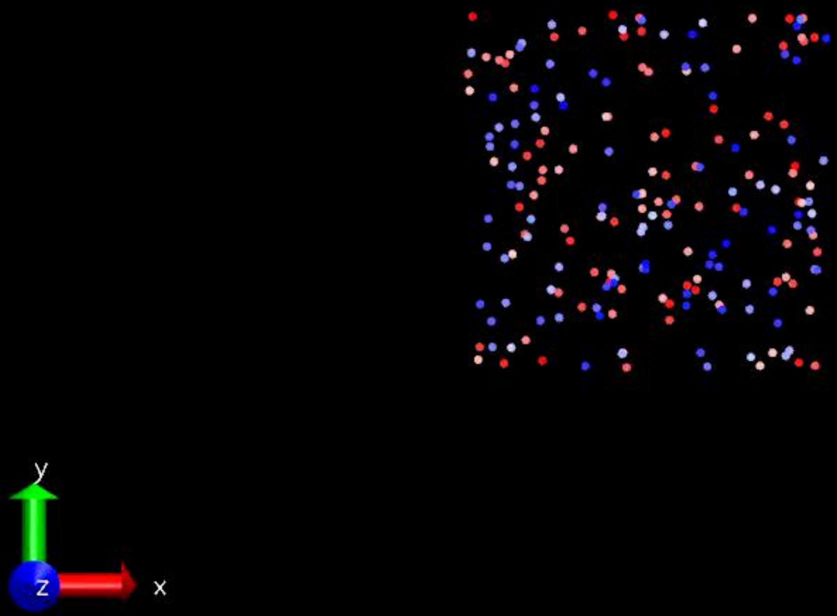
Statistical Physics



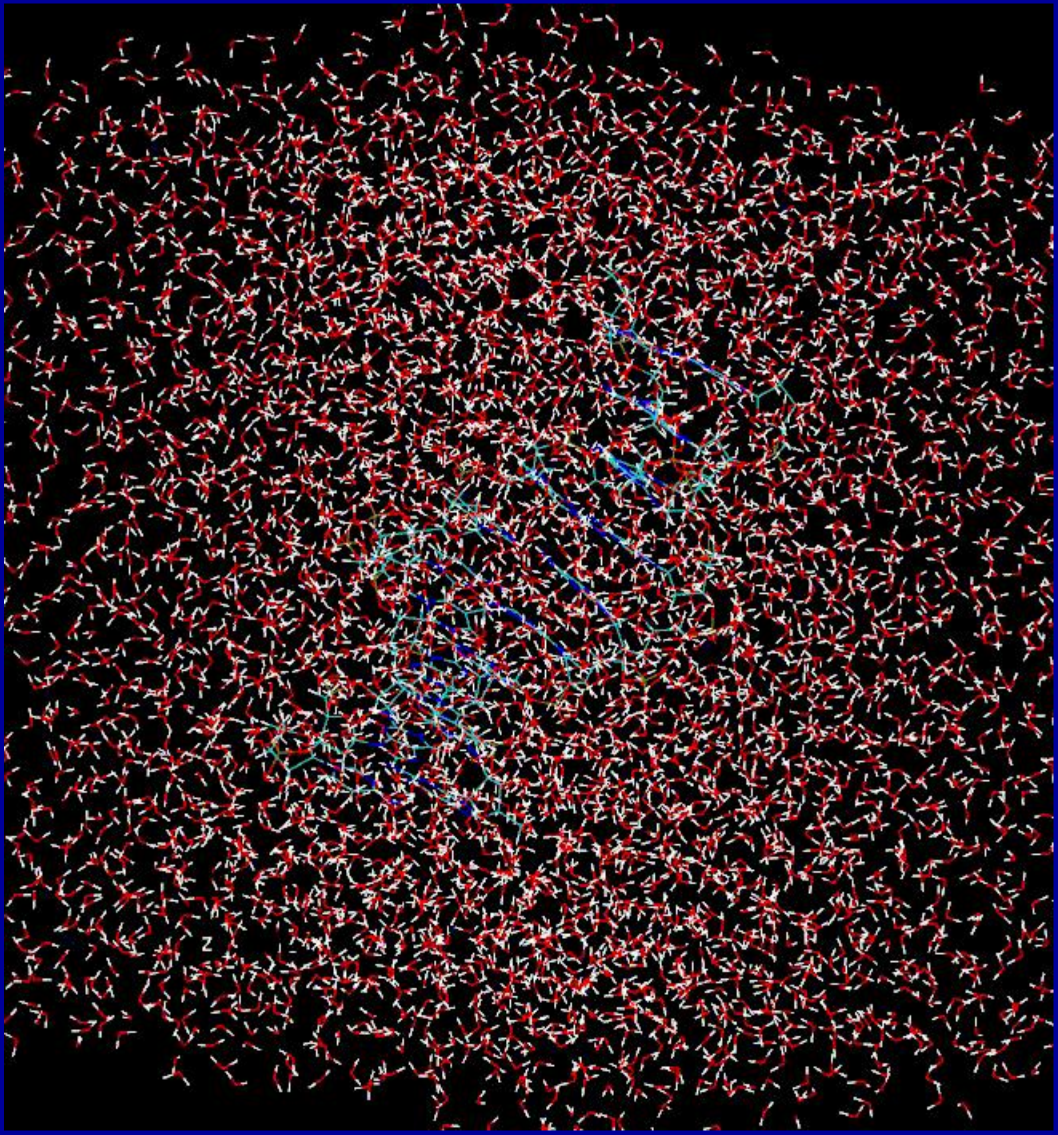
Statistical Physics



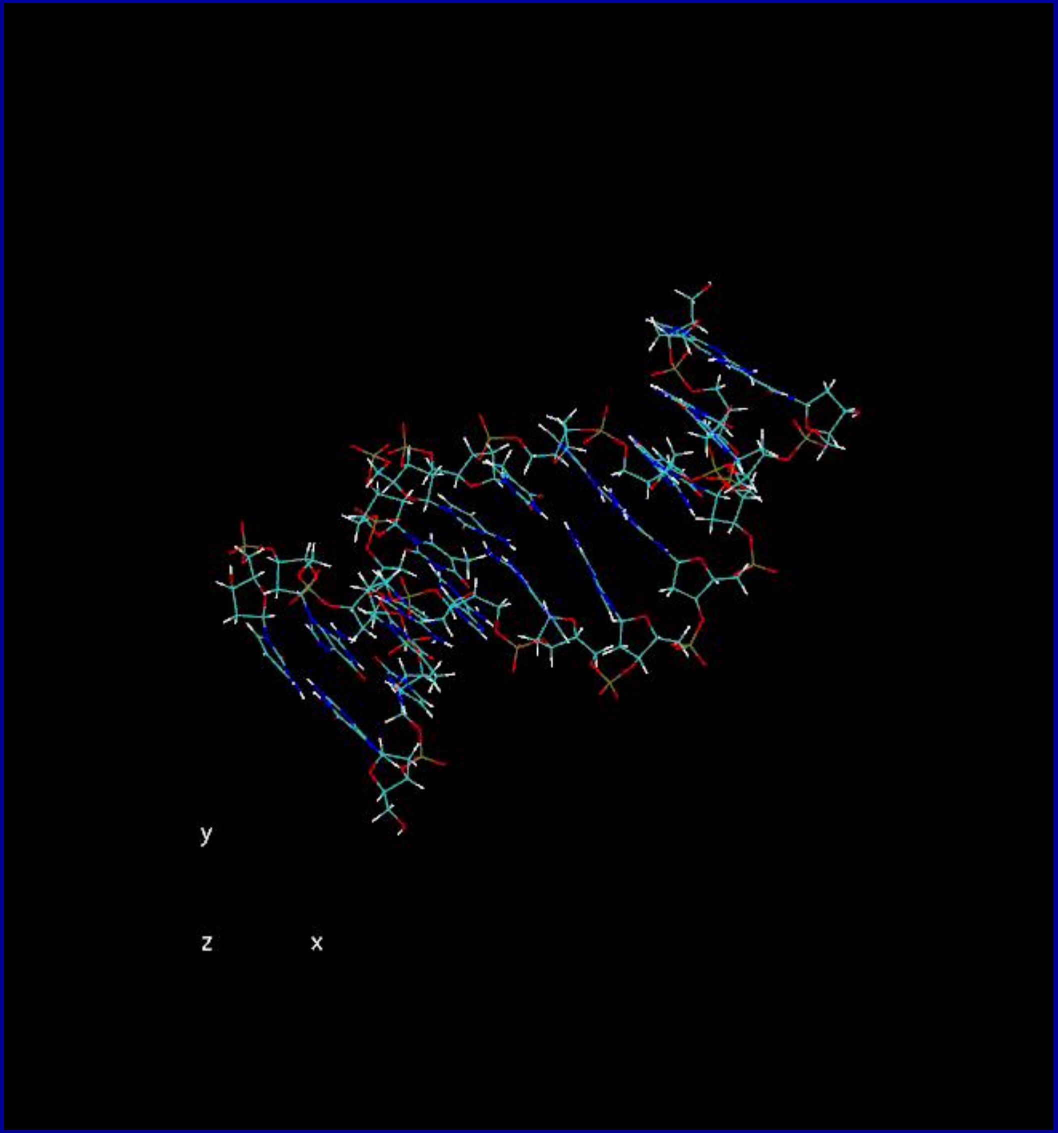
Statistical Physics



Statistical Physics



Statistical Physics



Statistical Physics

Physics → **set up a model** to solve the "common properties" for multi-body systems.

Pressure, temperature, heat capacity etc;

Structure, magnetism, dielectric properties, heat/electron transportation, phase transition

Statistical Physics covers extensive objects

From classic particles to quantum ones

ideal gas electron/photon/phonon

From solid to liquid, to glass, to polymers

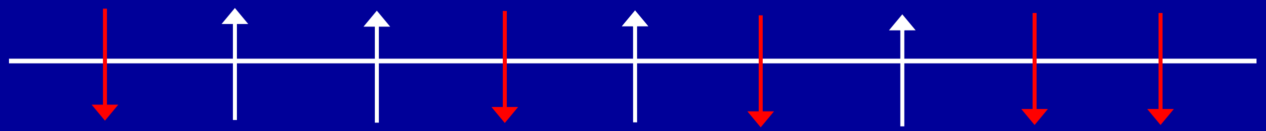
order crystal → noncrystal with local order

From phys to chem, to bio systems

Why is statistical physics important?

Paradigm example 1

<u>1, Ferromagnetism (FM)</u>. Ising model



Hamiltonian $H = -J \sum_{N\text{-}N} s_i \bullet s_j$

Partition function $Z = \sum_{\text{all possible configuration}} \exp(-H/k_BT)$

1D: Ising, analytical solution and no ferromagnetic transition

2D: Peierls, exists ferromagnetism transition in high dimension

Kramers, Wannier, primary solution for 2D, FM transition

Onsager, strict solution for 2D, FM transition

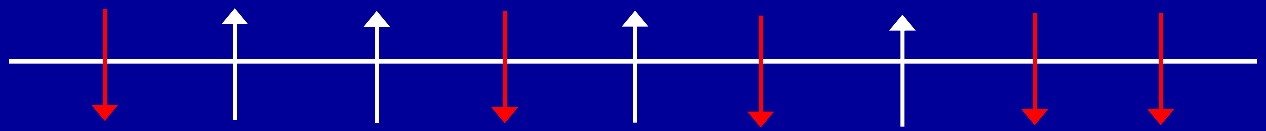
3D: no strict analytical solution until now

Further reading: 《热力学与统计力学》 顾莱纳等，北大出版社

Why is statistical physics important?

