European Territorial Cooperation Programme
Greece-Bulgaria 2007-2013
INVESTING IN OUR FUTURE

ICoSCIS

European Territorial Cooperation Progamme
Greece - Bulgaria 2007 - 2013
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Introduction to complex science

Introduction to complex science

Course outline

1. What is Complexity Science?
2. Elementary Statistical Physics
3. Phase transitions
4. Diffusion theory
5. Percolation theory

Introduction to complex science – What is complexity science?

Outline

1. What is a system
2. Examples of systems
3. Simple vs complex systems
4. So, what is complex systems?
5. Complex Systems

   Main properties

Bibliography

Introduction to complex science – What is complexity science?

What is a system

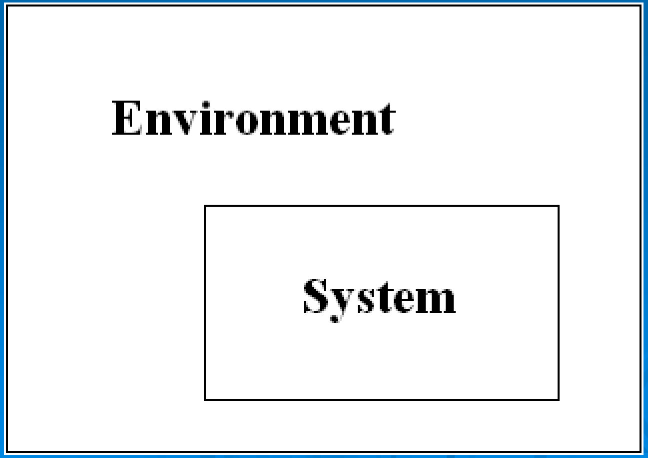
A delineated part of the universe which is distinguished from the rest by a real or imaginary boundary

Closed systems

Only internal interactions are taken into account

Open systems

In permanent interaction with the environment



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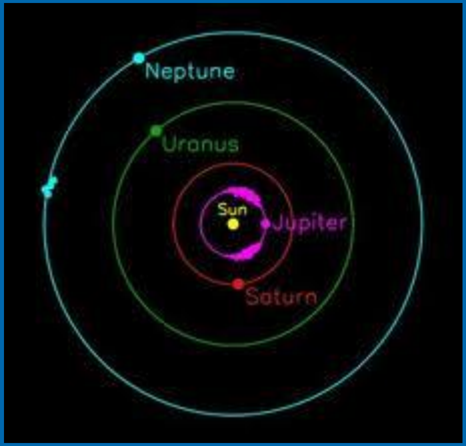
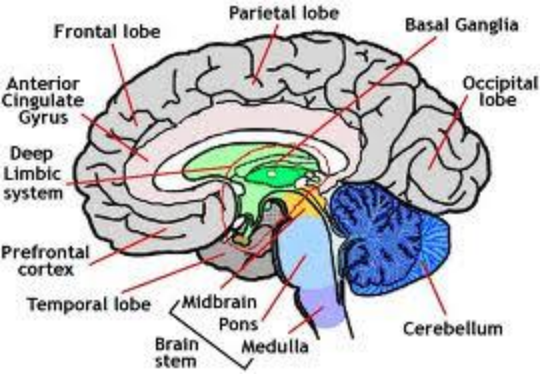
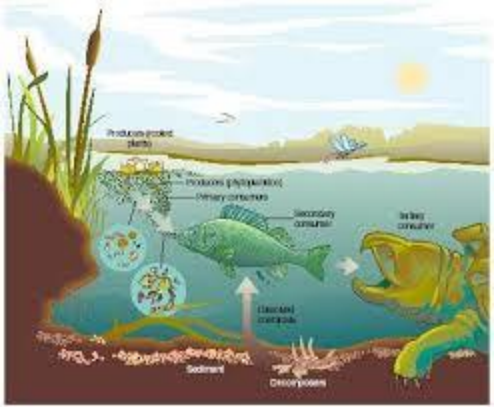
Examples of systems







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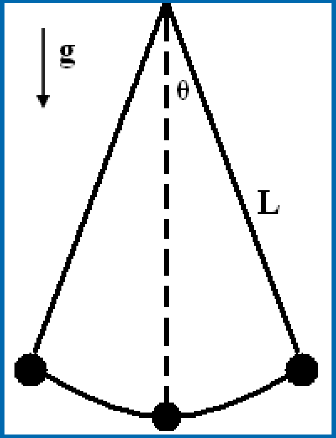
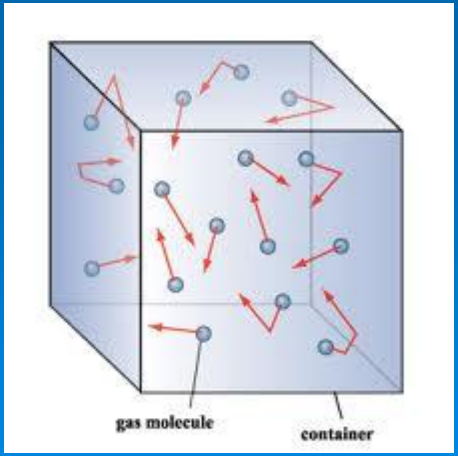
Simple vs Complex systems



We can predict the movement of the mass by simple physical laws

$$T \approx 2\pi\sqrt{\frac{L}{g}}, \quad \theta \;\; small$$



Consists of many colliding particles

We can predict macroscopic quantities like pressure, but not the actual trajectory of all the particles (of the order of N_A)

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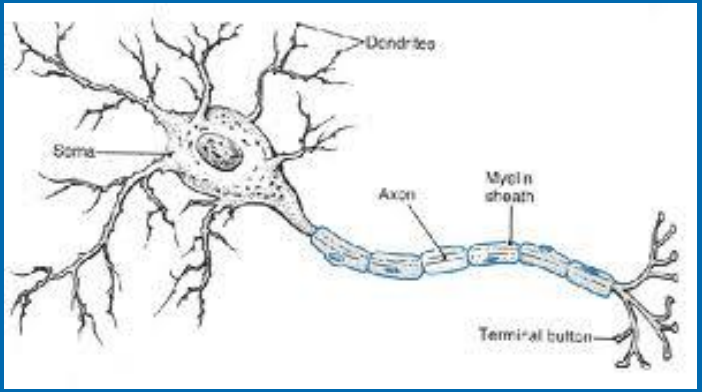
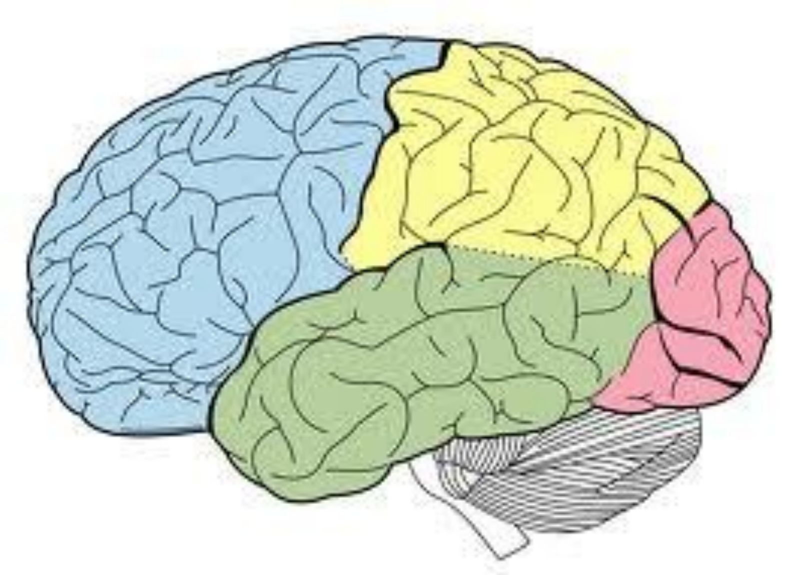
So, what is a complex system?





Many neuronal models have been proposed, but brain functionality cannot be inferred directly from the parts.

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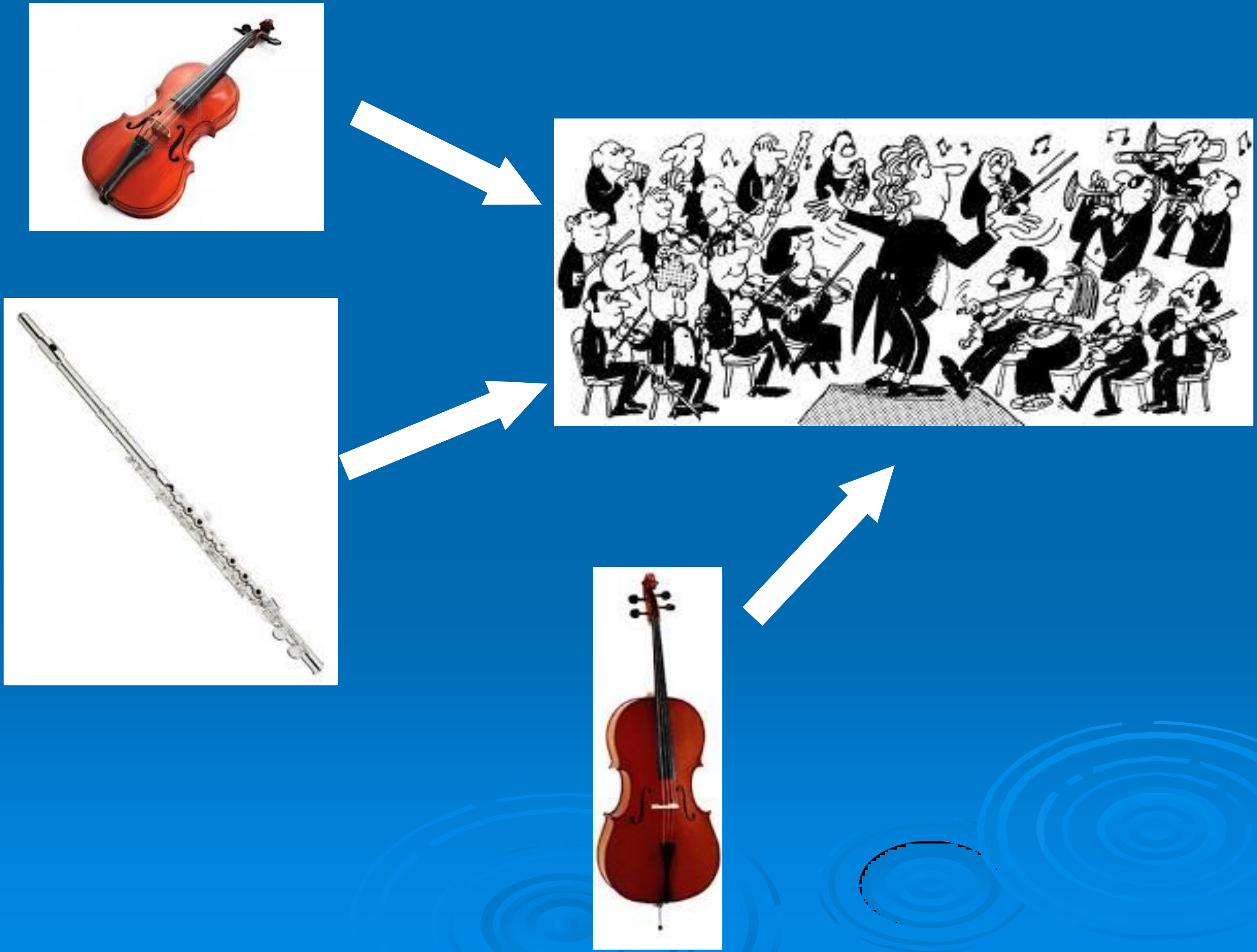

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Complex system

A system formed out of many components whose behavior is emergent, that is the behavior of the system cannot simply inferred from the behavior of its components

Can you predict the behavior of a human, just by knowing the functionality of its individual organs?

Main properties of complex systems

Interdependent parts

Emergence, i.e. self-organizing collective behavior difficult to anticipate from the knowledge of the parts behavior.

The emergent behavior does not result from the existence of a central controller.

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Outline

1. Probability basics
2. Modern probability theory
3. Hamiltonian of a system
4. Introduction to statistical mechanics
    - microstate
    - ensemble
    - partition function
    - types of ensembles

Bibliography

Introduction to complex science – Elementary Statistical Physics

Take a string composed of 3 characters A, B and C

$$AABCABBCCAABCBCBAA$$

Which is the relative frequency of each character in the string ?

$$f_A = \frac{N(A)}{N} = \frac{7}{17} \qquad f_B = \frac{N(B)}{N} = \frac{5}{17} \qquad f_C = \frac{N(C)}{N} = \frac{5}{17}$$

In total

$$\sum_{i=\{A,B,C\}} f_i = 1$$

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More generally, consider a collection of possible outcomes

$$\{A_1, A_2, \ldots, A_k, \ldots A_L\}$$

In an experiment, we may have the following succession of outcomes

$$A_1 A_2 A_1 A_4 \ldots A_k A_7 \ldots A_L \ldots .$$

Assuming that the number of repetitions N is very large, the probability of getting an outcome A_k, p_k, is

$$p_k = \lim_{N\to\infty} \frac{N(A_k)}{N}$$

In the previous example, considering that the same sequence of characters is repeated practically infinitely, we have

$$p_A = f_A,\ p_B = f_B,\ p_C = f_C$$

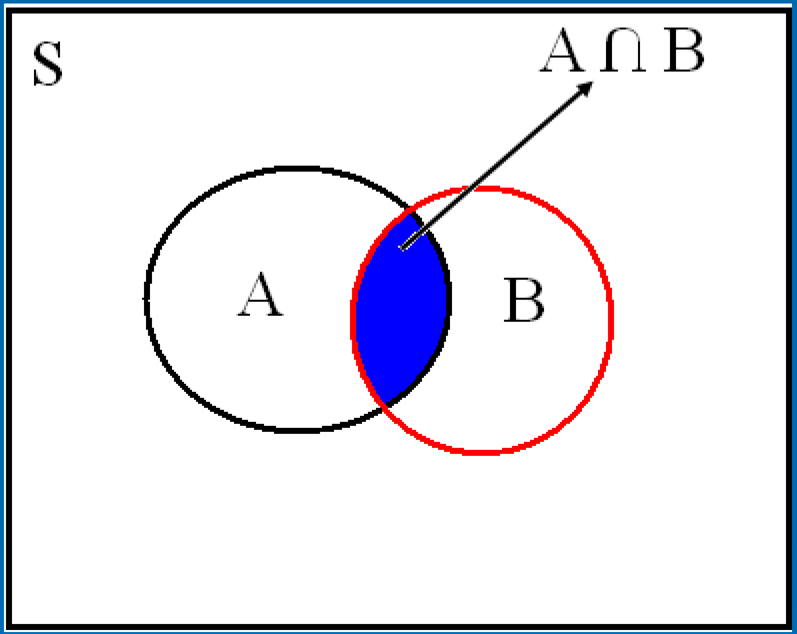
Probabilities using set theory

S : Event space

A,B : Elementary events

Ø : empty set

$$\left.\begin{array}{l} P(S) = 1 \\ \\ P(\oslash) = 0 \end{array}\right\} \Rightarrow 0 \leq P(A) \leq 1$$



A OR B = A ∪ B

A AND B = A ∩ B

$$\{A \cup B\} = \{A\} \cup \{B\} - \{A \cap B\}$$

$$P(A \cup B) = P(A) + P(B) - P(A \cap B)$$

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Problem

Consider a box which contains 4 black and 5 white balls. A person put his hand inside, without being able to observe the containment.

(a) *What is the probability of taking a black ball?*

(b) *The same person drags a ball, without putting it back. Then, he repeats the same procedure. What is the probability that he gets a black ball? What is the probability that he takes out a white ball, given that he has drawn a black ball at his first attempt?*

Solution

(a) Defining the events:

A: “drag a white ball”

B: “drag a black ball”

N_w **:** number of white balls

N_b **:** number of black balls

N **:** total number of balls

$$P(A) = \frac{N_w}{N} = \frac{5}{9}$$

$$P(B) = \frac{N_b}{N} = \frac{4}{9}$$

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A and B : mutually exclusive

$$A \cap B = \oslash \Rightarrow P(A \cap B) = 0 \Rightarrow P(A \cup B) = P(A) + P(B)$$

For more mutually exclusive events

$$P(A_1 \cup A_2 \cup \ldots \cup A_N) = P(A_1) + P(A_2) + \ldots + P(A_N)$$

If A an event and Ā its complementary, we have

$$\left.\begin{array}{l} A \cap \bar{A} = \oslash \\ A \cup \bar{A} = S \end{array}\right\} \Rightarrow P(A) = 1 - P(\bar{A})$$

E.g. : in a coin flip, we have two possible outcomes, “heads” or “tails”. The appearance of “heads” excludes “tails” and vise versa. That is A=“heads” and Ā=“tails”. Thus if P(A)=p, then P(Ā) = 1- P(A) = 1- p

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The probability of the combination of two events (that is, of the simultaneous occurrence of both of them) is equal to the probability of one of them multiplied by the probability of the other provided that the first event has occurred.

$$P(A \cap B) = P(A) \cdot P(B|A)$$

Conditional probability $P(B|A)$

EXAMPLE

Let the urn contain 3 white balls and 4 black balls. Two balls are extracted one after the other. Find the probability that both these balls will be white.

Solution

$A = \{first\ ball\ white\}$

$B = \{second\ ball\ white\}$

$$P(A \cap B) = P(A)P(B|A) = \frac{3}{7} \cdot \frac{2}{6} = \frac{1}{7}$$

Generally

$$P(A \cap B) = P(A) \cdot P(B|A) = P(B) \cdot P(A|B)$$

Two events A and B are said to be independent if and only if

$$P(A \cap B) = P(A)P(B)$$

This means that $P(B|A) = P(B) \; and \; P(A|B) = P(A)$

Example

What is the probability of having “head” in the 2nd coin toss if we had “tails” in the 1rst attempt?

Each coin toss is independent from its previous ones. So, the probability of having “tails” is not affected by the fact that we had “heads” before. Thus:

$$P(B|A) = P(B) = 1/2$$

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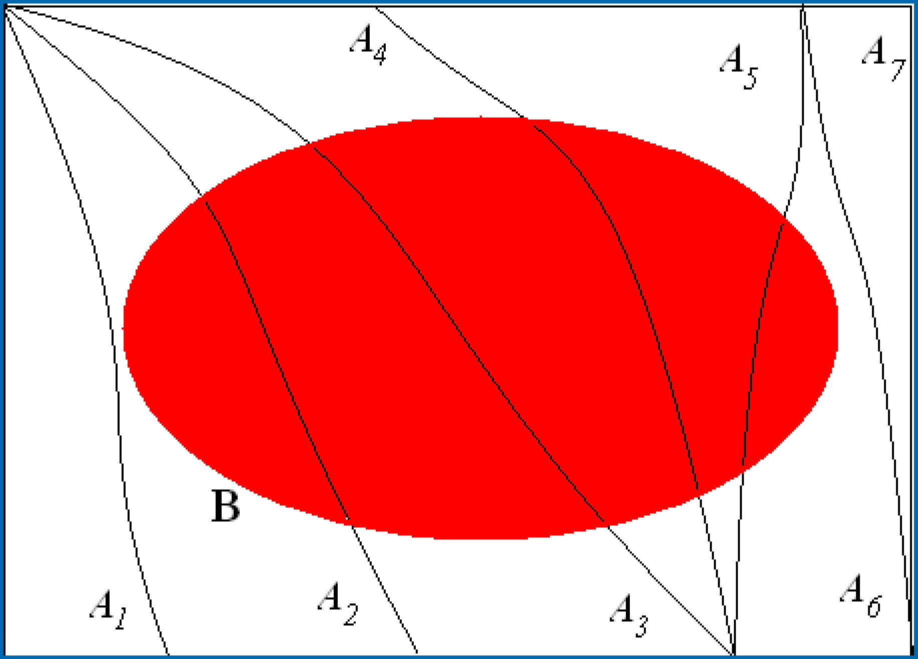
Consider the event space S which can be divided into 7 mutually exclusive events

$$P(A_i \cap A_j) = 0 \ \ \forall \ \ i, j$$

$$S = \cap_{i=1}^{7} A_i$$

$$\sum_{i=1}^{7} P(A_i) = P(S) = 1$$



$$P(B) = \sum_{i=1}^{7} P(B|A_i)P(A_i)$$

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General multiplication rule

$$P(A_1 \cap A_2 \cap \ldots \cap A_n) = P(A_1) \cdot P(A_2|A_1) \cdot P(A_3|A_1 \cap A_2) \cdots P(A_n|A_1 \cap A_2 \cap \ldots A_{n-1})$$

Example

Let five balls in the urn be numbered. They are drawn from the urn one after the other. Find the probability that the numbers of the balls will appear In the increasing order.

Solution

$$P(1,2,3,4,5) = P(1) \cdot P(2|1) \cdot P(3|1,2) \cdot P(4|1,2,3) \cdot P(5|1,2,3,4) = (1/5) \cdot (1/4) \cdot (1/3) \cdot (1/2) \cdot 1 = 1/120$$

Another way is to consider all the possible permutations, which are

$$n = \prod_{k=1}^{5} C(k,1) = C(5,1) \cdot C(4,1) \cdot C(3,1) \cdot C(2,1) \cdot C(1,1) = 5 \cdot 4 \cdot 3 \cdot 2 \cdot 1 = 120$$

Only one combination of the 120 is the proper, thus P(1,2,3,4,5)=1/n =1/120

Problem

A rifleman takes four shots at a target. The hit or miss in every shot does not depend on the result of the previous shots (that is, the shots are mutually independent). The probability of a hit in each shot is 0.3. Find the probability that the rifleman hits the target at least once.

Solution

We must calculate the following event:

$$C = \{(hit \cap hit \cap hit \cap hit) \cup (hit \cap hit \cap hit \cap missed) \cup ((hit \cap hit \cap missed \cap hit) \cup \dots\}$$

The above event must contain 15 sub – events, making calculations very tiring

Instead, let’s try to calculate the complementary event $\bar{C}$ which is stated as “all targets are missed” . That is:

$$\bar{C} = \{missed \cap missed \cap missed \cap missed\}$$

So

$$\begin{aligned} &P(\bar{C}) = P(\{missed \cap missed \cap missed \cap missed\}) \\ &= P(missed) \cdot P(missed) \cdot P(missed) \cdot P(missed) \\ &= (1-p)^4 = 0.7^4 = 0.24 \end{aligned}$$

and

$$\begin{aligned} &P(C) = 1 - P(\bar{C}) \\ &= 1 - 0.24 = 0.76 \end{aligned}$$

If an opposite event divides into a smaller number of variants than the event in question, we should shift to the opposite event.

Modern probability theory

Random Variable (RV) : *a quantity that , as a result of an experiment, it may take on various values which are unknown beforehand*

E.g: number of “heads” in a series of coin tosses

Discrete RV: *the possible values are separated by some interval*

e.g. the number of people wearing hats in a room

Continuous RV: *continuously filling a certain interval*

e.g. the height of people living in a city

Uppercase letters are used for the symbolic representation of a RV while *lowercase* ones are used for the possible values of the RV

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Distribution function

Describes the distribution of the probabilities among the values of a random variable

For discrete RV's: distribution series

x_i	x_1	x_2	….	x_n
p_i	p_1	p_2	….	p_n

$$p_i = P(X = x_i)$$

$$\sum_i p_i = 1$$

PROBLEM 1

Three independent shots are taken at a target; the probability of a hit each time is *p* = 0.4. Discrete RV X is the number of hits. Construct its distribution series.

Solution

The possible outcomes are: 0,1,2 and 3. Thus, X, takes on that values.

Now, what is the probability of each case?

By letting + the successful shot and – the missed target, we have:

$$x = 0 \Rightarrow (-\ AND\ -\ AND\ -)$$

Each shot is independent from the succeeding, thus

$$P(X=0) = P(-\ AND\ -\ AND\ -) = P(-)P(-)P(-) = (1-p)^3$$

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By the same treatment, we have

$$P(X = 1) = 3(1 - p)^2 p$$

$$P(X = 2) = 3(1 - p)p^2$$

$$P(X = 3) = p^3$$

The results are summarized in the following table

x_i	0	1	2	3
p_i	0.216	0.432	0.288	0.064

Homework

A sportsman makes several attempts to throw a ball into a basket. At every attempt (independently of the others) a success occurs with the probability $p = 0.2$. As soon as the ball gets into the basket the exercise is stopped. Discrete RV X is the number of trials to be made. Construct the distribution series for RV X.

For continuous RV’s: probability density function

Probability density *of a continuous random variable* X *is the limit of the ratio of the probability of getting* RV X *into a small interval in the vicinity of point x to the length of this interval as the latter tends to zero.*

$$f(x) = P(x \leq X < x + dx)$$

Consider the height of a man

- *Divide the whole range of values into certain intervals* (they may differ)
- *Calculate how many values are put into each interval and divide by the total number of experiments made.*
- *Calculate the frequency density for each interval; for this purpose divide the frequency by the length of the interval*

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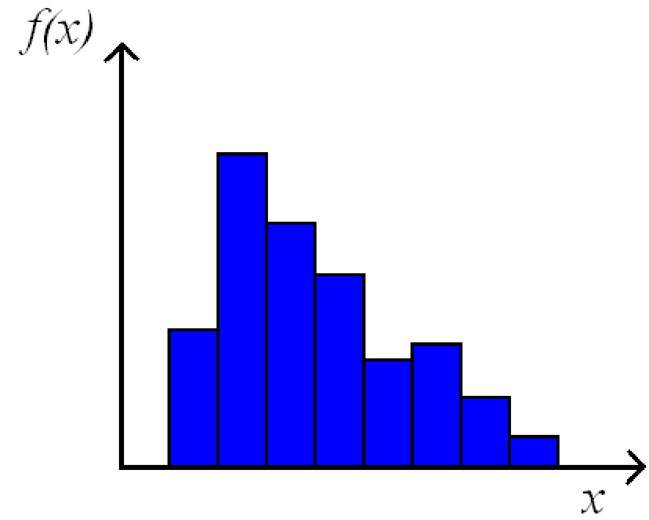
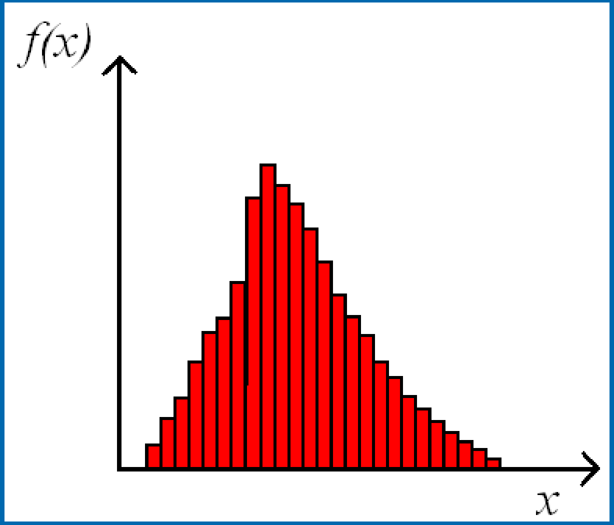
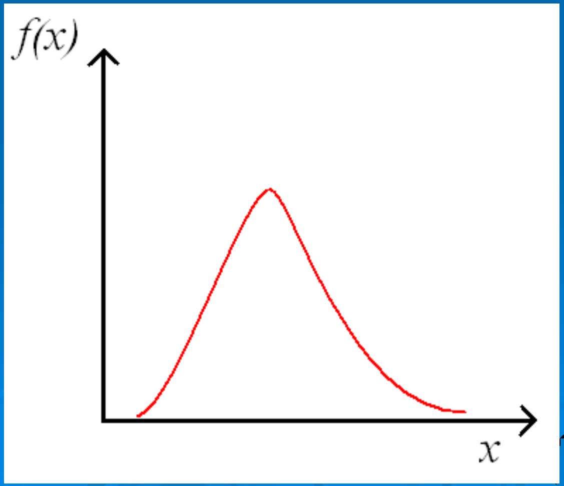