Paradigm example 1

1, Ferromagnetism (FM). 1D Ising model



$$Z=\sum_{s_1}\sum_{s_2}\dots\sum_{s_N} e^{\beta J s_1 s_2} e^{\beta J s_2 s_3}\dots e^{\beta J s_{N-1} s_N} \qquad s=1 \text{ or } -1$$

$$=\sum_{s_1}\sum_{s_2}\dots e^{\beta J s_1 s_2} e^{\beta J s_2 s_3}\dots\sum_{s_N} e^{\beta J s_{N-1} s_N}$$

$$=\sum_{s_1}\sum_{s_2}\dots e^{\beta J s_1 s_2} e^{\beta J s_2 s_3}\dots\left((e^{\beta J}+e^{-\beta J})\right)$$

$$=2^N(\cosh\beta J)^{N-1}$$

《Thermal Physics》 Schroeder，Addison Wesley Longmann

Why is statistical physics important?

Paradigm example 1

Statistical theory of equations of state and phase transitions. II. Lattice gas and Ising model

TD Lee, CN Yang - Physical Review, 1952 - APS

The problems of an Ising model in a magnetic field and a latticegas are proved mathematically equivalent. From this equivalence an example of a two-dimensional lattice gas is given for which the phase transition regions in the p —v diagram is exactly calculated. A theorem is proved which …

☆ 99 被引用次数：2037 相关文章 所有 12 个版本

The spontaneous magnetization of a two-dimensional Ising model

CN Yang - Physical Review, 1952 - APS

' 'T is the purpose of the present paper to calculate the - ~ spontaneous magnetization (ie, the intensity of magnetization at zero external field) of a two-dimen- sional Ising model of a ferromagnet. Van der Waerden' and Ashkin and Lamb' had obtained a series. expansion of the …

☆ 99 被引用次数：1163 相关文章 所有 5 个版本

Solving the 3D Ising model with the conformal bootstrap

S El-Showk, MF Paulos, D Pol

We study the constraints of crc

theories. In doing so we derive

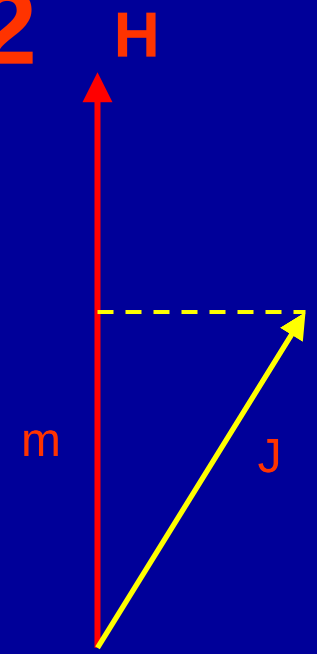
functions of scalars and preser

☆ 99 被引用次数：420

In this paper, we will be aiming for a solution of the 3D Ising model *in the continuum limit* and *at the critical temperature* $T = T_c$. While the 2D Ising model was solved exactly *on the lattice* and *for any temperature* by Onsager and Kaufman in the 1940s, the 3D lattice case has resisted all attempts for an exact solution. Istrail [28] proved in

Why is statistical physics important?

Paradigm example 2



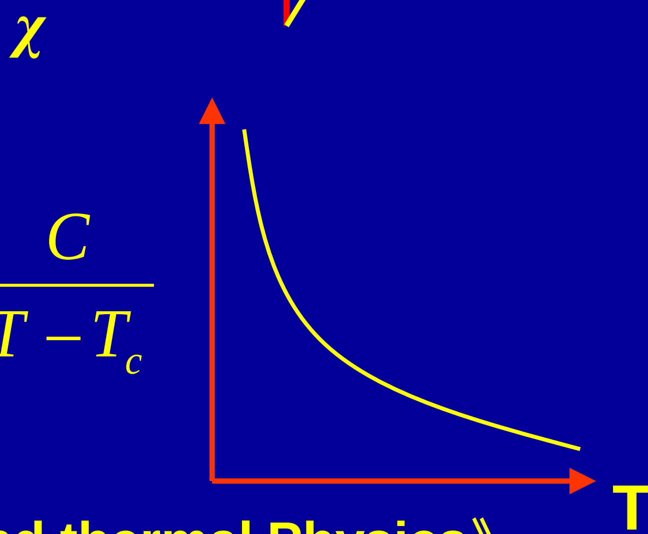
2, Paramagnetism. model

$$E = -g\mu_0 \mathbf{J} \bullet \mathbf{H} = -\underbrace{g\mu_0 J_z}_{\mu_z} H$$

$$\overline{\mu}_z = \frac{\sum_{-J}^{J} \mu_z \exp(\mu_z H / k_B T)}{\sum_{-J}^{J} \exp(\mu_z H / k_B T)}$$

$$M = N * \overline{\mu_z}$$

$$\chi = \frac{C}{T - T_c}$$

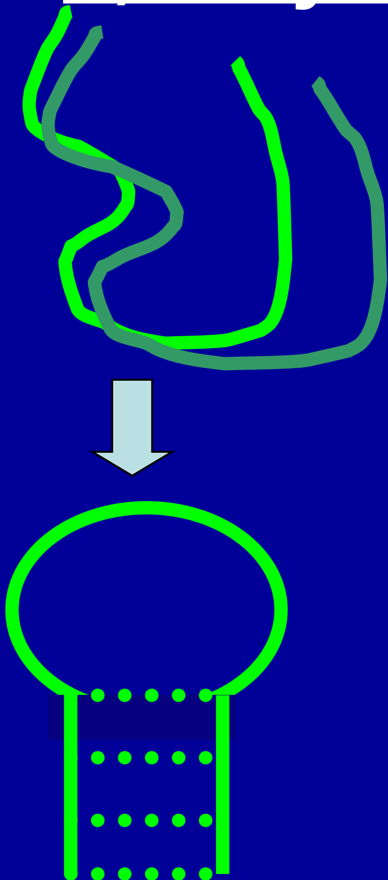


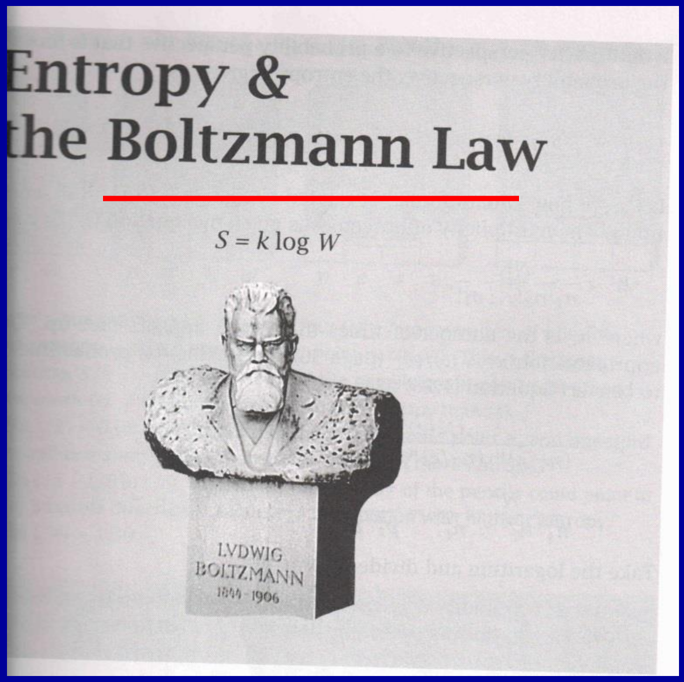
Further reading: 《**Fundamentals of statistical and thermal Physics**》 **by F. Reif**

Why is statistical physics important?

Paradigm example 3

3, Polymer. Lattice model

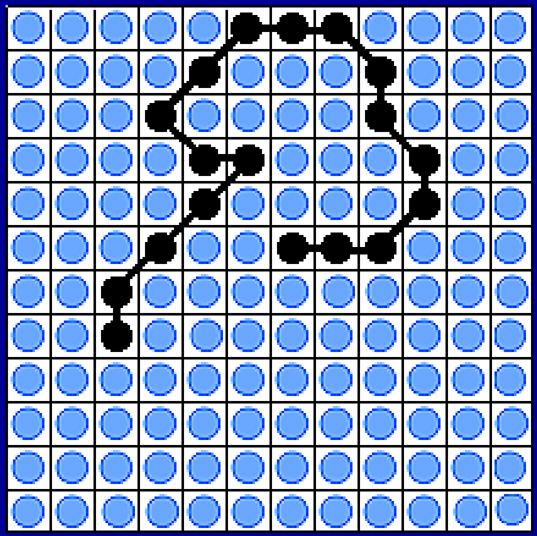




$$S = k_B \ln Q$$

?

Q can be counted based on



Further reading: 《**Molecular driving force**》 **Dill et al，Taylor , 2010**

Why is statistical physics important?