Increasing the number of people participating in the experiment leads to a smoother histogram



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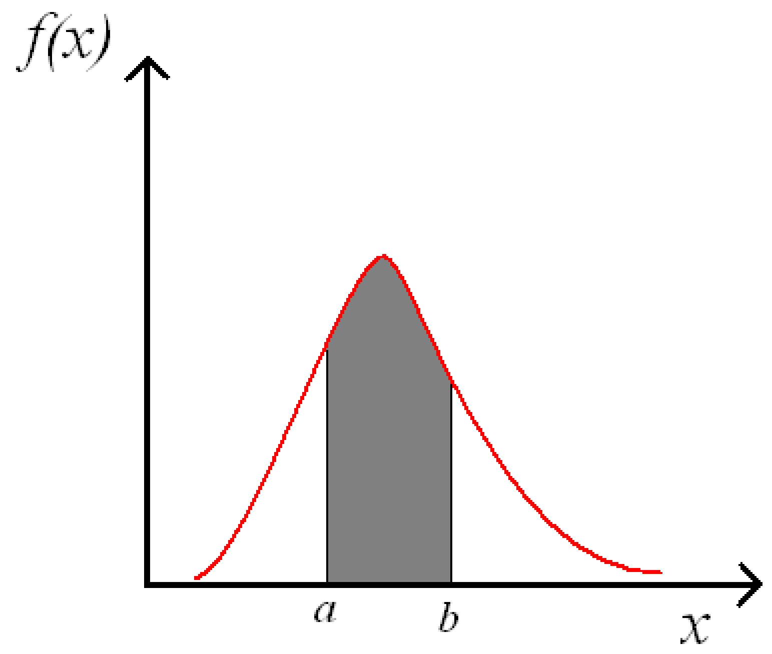
How to calculate the probability of an event of the form *a* ≤ *X* < *b*, given f(x)?

$$P(a \leq X < b) = \int_a^b f(x)dx$$



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Basic characteristics of RVs

Expectation

$$E[X] = \sum_{i=1}^{n} x_i p_i$$

discrete RV

$$E[X] = \int_{-\infty}^{+\infty} x f(x) dx$$

continuous RV

For PROBLEM 1, find the expectation value of X

Solution

$$E[X] = \sum_{i=0}^{3} x_i p_i = x_0 p_0 + x_1 p_1 + x_2 p_2 + x_3 p_3$$
$$= 0 \cdot 0.216 + 1 \cdot 0.432 + 2 \cdot 0.288 + 3 \cdot 0.064 = \boxed{1.2}$$

Expectation value need not be a member of the possible outcomes (e.g. S ={0,1,2,3})

Given a set of N observed values and for the sake of simplicity can only be discrete and countable, we can approximate the expectation by the arithmetic mean for the dataset, that is

$$E[X] \approx \bar{X}$$

for relatively large N

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Basic characteristics of RVs

Variance

$$\sigma^2 = D[X] = \sum_{i=1}^{n} (x_i - E[X])^2 p_i$$

discrete RV

$$\sigma^2 = D[X] = \int_{-\infty}^{+\infty} (x - E[X])^2 f(x)dx$$

continuous RV

It can be shown that $\sigma^2 = D[X] = E[X^2] - E[X]^2$

where

$$E[X^k] = \begin{cases} \sum_{i=1}^{n} x_i^k p_i \\ \int_{-\infty}^{+\infty} x^k f(x)dx \end{cases}$$

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For PROBLEM 1, find the variation of X

Solution

$$D[X]=\sum_{i=0}^{3}\left(x_i-E[X]\right)^2p_i$$
$$=(0-1.2)^2 0.216+(1-1.2)^2 0.432+(2-1.2)^2 0.288+(3-1.2)^2 0.064$$
$$=0.72$$

Given a set of N observed values and for the sake of simplicity can only be discrete and countable, we can approximate the variation by averaging the squares of the deviations of the values in the dataset from their arithmetic mean, that is

$$D[X]\approx\frac{1}{N}\sum_{k=1}^{N}\left(x_k-\bar{X}\right)^2$$

for relatively large N

Standard deviation $\sigma=\sqrt{D[X]}$

Practically, the 99% of the values of a RV X reside inside the range

$$E[X]-3\sigma_X<x<E[X]+3\sigma_X$$

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Other properties of expectation and variance

Additivity

Given *N* RVs $X_1, X_2, \ldots, X_N$ it can be shown that for the sum of the RVs

$$X = X_1 + X_2 + \ldots + X_N$$

the *expectation* value of the new RV *X* is

$$E[X] = \sum_{i=1}^{N} E[X_i]$$

and the *variance* (given that $X_1, X_2, \ldots, X_N$ *are independent RVs*) is

$$D[X] = \sum_{i=1}^{N} D[X_i]$$

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Multiply by a constant factor c

Given *a RV X´= cX,* where *c constant, it can be shown that* the *expectation* value is $E[X'] = cE[X]$

and the *variance* $D[X'] = c^2 D[X]$

PROBLEM 2

Let N independent trials be made, in each of which event A occurs with probability p. We consider a random variable P, the frequency of event A in this series of trials. Find approximately the range of possible values of RV P**

Solution

XX_i***:*** *occurrence of A in a single experiment*

X: *number of occurrences of A in N realizations* → $X = X_1 + X_2 + \ldots + X_N$

$E[X_i] = 0 \cdot (1-p) + 1 \cdot p$ → $E[X] = \sum_{i=1}^{N} E[X_i] = N \cdot p$

$D[X_i] = p(1-p)$ → $D[X] = \sum_{i=1}^{N} D[X_i] = N \cdot p \cdot (1-p)$

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PROBLEM 2 (cont’)

P*: frequency of occurrence of A in the sequence of N realizations **(X/**N)

c=1/N →

$$E[P^*] = E[\frac{X}{N}] = \frac{1}{N}E[X] = \frac{Np}{N} = p$$

$$D[P^*] = D[\frac{X}{N}] = \frac{1}{N^2}D[X] = \frac{Np(1-p)}{N^2} = \frac{1}{N}p(1-p)$$

Some basic distributions

- **Binomial** $P(k) = \binom{N}{k} p^k (1-p)^{N-k}$
- **Uniform** $P(k) = \begin{cases} \frac{1}{b-a}, & a \le k \le b \\ 0, & elsewhere \end{cases}$
- **Poisson** $P(k) = \frac{e^{-\lambda}\lambda^k}{k!}$

It can be shown that for $N \to \infty$ and $Np \to \lambda$ that the Poisson distribution can be recovered from the binomial distribution

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Some basic distributions (cont')

- **Normal (or gaussian)**

$$P(k) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(k-m)^2/2\sigma^2}$$

- **Power – law**

$$P(k) = ck^{-\gamma}$$

Central – limit theorem

If we add up a large number of independent (or weakly dependent) random variables comparable by the order of variances, then the *distribution of the sum will be close to the normal distribution, irrespective of the distributions of the addends,* and the closer the greater number of random variables are added up.

Note that the CLT is applicable only for RVs that exhibit finite mean values and variances, i.e. it cannot be applied for a power – law distribution

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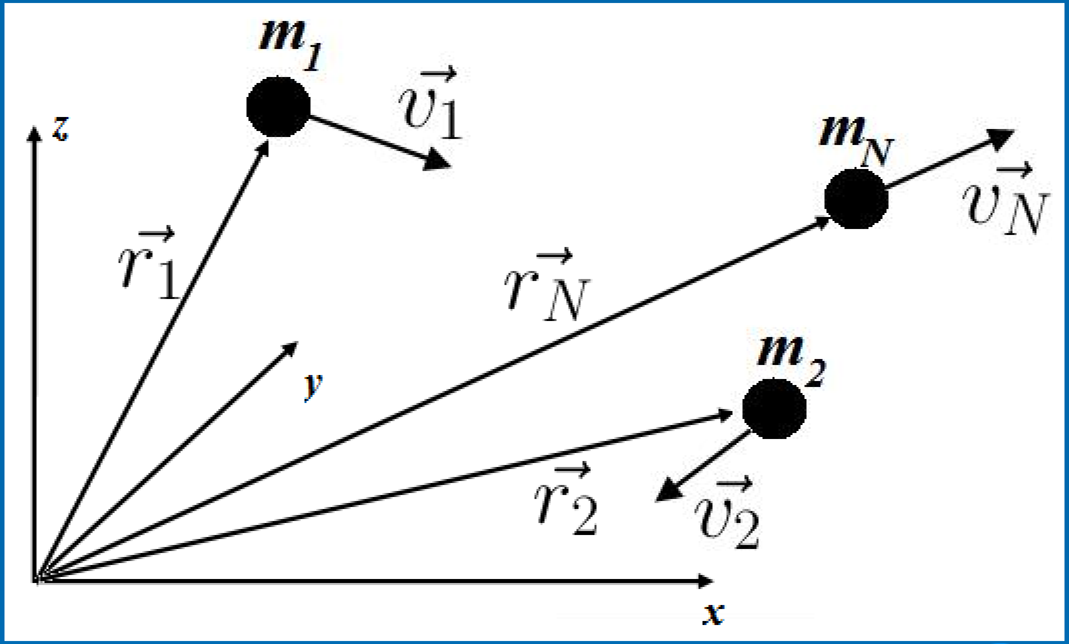
To study the properties of a system, it is important to calculate its energy

Potential Energy

$$V = V(\vec{r_1}, \vec{r_2}, \dots, \vec{r_N}, t)$$

Kinetic Energy

$$T_i = \frac{1}{2} m_i \vec{v_i}^2 = \frac{\vec{p_i}\vec{p_i}}{2m_i}$$



Total system's energy (Hamiltonian)

$$H = T + V = \sum_{i=1}^{N} T_i + V$$

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For a non – interacting system

$$V(\vec{r_1}, \vec{r_2}, ..., \vec{r_N}, t) = V_1(\vec{r_1}, t) + V_2(\vec{r_2}, t) + ... + V_N(\vec{r_N}, t)$$

$$\Rightarrow V(\vec{r_1}, \vec{r_2}, ..., \vec{r_N}, t) = \sum_{i=1}^{N} V(\vec{r_i}, t)$$

The total energy may be written as

$$H = \sum_{i=1}^{N} \left[\frac{\vec{p_i}\vec{p_i}}{2m_i} + V_i(\vec{r_i}, t) \right]$$

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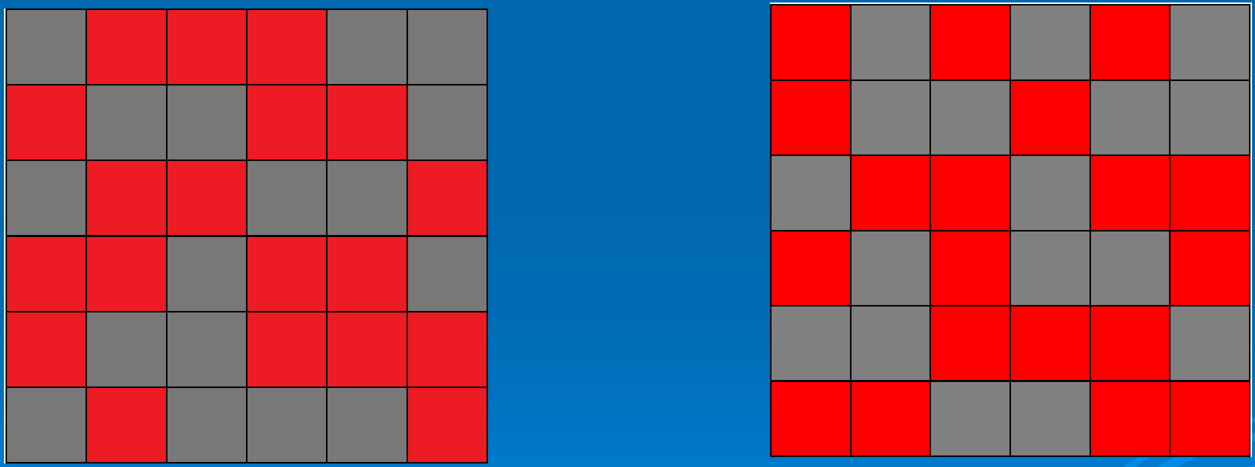
Introduction to statistical mechanics

Statistical mechanics **applies probability theory to study the thermodynamic behavior of the system composed of a large number of particles**

Basic notions

microstate: one of the possible configurations of a collection of particles in a given environment



In the above example, we have 19 red shells and 17 grey shells (representing for example "up" and "down" spins respectively) in two different possible microstates.

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Ensemble

The set of all possible realizations that a system might be

Three basic types of ensembles in statistical mechanics

Microcanonical

describes a completely isolated system, having constant energy, as it does not exchange energy or mass with the rest of the universe. N, V, E constant.

Canonical

describes a system in thermal equilibrium with its environment. It may only exchange energy in the form of heat with the outside. N, V, T constant.

Grand canonical

used in open systems which exchange energy and mass with the outside. V, T, μ constant.

Each ensemble is connected to a specific partition function

Partition function

Measure of the number of states accessible to the system at a given temperature

Encodes the underlying physical structure of the system

- **Microcanonical Ensemble**

$\Omega(E)$ **Number of states at a given energy E**

The (statistical) entropy of the system is given by

$$S = -k_B \sum_s p_s \ln p_s = -k_B \sum_s \frac{1}{\Omega(E)} \ln(\frac{1}{\Omega(E)})$$

$$\Rightarrow S = k_B \ln \Omega(E)$$

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- **Canonical Ensemble**

$$p_s = e^{-\beta E_s} / \sum_s e^{-\beta E_s} = Z^{-1} e^{-\beta E_s}$$

where $Z = \sum_s e^{-\beta E_s}$ **is the partition function**

The (statistical) entropy of the system is given by

$$S = -k_B \sum_s p_s \ln p_s = k_B lnZ + k_B \beta \sum_s E_s p_s$$

$$\Rightarrow S = k_B lnZ + k_B \beta < E >$$

It follows that

$$F =< E > -TS =< E > -k_B T(\ln Z + \beta < E >)$$

$$\Rightarrow F = -(1/\beta) \ln Z$$

the well – known relation for the free energy F

Introduction to complex science – Elementary Statistical Physics

- **Grand Canonical Ensemble**

It can be shown that the partition function is given by the following relation

$$\Xi = \sum_{s} \exp(\beta(\sum_{j=1}^{n} \mu_j N_{sj} - E_s))$$

where N_{sj} the number of jth particles in the sth configuration

In the *thermodynamic limit*, the macroscopic behavior of the system does not depend on the particular ensemble for its description.

So, we can use the ensemble which allows to calculate the properties of the macroscopic system more easily

Introduction to complex science – Elementary Statistical Physics

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http://en.wikipedia.org/wiki/Statistical_mechanics

http://en.wikipedia.org/wiki/Statistical_ensemble

Introduction to complex science – Phase Transition

Outline

1. What is a phase?
2. What is a phase transition
    - -Examples of phase transitions
    - A. Liquid - gas transition (Vaporization)
    - B. Ferromagnetic – paramagnetic transition
3. State variables
4. Phase diagram
5. Order of transition
6. Critical Phenomena
    - - behavior near criticality
    - - critical exponents
    - - pair – correlation function

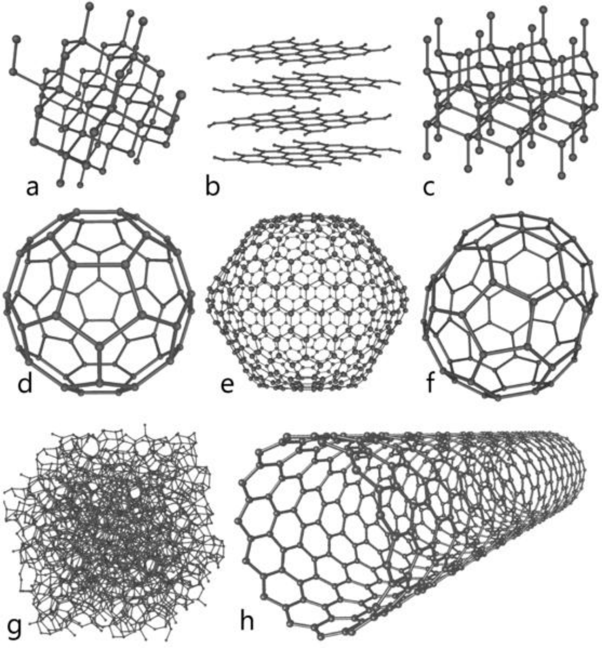
Bibliography

Introduction to complex science – Phase Transition

What is a phase?

A state of a system where its properties are the same for every part of it

The most common phases are: <u>Solid</u>, <u>Liquid</u> and <u>Gas</u> . Phases can also be defined according to other aspects, such as different structure (e.g. graphite – diamond phase for carbon)



Introduction to complex science – Phase Transition

Introduction to complex science – Phase Transition

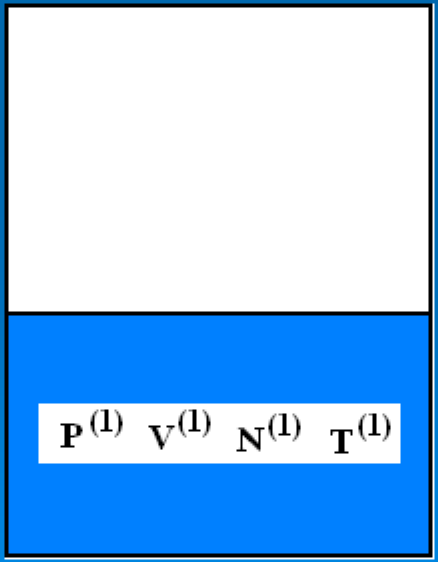
What is a phase transition?

The transition of a system from its current phase to another

Examples of phase transitions

A. Liquid - gas transition (Vaporization)

Consider a one-component system at temperature T.



At temperature T below T_{boil}, the system is at its liquid phase

By heat transfer from its surrounding environment, the temperature of the system increases.

At $T=T_{boil}$, with further heating, the temperature of the liquid phase system is held constant.

This amount of thermal energy (called latent heat) is used to change the phase of the system from liquid to gaseous

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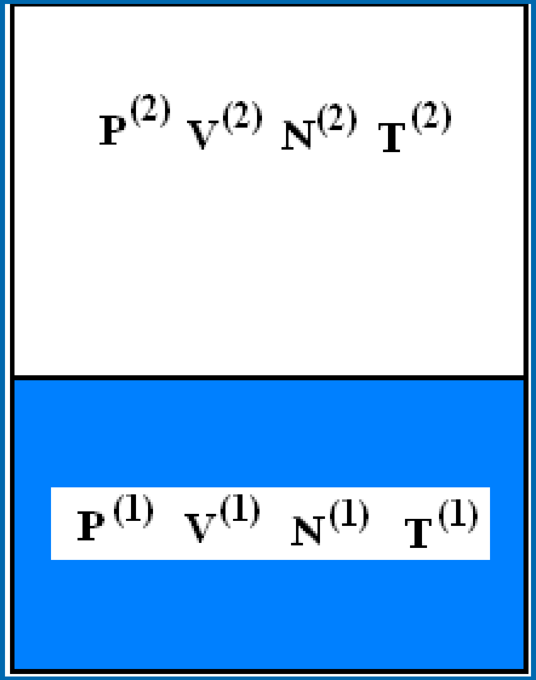
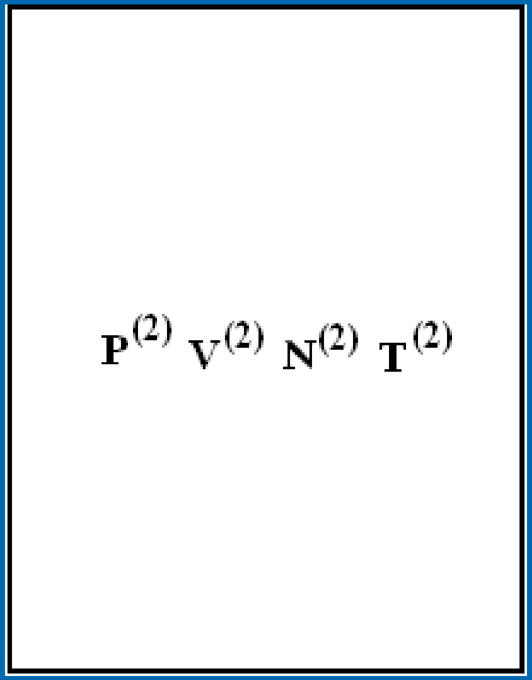


At an intermediate state (coexistence of 2 phases)



Complete transition to the gaseous phase

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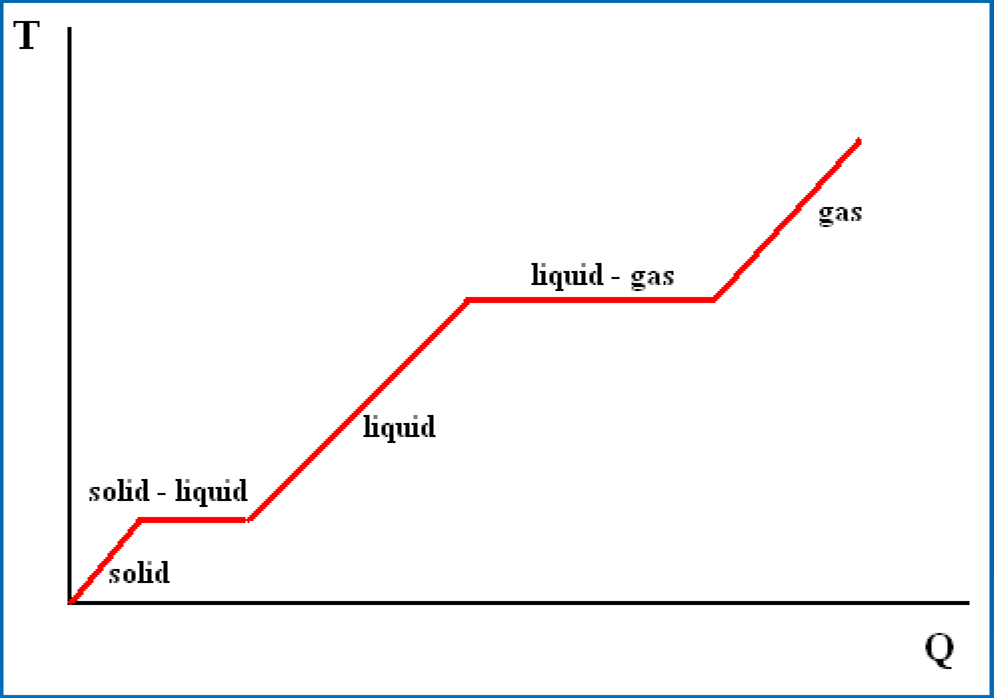

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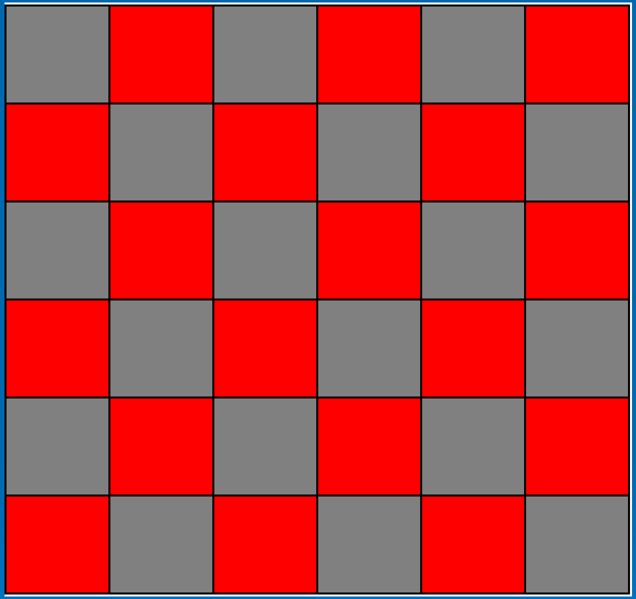
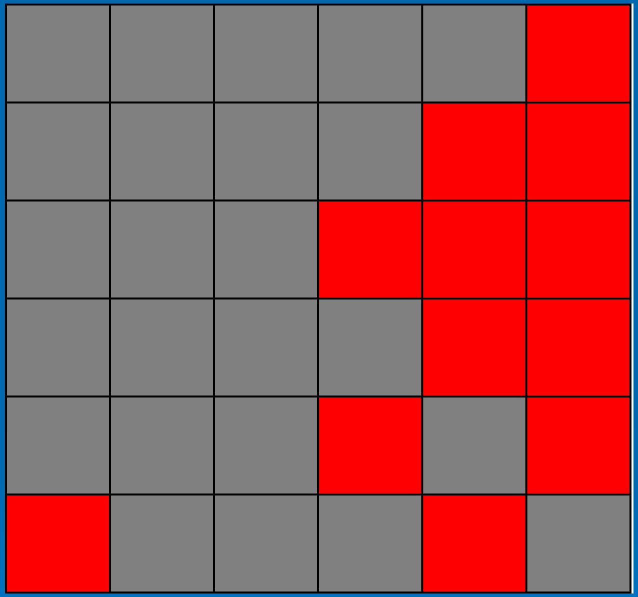
B. Ferromagnetic – Paramagnetic transition

Consider a 2 D lattice. Each site can be occupied by either an up or down spin, denoted by grey and red respectively.