Paradigm example 3

3, Polymer.   Lattice model

Thermodynamics of high polymer solutions

PJ Flory - The Journal of Chemical Physics, 1941 - aip.scitation.org

Interest in the separation of isotopes and in the theory of vapor pressures of non-polar

Thermodynamics of high polymer solutions

PJ Flory - The Journal of chemical physics, 1942 - aip.scitation.org

A statistical mechanical treatment of high polymer solutions has been carried out on the basis of an idealized model, originally proposed by Meyer, which is analogous to the one ordinarily assumed in the derivation of the``ideal''solution laws for molecules of equal size …

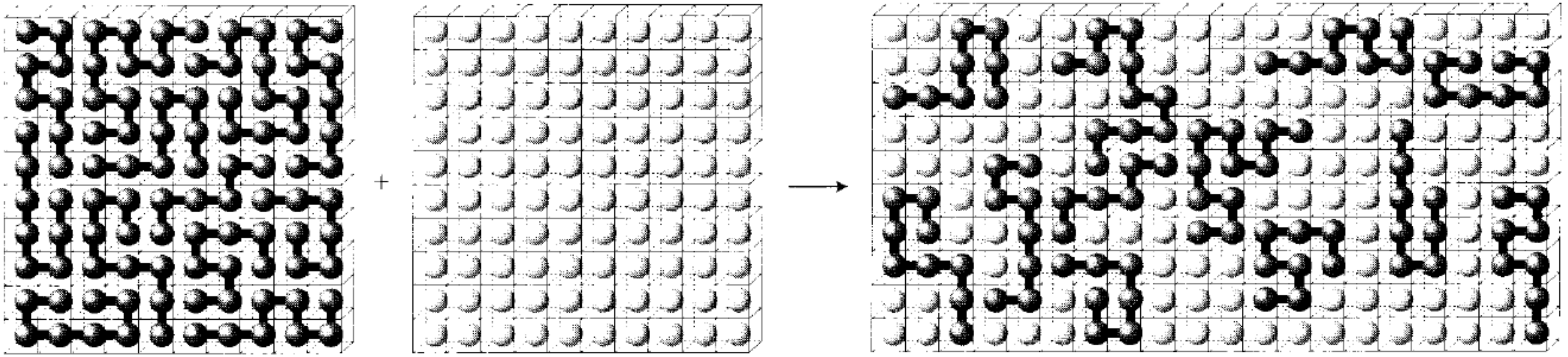


Figure 31.5 A lattice model for mixing n_p polymer molecules, and n_s solvent molecules, to get a solution of n_p polymer molecules and n_s solvent molecules.

Why is statistical physics important?

Paradigm example 4

4, Stochastic process. **Langevin equation**

Brownian motion

$$m\frac{d^2\vec{r}}{dt^2} = -a\frac{d\vec{r}}{dt} + \vec{F}(t)$$

$t>>t_0$, $<r>^2 = 6Dt$

$t<<t_0$, $<r>^2 = v^2t^2$

Fluctuation of electric current

$$L\frac{dI(t)}{dt} = -aI + V(t)$$

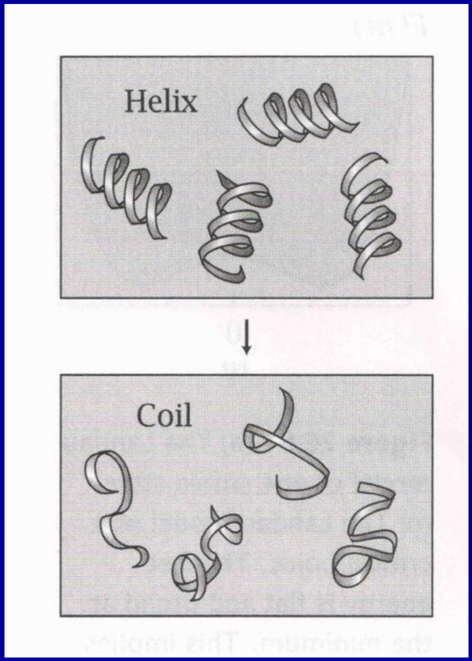
$t >>$♦, $I^2 = kT/L$

Further reading: 《热力学与统计物理学》 林宗涵，北大出版社

Why is statistical physics important?

Paradigm example 5

5, peptide helix-coil transition.



1, Non-cooperative model:

q_H----probability for H state

q_C---- probability for C state

The partition function is:

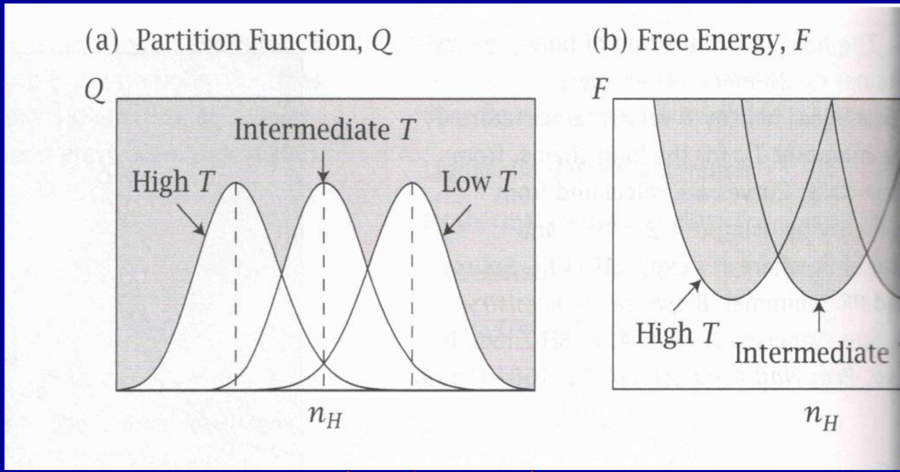
$$Z = \sum_{n_H=0}^{N} q_c^{n_c} q_H^{n_H} \frac{N!}{n_C! n_H!} = (q_C + q_H)^N$$

$$q_c \propto \exp(-G_c / k_B T)$$

$$q_H \propto \exp(-G_H / k_B T)$$

$$q_c + q_H = 1$$

$$q_H / q_c = \exp(-\Delta G_{H-c} / k_B T)$$



连续相变

Why is statistical physics important?

Paradigm example 5

5, peptide helix-coil transition.