$T>T_C$



$T<T_C$

The interactions are only between nearest neighboring spins, with no external magnetic field application

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The net magnetization for the system is given by the relation

$$\langle M \rangle = \sum_i s_i$$

where **s_i** receives the value **+1** for the up direction and **-1** for the down one

At $T > T_C$, we can calculate from the given instant that

$$\langle M \rangle = \sum_i s_i = 18 \cdot (-1) + 18 \cdot (+1) = 0$$

However, at $T < T_C$, we have

$$\langle M \rangle = \sum_i s_i = 12 \cdot (-1) + 24 \cdot (+1) = 12$$

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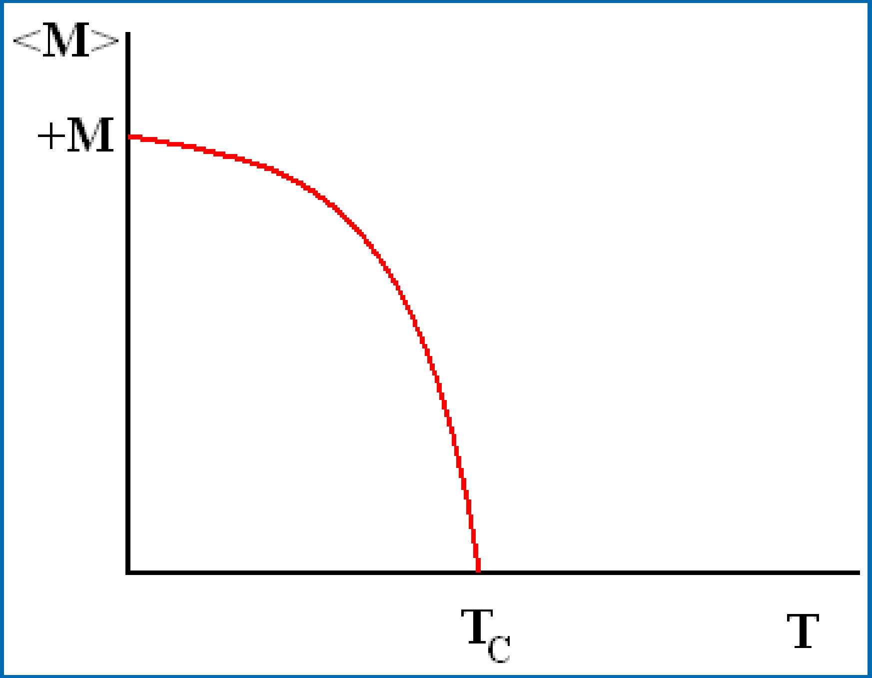

We observe that above a critical temperature T_C, the system is composed of random up and down spins. On average, the magnetization of the system is 0. By reducing the temperature below T_C, an ordered phase appears, giving rise to a non-zero net magnetization. Thus, we can state that the system undergoes a phase transition from the paramagnetic to ferromagnetic phase, as T is reduced below T_C.

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State variables

A set of quantities, which uniquely characterize the state of a thermodynamic system.

For example, in a fluid system, these variables could be pressure (P), volume (V), temperature (T), number of molecules (N).

These quantities are linked with each other by the famous equations of state. E.g., for the monoatomic gases, we have:

$$PV = NRT$$

or ,taking into account the interactions between molecules, we have the famous van der Waals equation of state for a non-ideal gas

$$P_{vdW} = \frac{Nk_BT}{V - Nb} - \frac{N^2\alpha}{V^2}$$

Generally, $f(P, V, T, N) = 0$

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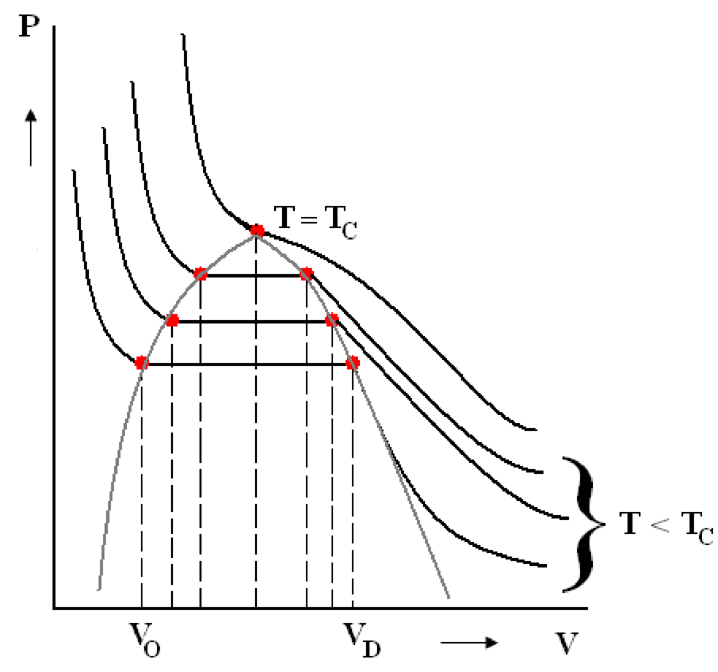
Phase diagram

The changing pattern of a state variable with respect to the others.

For convenience, we use 2-d diagrams, i.e. we measure the change of one variable with respect to another one, holding a second variable constant.



P-V diagram for different values of T

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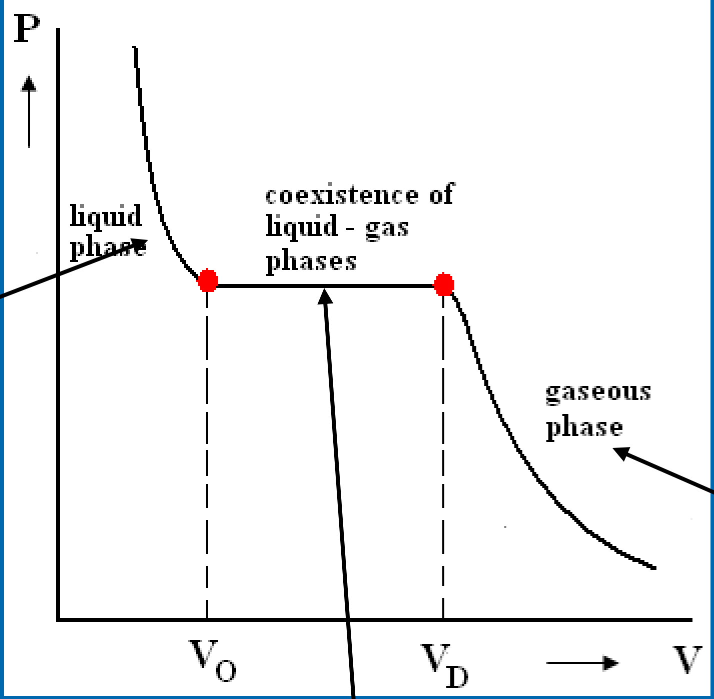

High pressure – low volume regime

Condensed phase

Region of phase coexistence

Low pressure – high volume regime

Dilute phase

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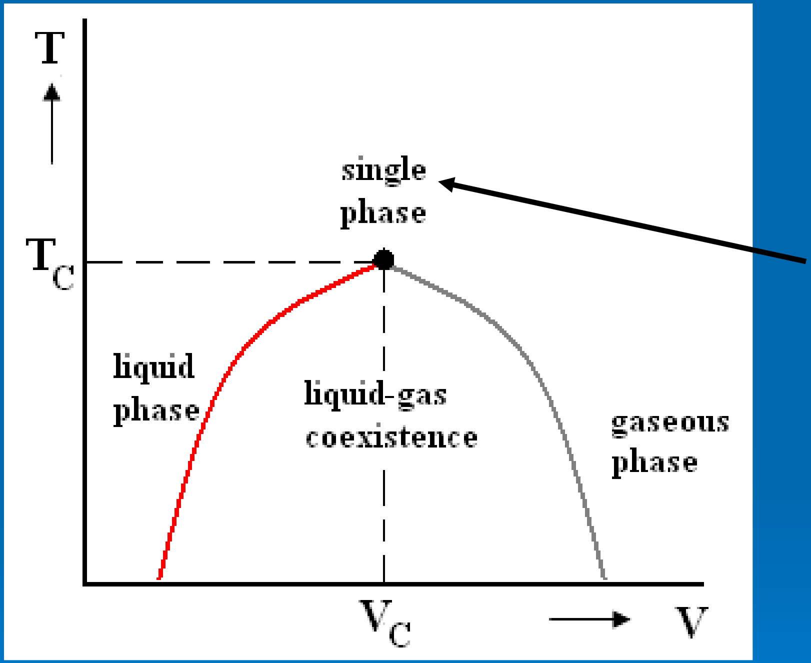
We can construct the T-v phase diagram, by connecting the red dots in the P-v diagram



Typical T- V diagram

Above T_C, we can move continuously from the gaseous phase to liquid phase and vice versa

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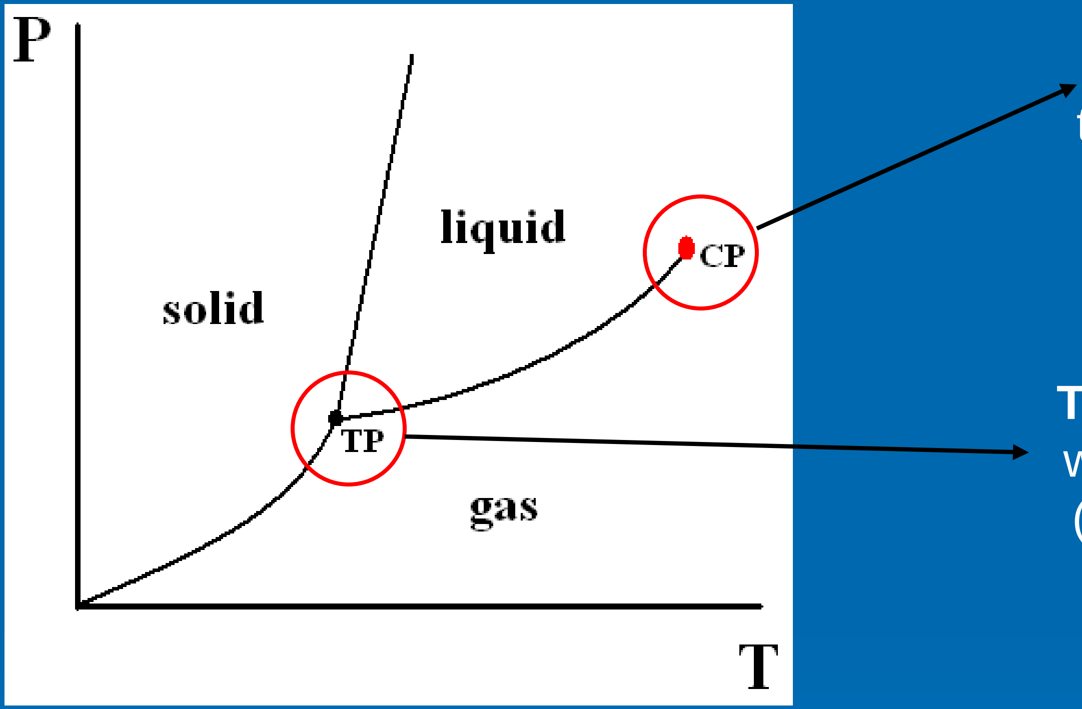

Critical point: the transition between liquid and gaseous phase is continuous

Triple point: the (P,T) values where the 3 different phases (solid, liquid, gas) coexist in equilibrium

Typical P- T diagram

Coexistence curves

- Melting curve (**Solid→Liquid**)
- Vapor pressure curve (**Liquid→Gas**)
- Sublimation curve (**Solid→Gas**)

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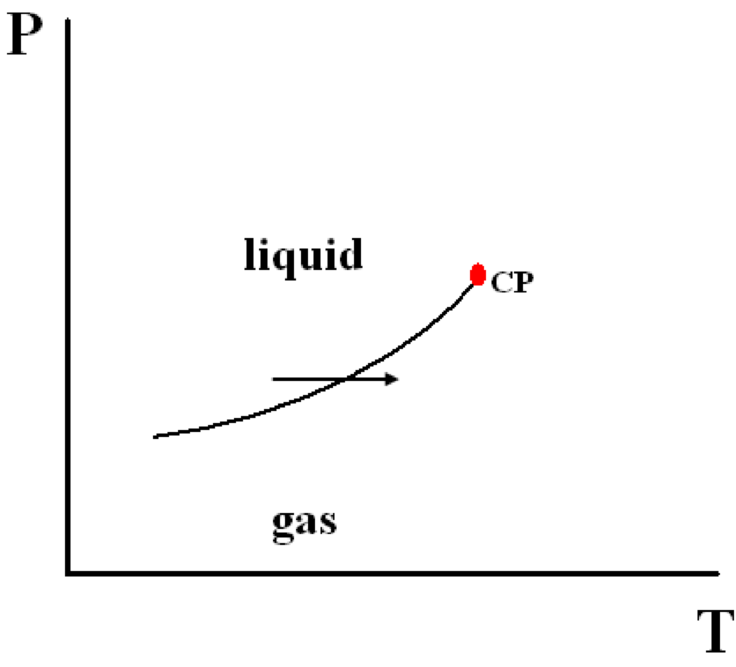

Latent heat: the amount of energy necessary for the transition from one phase to another

Consider that we are initially in the liquid phase. We move according to the direction of the arrow. We transfer heat, keeping the volume constant

While heat is provided to the system, its temperature rises. However, there is a point (the well – known boiling point) for which, upon further increase of heat transfer, the temperature of the system remains the same. This energy, provided as heat, is the abovementioned latent heat. There, we have a phase change (in the figure, the liquid to gas transition). The transition is discontinuous. When the substance is completely changed to gas, further heating leads to temperature rising.