2, Maximum-cooperative model: two-state model

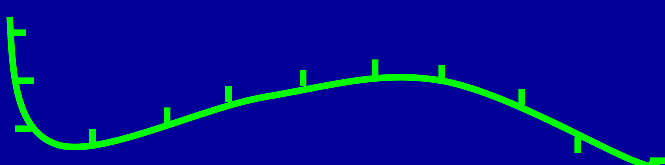
q_H----probability for H state

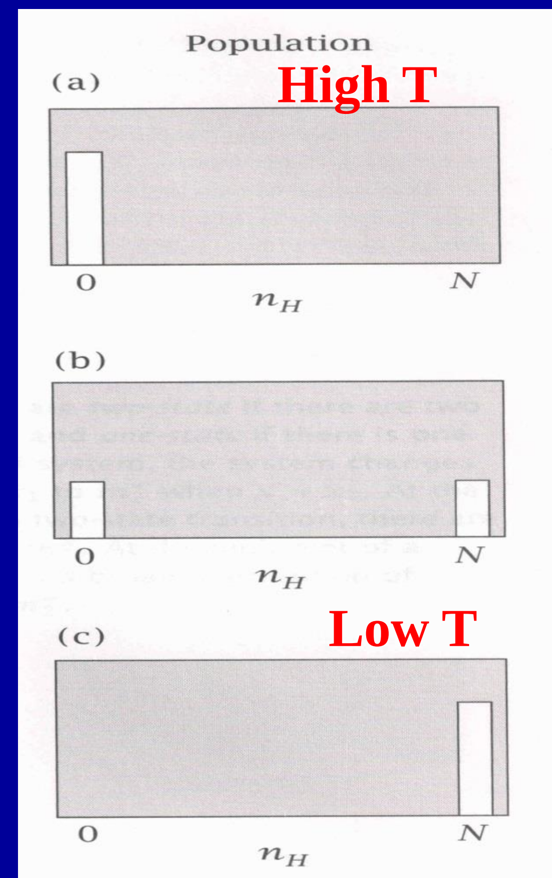
q_C---- probability for C state

The partition function is:

$$Z = q_C^N + q_H^N$$

非连续相变





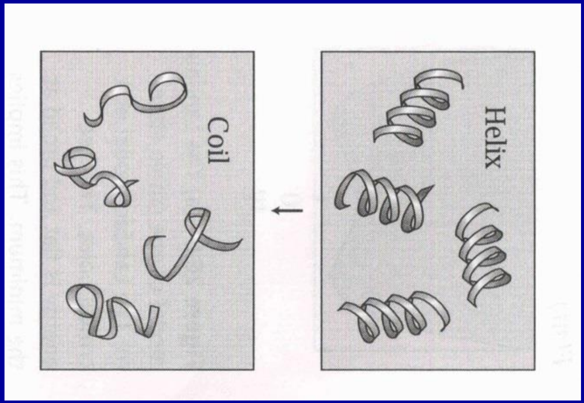
Why is statistical physics important?

Paradigm example 5

5, peptide helix-coil transition.

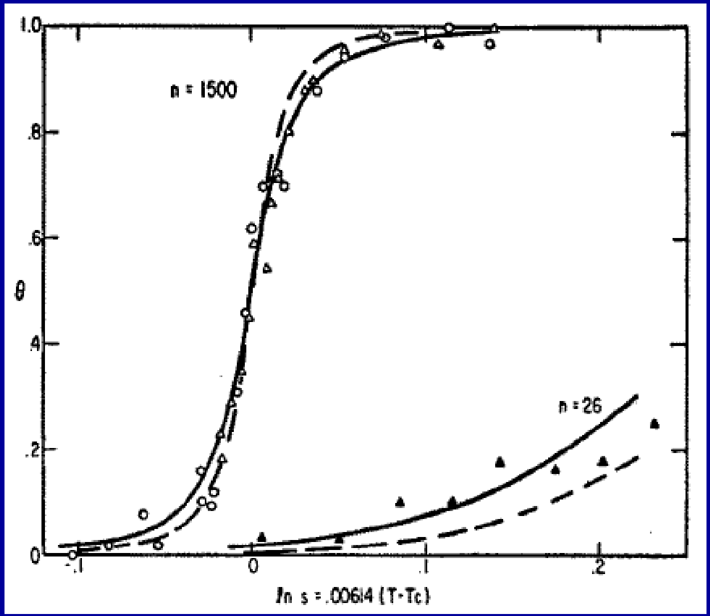
3, Ising-like model

j-1	j	统计权重
C	C	q(C|C)=1
H	C	q(C|H)=1
C	H	q(H|C)=σs
H	H	q(H|H)=s



N-mer peptide partition function:

$$Z_N = [1, \sigma s] \underbrace{\begin{bmatrix} 1 & \sigma s \\ 1 & s \end{bmatrix} \cdots\cdots \begin{bmatrix} 1 & \sigma s \\ 1 & s \end{bmatrix}}_{N-1} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



Zimm & Bragg, *J. Chem. Phys*. 31: 526-535, 1959

Why is statistical physics important?

Paradigm example 5

5, peptide helix-coil transition.

3, Ising-like model

Theory of the phase transition between helix and random coil in polypeptide chains

BH Zimm, JK Bragg - The journal of chemical physics, 1959 - aip.scitation.org

The transition between the helical and randomly coiled forms of a polypeptide chain is discussed by reference to a simple model that allows bonding only between each group and the third preceding. Two principal parameters are introduced, a statistical parameter that is …

Zimm & Bragg, *J. Chem. Phys*. 31: 526-535, 1959

Why is statistical physics important?

Paradigm example 6

6, Protein folding. HP model

氨基酸：H型　和　P型

（疏水）（亲水）

肽 链：　H、P的分子链

最近邻模型：

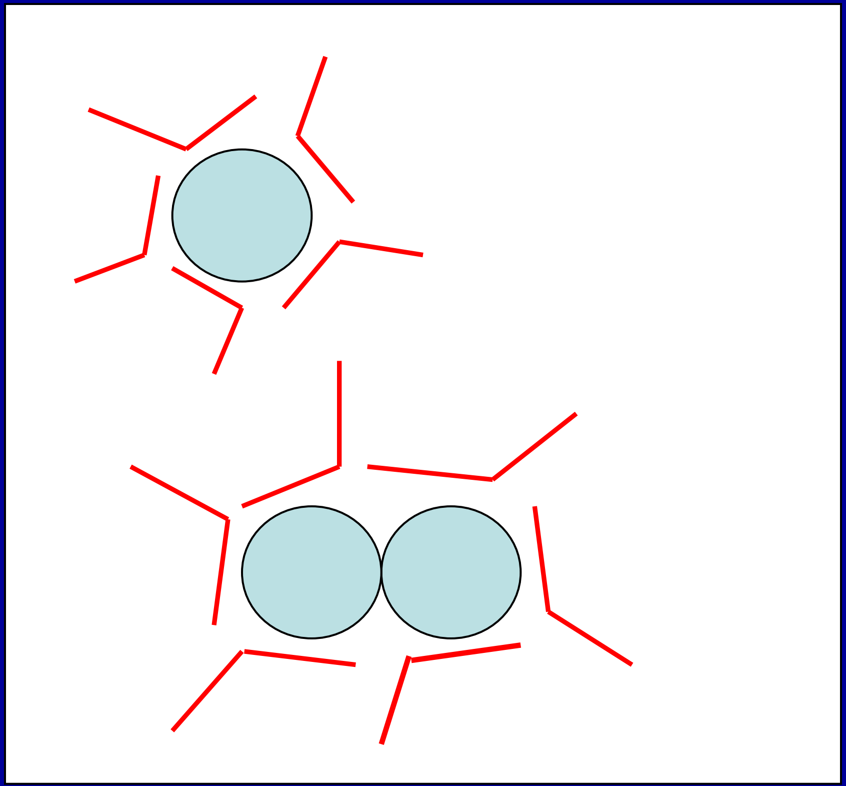
$$\varepsilon(\mathrm{HH}) = -1$$

$$\varepsilon(\mathrm{HP}) = 0$$

$$\varepsilon(\mathrm{PP}) = 0$$

自回避行走

低能态



配分函数：

$$Z = \sum_{\text{all conformations}} e^{-U/k_B T}$$

Dill et al, *Protein Sci.* 4: 561-602, 1995

Why is statistical physics important?
Paradigm example 6

6, Protein folding. HP model

Amino acid：H- & P- type
（疏水）（亲水）

peptide： H、P chain

Nearest neighbor model：

$$\varepsilon(\mathrm{HH}) = -1$$
$$\varepsilon(\mathrm{HP}) = 0$$
$$\varepsilon(\mathrm{PP}) = 0$$

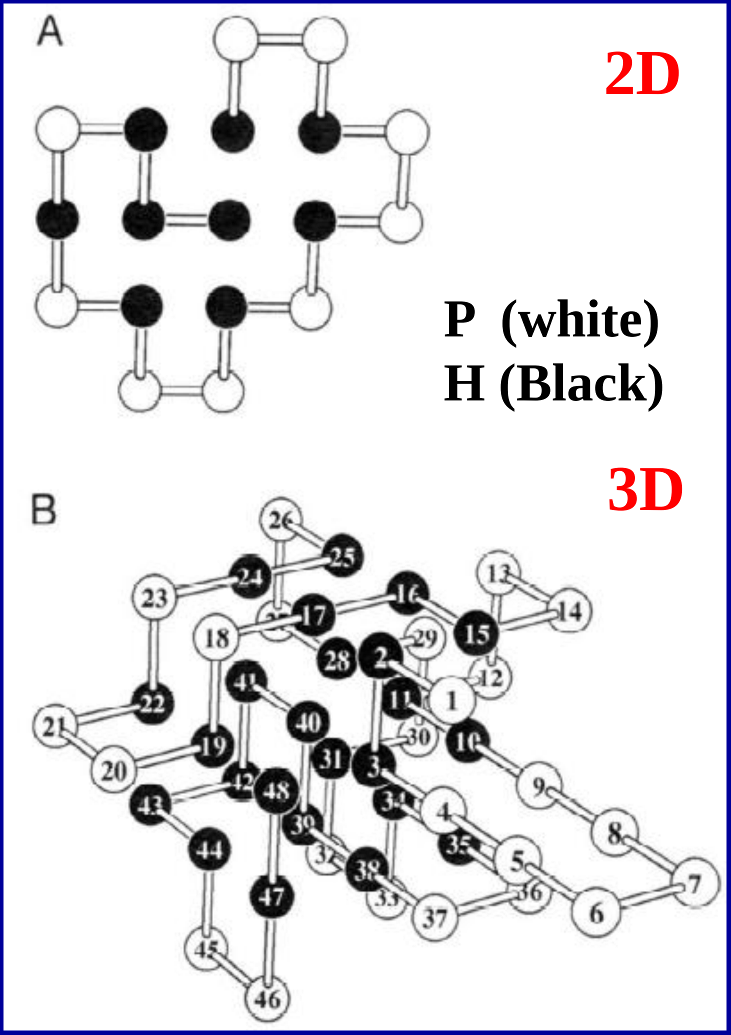
Self-avoiding walk

low energy state

配分函数：

$$Z = \sum_{\text{all conformations}} e^{-U/k_B T}$$

Dill et al, *Protein Sci.* 4: 561-602, 1995

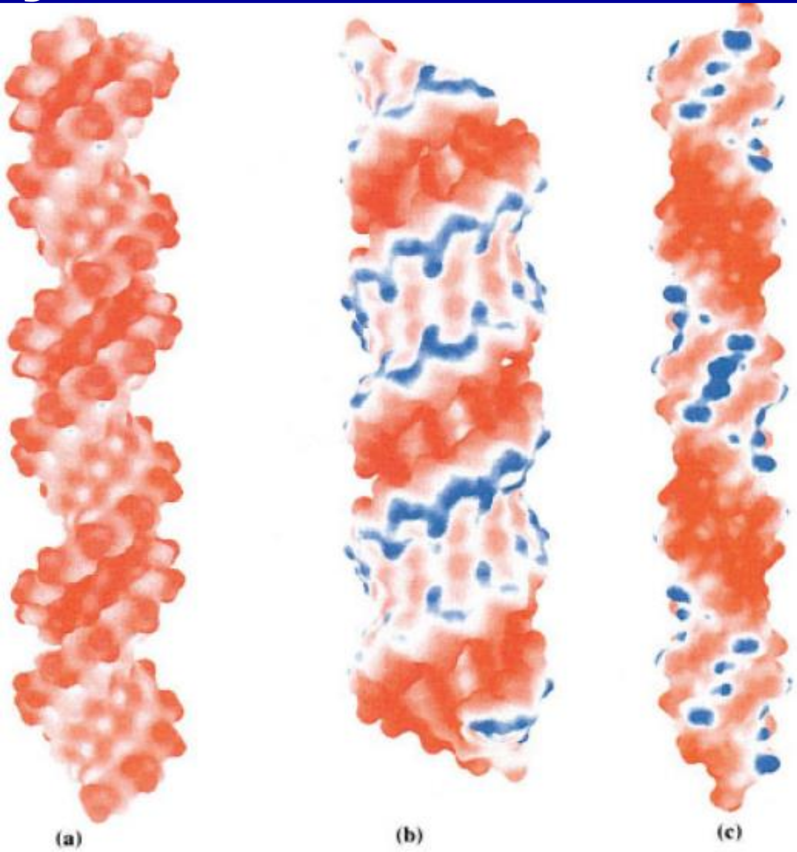


Why is statistical physics important?
Paradigm example 7

7, Electrostatics. PB theory

$$\begin{cases} \nabla \cdot \varepsilon_0 \varepsilon \nabla \psi = 4\pi\rho \\ \rho = \left(\rho_f + \sum_\alpha z_\alpha e c_\alpha^0 \mathrm{e}^{-z_\alpha e\psi / k_B T} \right) \end{cases}$$

$$G / k_B T = \tfrac{1}{2} \int \psi (\rho_f + \rho_m) dv$$
$$+ \int \sum_i (c_i \ln \frac{c_i}{c_i^0} - c_i + c_i^0) dv$$