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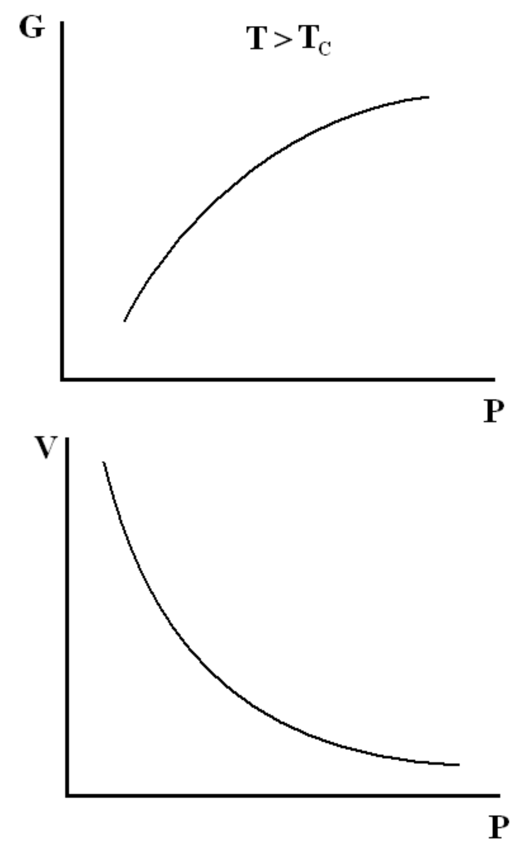
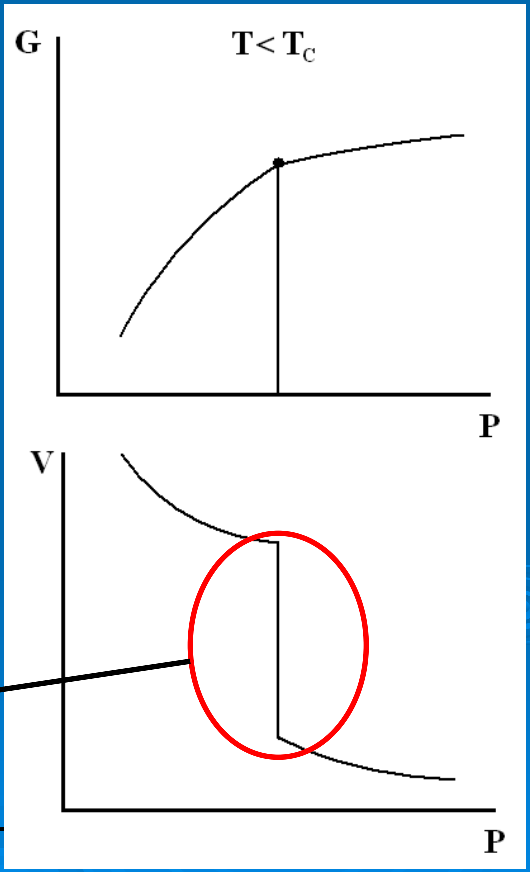
Order of transition

In thermodynamics, the order of the phase transition is related to the first derivatives of the Gibbs free energy,



$$G = G(T,P)$$

$$V = \left(\frac{\partial G}{\partial P}\right)_T$$



Discontinuity

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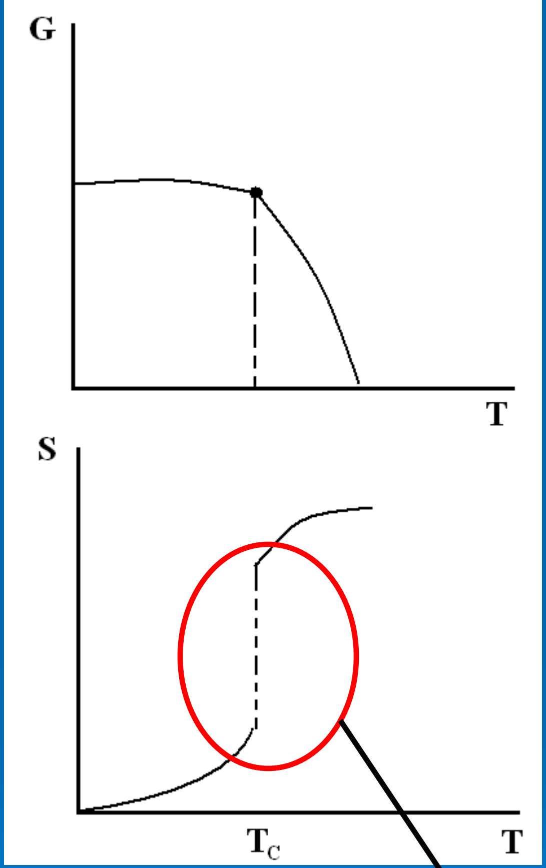
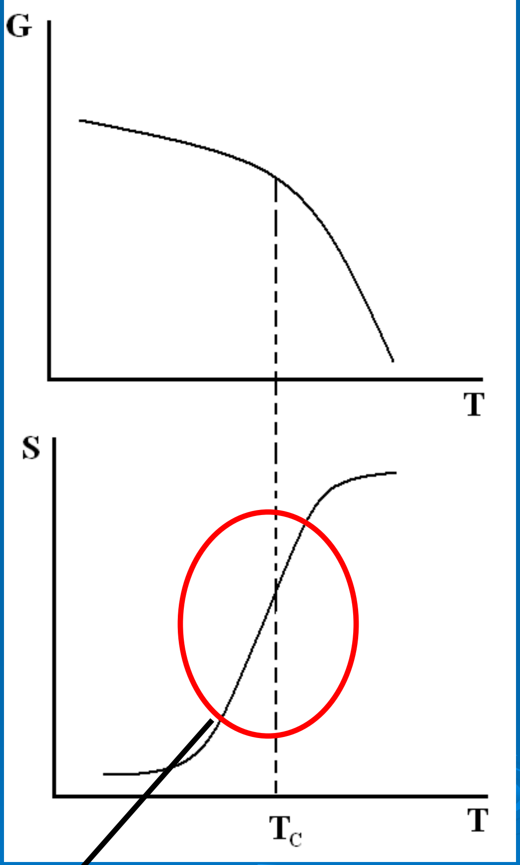


$$S = -\left(\frac{\partial G}{\partial T}\right)_P$$



Discontinuity

Continuity

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For thermodynamics, a phase transition is classified as follows

First order

The first derivatives of the Gibbs free energy are discontinuous.

Second order

The first derivatives of the Gibbs free energy are continuous, but the second order ones are discontinuous or infinite.

E.g, the entropy $S = -\left(\frac{\partial G}{\partial T}\right)_P$ is continuous while the specific heat $C \sim \left(\frac{\partial S}{\partial T}\right)_P = -\left(\frac{\partial^2 G}{\partial T^2}\right)_P$ is discontinuous

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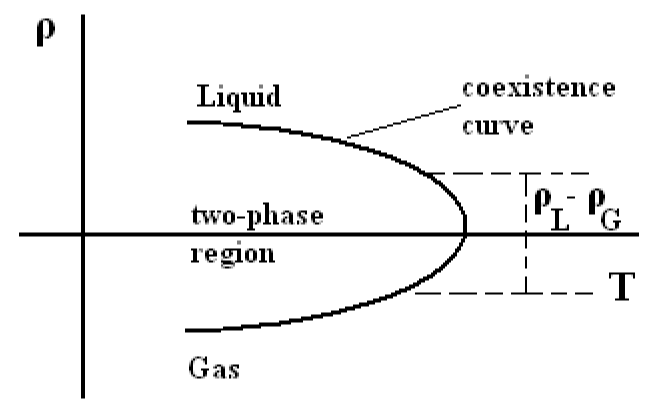
Critical phenomena

<u>Order parameter</u>: a property of a system which is non – zero in the “ordered phase” and zero in the disordered phase



For a fluid, such a parameter could be the difference between the density of the liquid and gaseous phase

$$\bar{\rho} = \rho_L - \rho_G$$

Following the above diagram, it is easy to verify that the difference of densities are 0 above a critical temperature T_C and non – zero above it

Introduction to complex science – Elementary Statistical Physics

Why are we interested to examine the behavior of a system at its critical point?

Understand better the basic phenomena

The striking similarity of systems near their critical point, yet being different in nature

Understand the “spontaneous” ordering of the system over a practically infinite length scale (e.g., how do spins align suddenly at T_C?)

Behavior near criticality

Lets define a dimensionless parameter t. For example $t= (T-T_C)/T_C$

Generally, a quantity near the critical point can be described by a function of the form

$$f(t) = A\,|t|^{\lambda}\,(1 + Bt^{\lambda_1} + \ldots), \quad \lambda_1 > 0$$

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For t → 0 $f(t) \to A\left|t\right|^{\lambda}$

Critical exponents

Given a quantity which can be described by a positive and continuous function *f* for small t, it can be shown that the following limit exists

$$\lambda = \lim_{t \to 0} \frac{\ln(f(t))}{\ln(|t|)}$$

λ is called the critical exponent of the quantity described by *f*

So, a set of indices which describe the behavior near the critical point of the various quantities of interest are called critical exponents

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For example, some relevant quantities of a magnetic system can be described at T_C by the following relations

Zero – field magnetization $M \sim (-t)^{\beta}$

Zero – field isothermal susceptibility $\chi_T \sim |t|^{-\gamma}$

$$t = \frac{T - T_C}{T_C}$$

Correlation length $\xi \sim |t|^{-\nu}$

The correlation length is a very important quantity for critical phenomena. It defines the length above which the pair - correlation function is negligible.

Pair – correlation function

Questions whether or not distant localities tend to act in unison for fluctuations of the same direction

$$\Gamma(\vec{r}) = \left\langle \delta M(\vec{0})\delta M(\vec{r}) \right\rangle$$

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Near the critical point, the correlation function can be written as

$$\Gamma(\vec{r}) \sim \frac{1}{|\vec{r}|^{d-2+\eta}} \exp(-|\vec{r}|/\xi)$$

where *η* is a critical exponent.

For $t \to 0$ we have $\xi \to \infty$ and $\Gamma(\vec{r}) \sim \frac{1}{|\vec{r}|^{d-2+\eta}}$

We focus to the determination of the critical point exponents for the following reasons

They are measurable while the complete function is not

There is a large number of relations between the exponents. We have to know only two of them in order to calculate the others for a given class

In the percolation chapter, we will have a closer look at these relations

Introduction to complex science – Phase Transition

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Introduction to complex science – Diffusion Theory

Outline

1. Random Walk

   - 1-d case

2. Diffusion Approximation

3. Relation to classical diffusion theory

   - Fick’s laws

3. Some examples using diffusion theory

   A. Diffusion of polymer chain in random media

   B. Diffusion of information in a complex network

   C. Diffusion of zooplankton

   D. Molecular crowding and protein diffusion

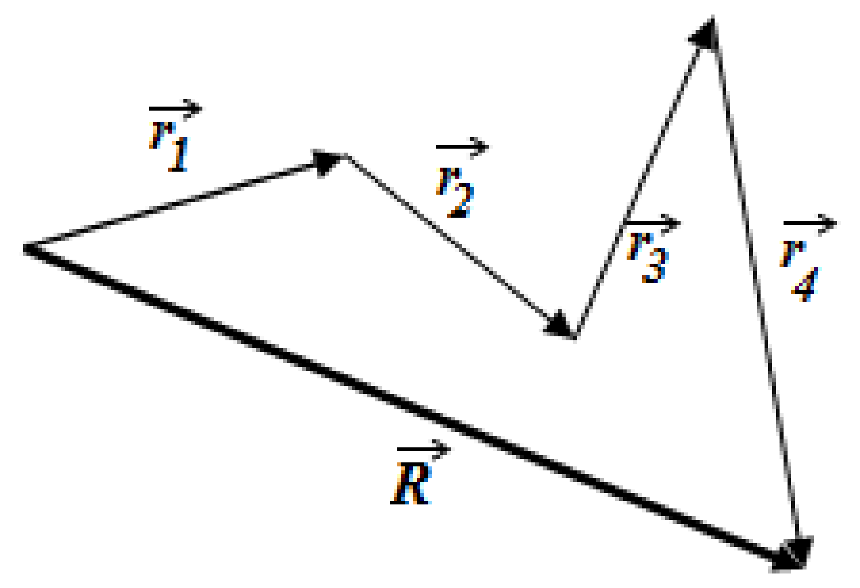
Bibliography

Introduction to complex science – Diffusion Theory

Random Walk

A stochastic process in which the action at the nth step depends only on the current state

$$Pr\left\{\vec{r}_{j+1}\middle|\vec{r}_j \cap \vec{r}_{j-1} \cap \ldots \cap \vec{r}_1\right\} = Pr\left\{\vec{r}_{j+1}\middle|\vec{r}_j\right\}$$



$$\vec{R} = \vec{r_1} + \vec{r_2} + \vec{r_3} + \vec{r_4}$$

$\vec{r_i}$ Random variable

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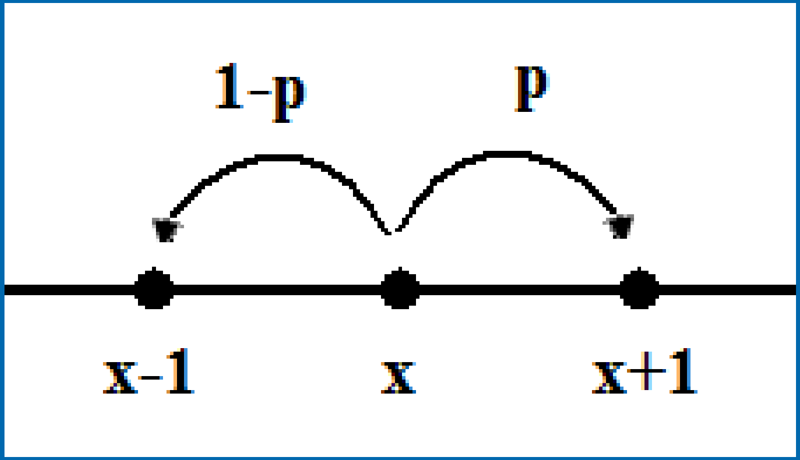
Random Walk – 1 d case