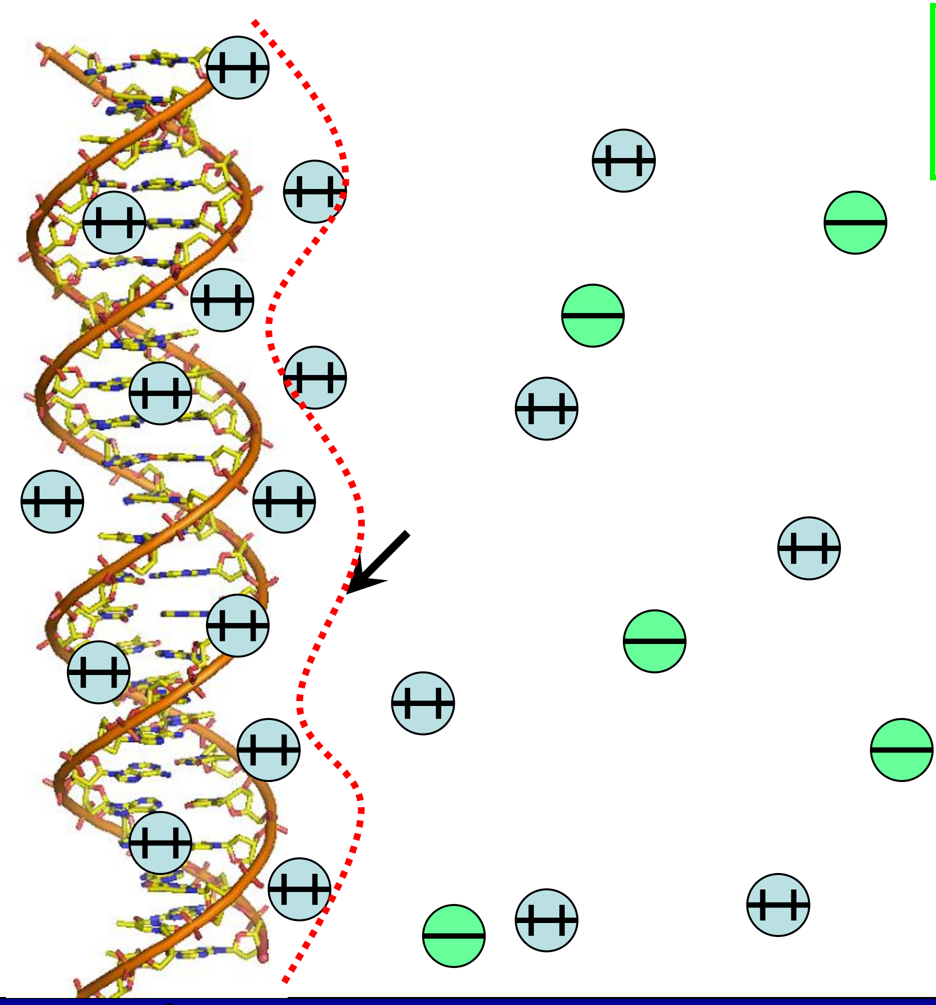


Further reading:
Sharp & Honig, *J. Phys. Chem.* 94, 7684, 1990; Baker et al, *PNAS* 98, 10037, 2000

Why is statistical physics important?

Paradigm example 8

8, Multivalent ion electrostatics. TBI theory



Nucleic acid—ion system (multi-body long-ranged)

Ions: strongly correlated +weakly correlated

Weakly correlated ions treated by mean field PB

Nucleic acid—ion system (few-body system)

Further reading: Tan & Chen, Journal of Chemical Physics 122, 044503, 2005

TextBooks for the course

《Fundamentals of statistical and thermal Physics》by F. Reif, a textbook at Berkeley

Books for references:

《热力学与统计物理学》胡承正，科学出版社，2009

《热力学与统计物理学》林宗涵，北大出版社，2007

《热力学与统计力学》 顾莱纳等，北大出版社

《Statistical Physics》Landau & Lifshitz

《量子统计物理学》杨展如，高等教育出版社，2012

TextBooks for availability

《Fundamentals of statistical and thermal Physics》 by F. Reif, a textbook at Berkeley

Outline 1

1 Introduction to statistical methods

Random walk and binomial distribution

General discussion of the random walk

2 Statistical description of systems of particles

Statistical formulation of the mechanical problem

Interaction between macroscopic systems

Outline 2

3 Statistical thermodynamics

Irreversibility and attainment of equilibrium

Thermal interaction between macro systems

General interaction between macro systems

Summary of Fundamental results

4 Macroscopic parameters and measurement

Outline 3

5 Simple application of macro-thermodynamics

Properties of ideal gases

General relation for homogeneous substance

Free expansion and throttling processes

Heat engine and refrigerators

6 Basic methods & results of statistical mechanics

Ensembles representative of situations of physical interests

Approximation methods

Outline 4

7 Simple applications of statistical mechanics

- General method of approach
- ideal monatomic gas
- paramagnetism
- kinetic theory of dilute gases in equilibrium

8 Equilibrium between phases/chemical species

- General equilibrium conditions
- Equilibrium between phases
- System of multi-components; chemical equilib.

Outline 5

9 Simple applications of statistical mechanics

General method of approach

ideal monatomic gas

paramagnetism

kinetic theory of dilute gases in equilibrium

10 Equilib. between phases or chemical species

General equilibrium conditions

Equilibrium between phases

System with multi components; chem. equilib.