Transition probabilities

$$Pr\{x \rightarrow x+1\} = p$$

$$Pr\{x \rightarrow x-1\} = 1-p$$

Consider each displacement as an independent random variable X_i. For n=1, we have $x=x_1$ (let p=1/2 and start from the origin)

$$p(x_1 = -1) = p(x_1 = 1) = 1/2$$

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For n=2, we have $x=x_1+x_2$

$$p(x = x_1 + x_2 = -2) = p(x_2 = -1|x_1 = -1)p(x_1 = -1) = p(x_2 = -1)p(x_1 = -1) = 1/2 \cdot 1/2 = 1/4$$

$$p(x = x_1 + x_2 = -1) = 0$$

$$p(x = x_1 + x_2 = 0) = p(x_2 = 1|x_1 = -1)p(x_1 = -1) + p(x_2 = -1|x_1 = 1)p(x_1 = 1) = p(x_2 = 1)p(x_1 = -1) + p(x_2 = -1)p(x_1 = 1) = 1/2 \cdot 1/2 + 1/2 \cdot 1/2 = 1/2$$

In the same manner

$$p(x = x_1 + x_2 = 1) = 0$$

$$p(x = x_1 + x_2 = 2) = 1/4$$

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From the previous presentation, one can see that at every time step n, the following evolutionary equation holds

$$p_{n+1}(x) = p(x \to x-1)p_n(x+1) + p(x \to x+1)p_n(x-1)$$

It can be shown that the probability of a 1-d random walker being after n steps at position x is given by

$$p_n(x) = \begin{cases} \binom{n}{\frac{n+x}{2}}2^{-n}, & n+x\ even \\ 0\,, n+x\ odd \end{cases}$$

This probability density is attributed to the drunkard's walk in 1-d dimension

<u>Generally</u>, the mean square displacement follows asymptotically a relation of the form

$$\langle R^2 \rangle \sim N^{\alpha}$$

with

$$\alpha \begin{cases} < 1(subdiffusive) \\ = 1(normal\ diffusive) \\ > 1(superdiffusive) \end{cases}$$

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Another quantity which is of great interest for a RW is the mean number of distinctly visited sites. Asymptotically, we have

$$S_N \sim \begin{cases} \left(\frac{8N}{\pi}\right)^{1/2}, & 1-d \\ \frac{\pi N}{\ln N}, & 2-d \\ N, & 3-d \end{cases}$$

Moving from discrete to continuous representation – The Diffusion Approximation

If the number of steps is very large, we can move from the discrete representation of RW to the diffusion process, where space and time are continuous.

This is not possible for all RW models.

The diffusion approximation can be used to tackle a broader range of physical problems compared to RW models

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The Diffusion Approximation

We focus on the 1-d case

The transition probabilities for moving from a given position to site j are

$$P_{j+1\to j} = p$$
$$P_{j-1\to j} = 1 - p$$

The evolutionary equation is given by

$$p_n(j) = P_{j+1\to j}\, p_{n-1}(j+1) + P_{j-1\to j}\, p_{n-1}(j-1)$$
$$\Rightarrow p_n(j) = p \cdot p_{n-1}(j+1) + (1-p) \cdot p_{n-1}(j-1)$$

Letting $\Delta x, \Delta t$ small, we can write $x = j\Delta x$ and $t = n\Delta t$

Thus $p_n(j) = p[n\Delta t, j\Delta x]$

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The evolutionary equation can be written as

$$p[n\Delta t, j\Delta x] = p \cdot p[(n-1)\Delta t, (j+1)\Delta x] + (1-p) \cdot p[(n-1)\Delta t, (j-1)\Delta x]$$

By series expansion around Δx=0 and Δt = 0, we have

$$p[n\Delta t, j\Delta x] \sim p(x,t) + \Delta t \frac{\partial p(x,t)}{\partial t} + \ldots$$

$$p[(n-1)\Delta t, (j\pm 1)\Delta x] \sim p(x,t) \pm \Delta x \frac{\partial p(x,t)}{\partial x} + \frac{1}{2}(\Delta x)^2 \frac{\partial^2 p(x,t)}{\partial x^2} + \ldots$$

The evolutionary equation takes the form

$$\frac{\partial p(x,t)}{\partial t} = (2p-1) \cdot \frac{\Delta x}{\Delta t} \frac{\partial p(x,t)}{\partial x} + \frac{1}{2} \frac{(\Delta x)^2}{\Delta t} \frac{\partial^2 p(x,t)}{\partial x^2}$$

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Defining

$$D = \lim_{\Delta x, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} \qquad v = \lim_{\Delta x, \Delta t \to 0} (2p-1)\frac{\Delta x}{\Delta t}$$

and ensuring that

$$1 - 2p = \frac{v\Delta x}{2D}$$

we have

$$p = \frac{1}{2}(1 - \frac{v\Delta x}{2D})$$

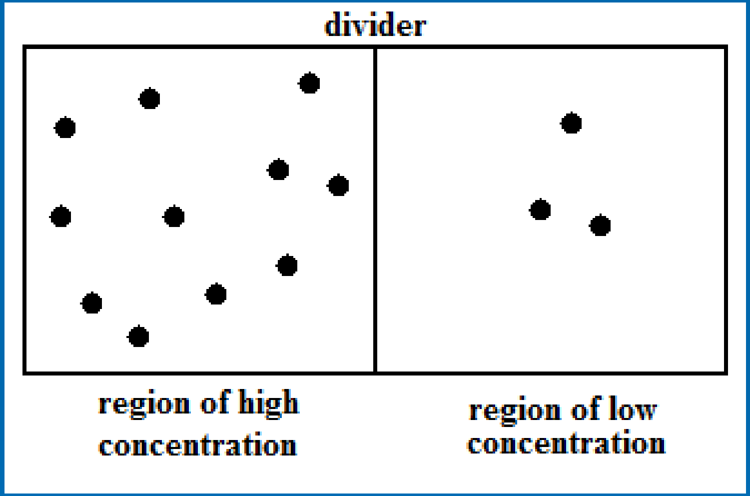
For Δx→0, p=1/2 and we arrive to the diffusion equation

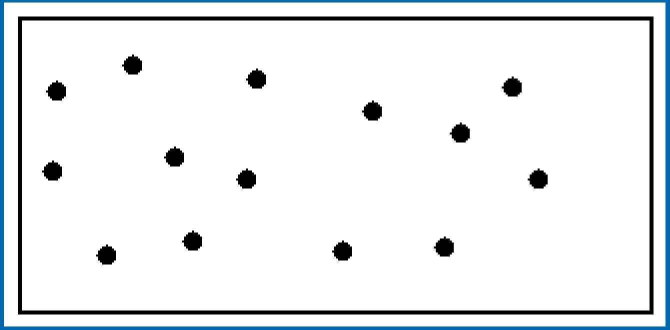
$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2} - v\frac{\partial p}{\partial x}$$

Introduction to complex science – Diffusion Theory

Relation to classical diffusion theory

In Latin, "diffundere" means "to spread out".





Removing the divider between high and low concentration region, we see that there is a flow from the former to the latter.

The flow tends to equalize the concentration.

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Fick’s Laws

First law

$$J = -v \frac{\partial \phi}{\partial x}$$

relates the diffusive flux to the concentration under the assumption of steady state

Second law

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2}$$

predicts how diffusion causes the concentration to change with time

A video showing the diffusion of colors in water

https://www.youtube.com/watch?v=o6nqYcrItiQ

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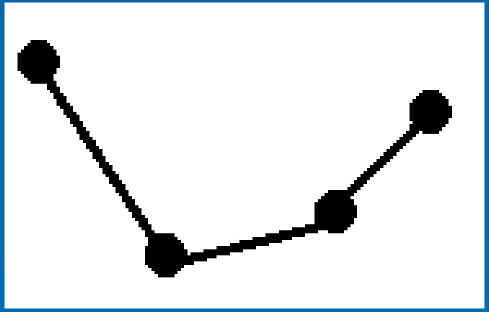
Some examples of using diffusion theory

A. Diffusion of a polymer chain in random media

Dynamic properties of a self-avoiding walk chain, which performs Brownian motion between randomly distributed impenetrable fixed obstacles, using Monte Carlo simulations



Molecule consist of beads (black circles) and links. The intersection of beads is forbidden.

Two cases investigated: (1) no intersection and (2) “weak” intersection of links

In both cases, it was proven that the diffusion process is slower than reptation and the chain diffusion is controlled by entropic barriers present in the system

M.Muthukumar and A.Baumgaertner, “Diffusion of a Polymer Chain in Random Media”,Macromolecules, vol.22, 1941-1946, 1989

Introduction to complex science – Diffusion Theory

B. Diffusion of information in a complex network

The effect of structural heterogeinity to the information diffusion is studied, using random walk methods.

By theoretical and numerical treatment, the following conclusions were drawn

Information does not distribute uniformly in heterogeneous networks

But this imposes congestion problems, because network nodes have finite capacities

The results have important implications in the design of networks such as WWW

J.D.Noh and H. Rieger, “Random Walks on Complex Networks”, PRL 92 (11), 118701, 2004

Introduction to complex science – Diffusion Theory

C .Diffusion of zooplankton

Examine the spatial distribution of motile zooplankton moving with a variety of idealized random motility modes

The model of “biodiffusion” (i.e. considering that the species diffuse normally) poorly describe the natural processes, because it captures only the dispersion and not the aggregation of the biological species under this study.

It must be taken into account the spatially varying environment

The results showed that the biological motility has been well described by the classical diffusion theory, however the behavior of biological agents cannot be treated in the same manner as molecules.

Even for a simple birth – death process, the use of concentration fields is not always successful.

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Introduction to complex science – Diffusion Theory

D. Molecular crowding and protein diffusion

Studying the diffusion of tracer proteins in highly – concentrated random-coil polymer and globular protein solutions

This setup is an simple but close to reality imitation of the conditions in cellular environments.

Results

Protein diffusion deviates from simple diffusion

Subdiffusive process

Very important for the improvement of drug delivery systems relying on the slow release of drugs from polymer matrices

D.S. Banks and C. Fradin, "Anomalous Diffusion of Proteins Due to Molecular Crowding", Biophys. Journal, vol 89, 2960, 2005

Introduction to complex science – Phase Transition

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D.S. Banks and C. Fradin, "Anomalous Diffusion of Proteins Due to Molecular Crowding", Biophys. Journal, vol 89, 2960, 2005

Introduction to complex science – Percolation

Outline

1. Historical Background
2. What is percolation – Why we study percolation?
3. Random percolation variants
4. Other types of percolation
5. Percolation theory
    - General
    - Scaling relations
    - Results at infinity
    - General properties of critical exponents
    - Results for the networks
    - General comments
    - Finite size effects

Bibliography for percolation theory

Percolation-Historical background

Paul Flory describes by means of statistics the vulcanization of rubber

[P.J. Flory, J. Am. Chem. Soc. ***63****, 3083 (1941) 1, 18]*

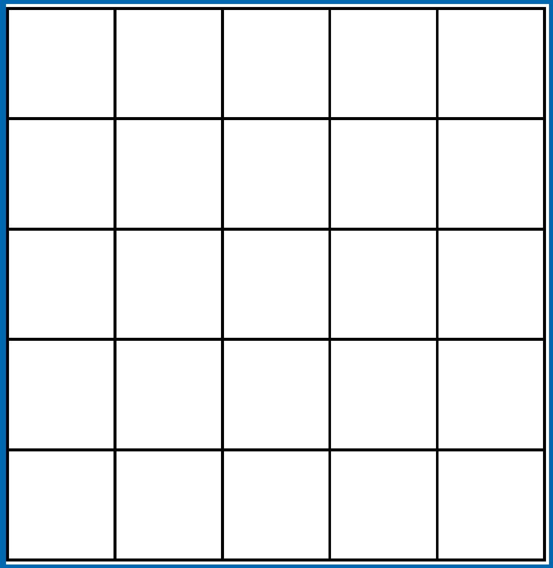
Similar treatment to the Cayley tree

***Broadbent* and *Hammersley* studied the influence of the random properties of a “medium” to the percolation of a “fluid” through it.**

*[*Broadbent S R and Hammenley J M *Proc. Camb. Phil. Soc. 53,* 629-41 (1957)*]*

Thereafter, many essays using percolation theory have been published, while the statistical properties of the model were made clear

What is percolation – Why we study percolation?



Consider an empty 2-D lattice with *L=5*

Total number of sites: 25

A site can be either occupied (with probability p) or empty (with probability 1-p)

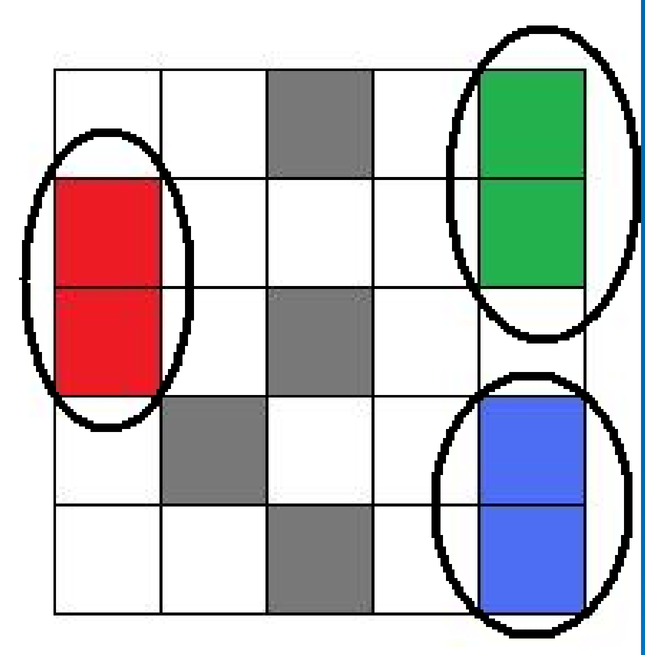
MAIN PROBLEM

Find the value of the probability p (termed p_c) for which the LxL lattice is spanned by a collection of nearest neighboring sites, forming a continuous path between the two sides of it (vertically, horizontally or both)

What is percolation – Why we study percolation?