Outline 6

9 Quantum statistics of ideal gases

Maxwell-Boltzman, Bose-Einstein, Fermi-Dirac

Black-body radiation

Conduction electrons in metals

10 System of interacting particles

Solids

Non-ideal classical gas

Ferromagnetism

Outline 7

15 Irreversible process and fluctuations

Transition probability and master equation

Simple discussion of Brownian motion

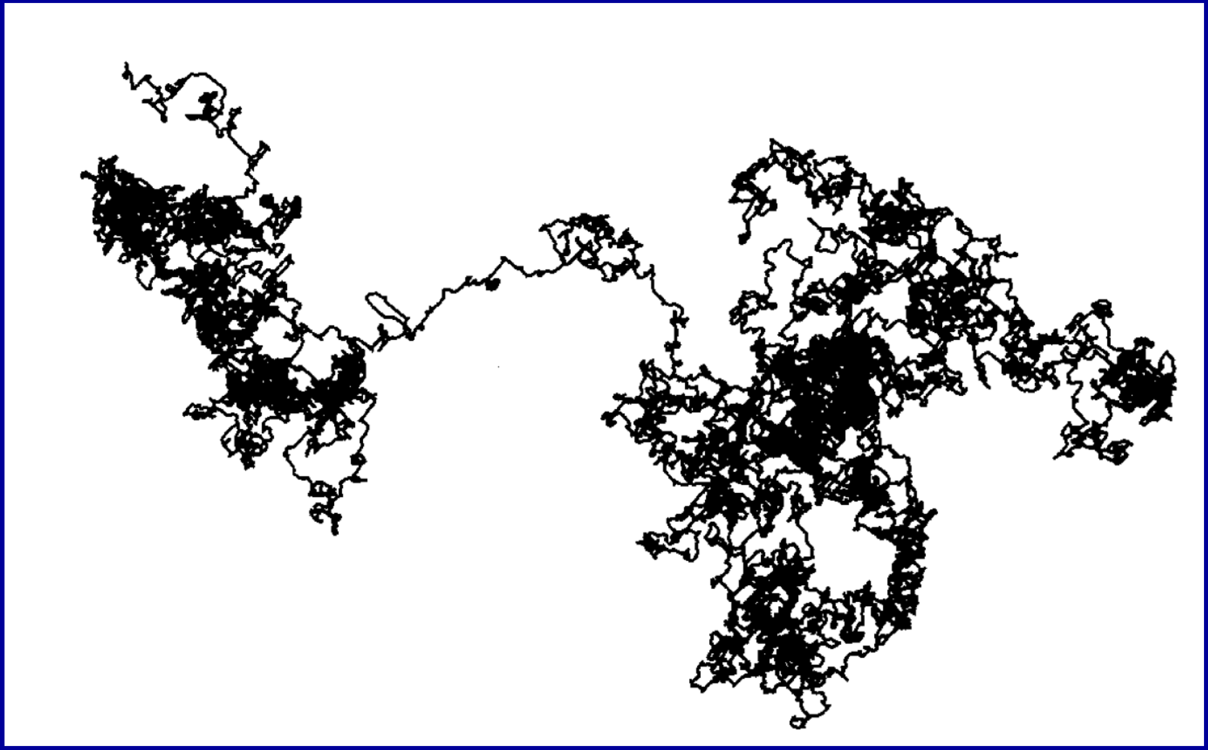
Detailed discussion of Brownian motion

Fourier analysis of random function

General discussion of irreversible process

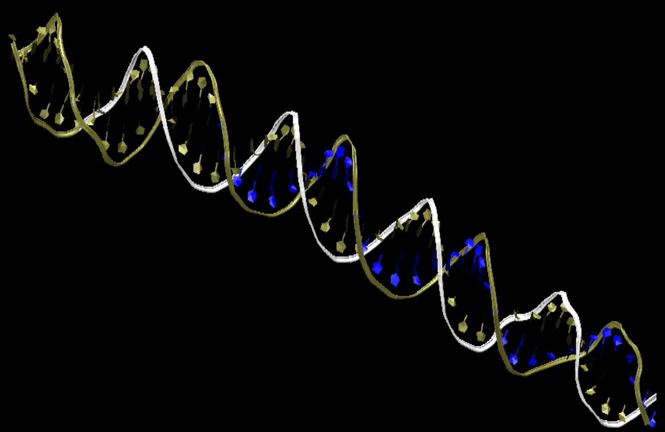
Question on class??

Which systems can be linked with random walk?

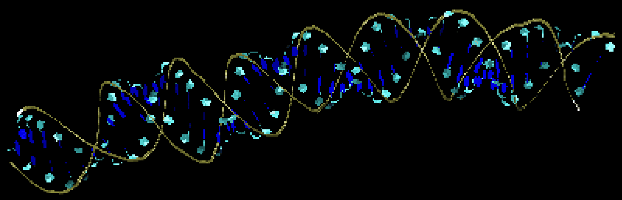


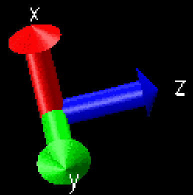
全原子动力学—DNA、RNA的柔性

DNA helix



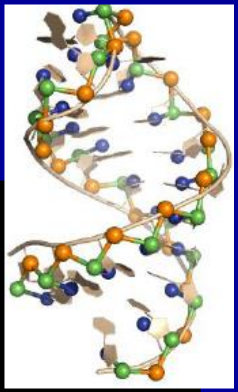
RNA helix

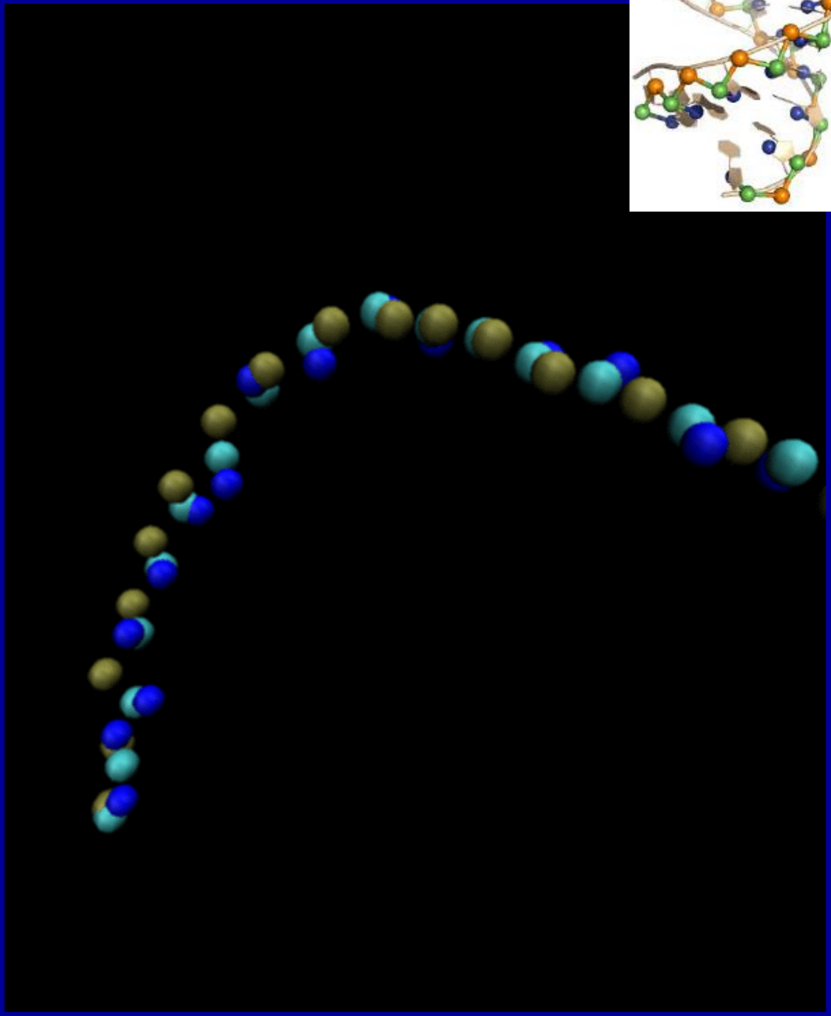




粗粒化模型—RNA结构预测

RNA hairpin





RNA pseudoknot