Basic notion

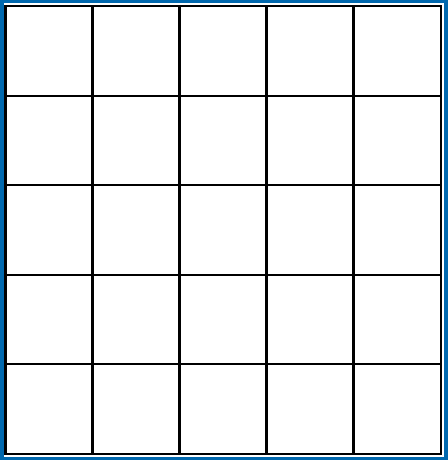
Cluster : *a set of occupied nearest neighboring sites*



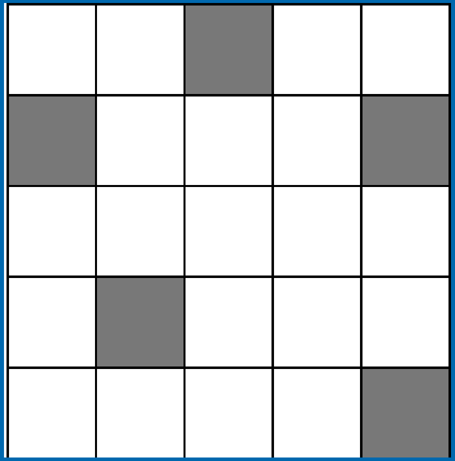
Percolation is a geometrical phase transition

Investigates the number and structure of these clusters as a function of their size

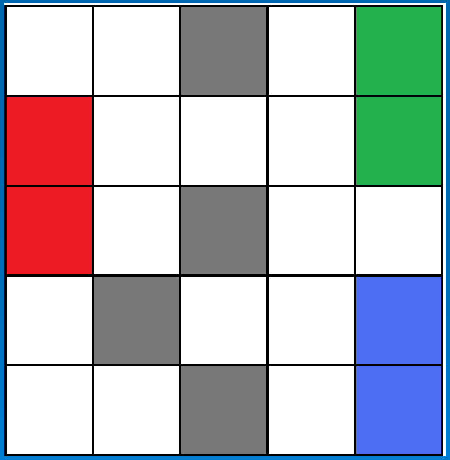
What is percolation – Why we study percolation?



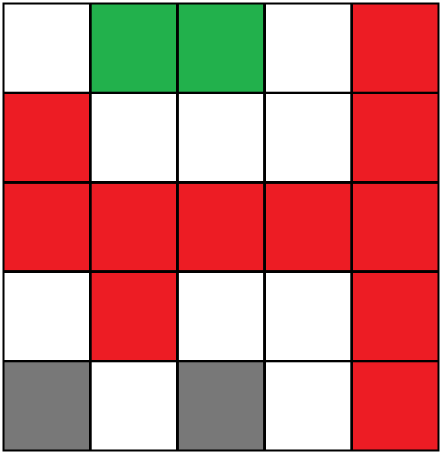
$p = 0/25$



$p = 5/25$



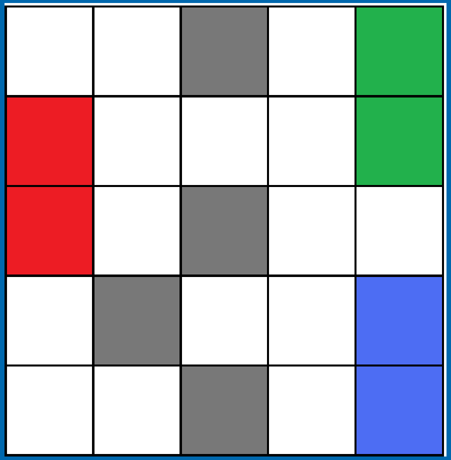
$p = 10/25$



$p = 15/25$

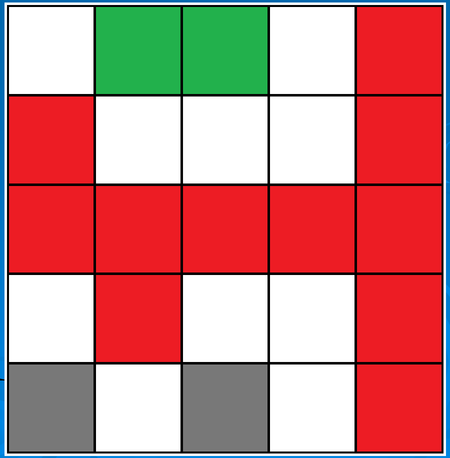
What is percolation – Why we study percolation?

From the previous figures for different values of occupation probability p, it is evident that we can divide the procedure in two regimes



1. **$p<p_c$: only small isolated clusters are formed**

Phase transition at p_c



2. **$p>p_c$: a spanning cluster exists, connecting the two vertical sides of the lattice**

What is percolation – Why we study percolation?

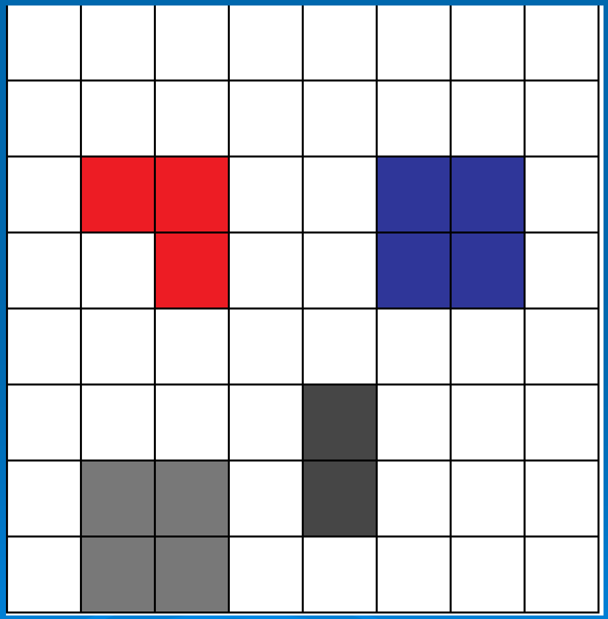
http://demonstrations.wolfram.com/PercolationOnASquareGrid/

Random percolation variants (I)

Site percolation

Each site can be either *occupied* (with probability p) or *empty* (with probability 1-p)

Bonds between all neighboring sites are present (for 2d lattice, there are 4 bonds per site)

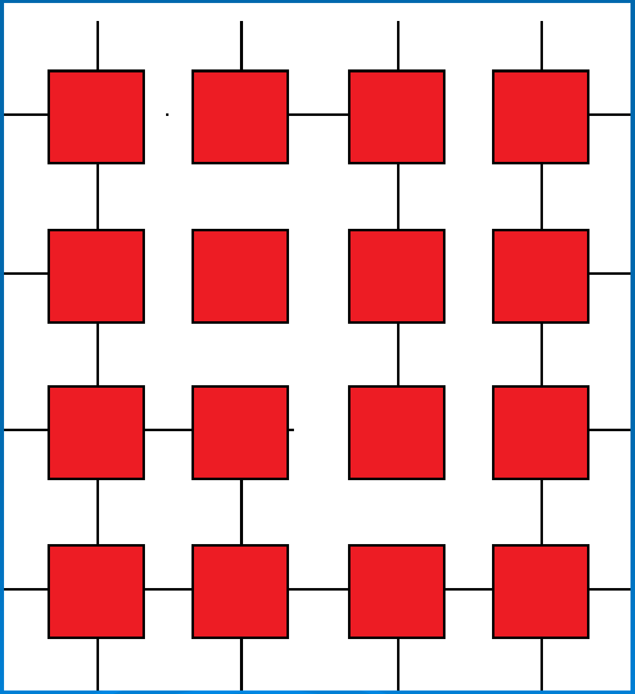


Random percolation variants (II)

Bond percolation

Each bond can be either occupied (with probability p) or empty (with probability 1-p)

<u>Sites are considered to be occupied</u>

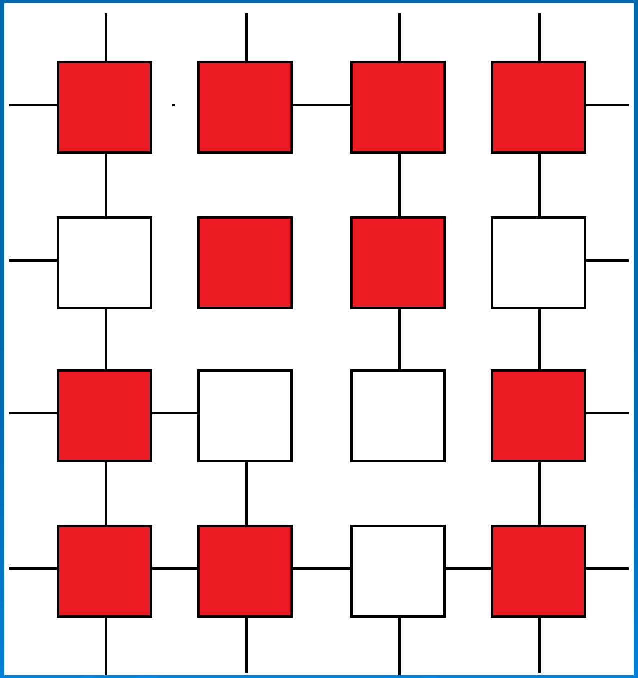


Random percolation variants (III)

Site/Bond percolation

Each site can be either *occupied* (with probability p) or *empty* (with probability 1-p)

Each bond can be either occupied (with probability q) or empty (with probability 1-q)

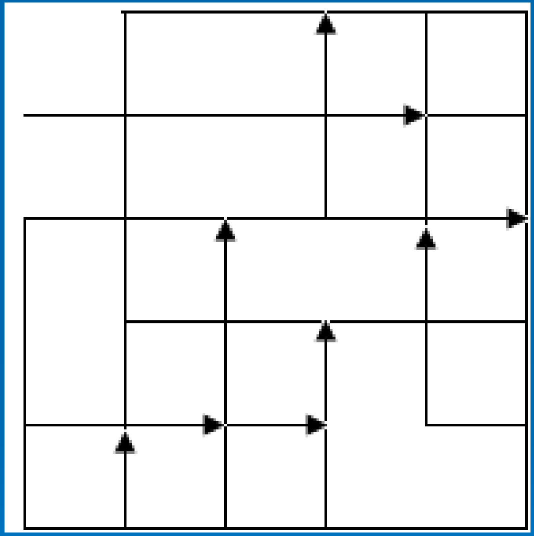


Other types of percolation

Other types of percolation

- Directed

The percolation process occurs only to a specified direction

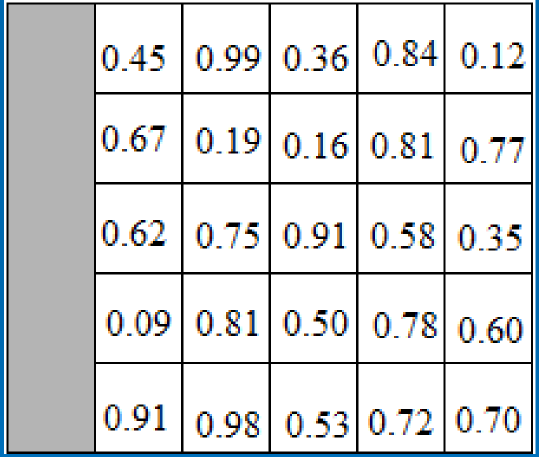


Although having a “percolating path”, we are restricted to follow the arrows, thus there is no way reaching from bottom to top.

Other types of percolation

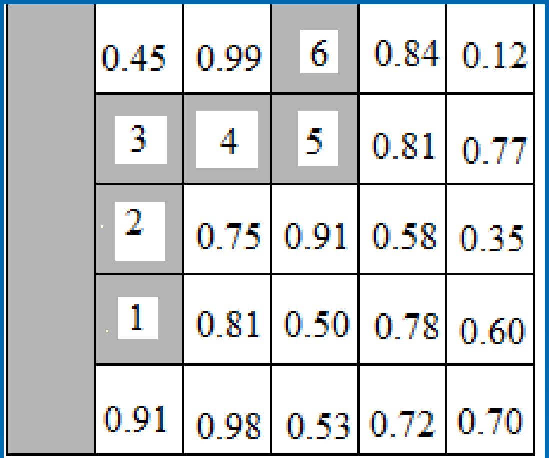
- Invasion

Proceeds by letting the displacing fluid grow each time step by occupying the accessible site along the front having the smallest random number.



	0.45	0.99	0.36	0.84	0.12
	0.67	0.19	0.16	0.81	0.77
	0.62	0.75	0.91	0.58	0.35
	0.09	0.81	0.50	0.78	0.60
	0.91	0.98	0.53	0.72	0.70

Initially



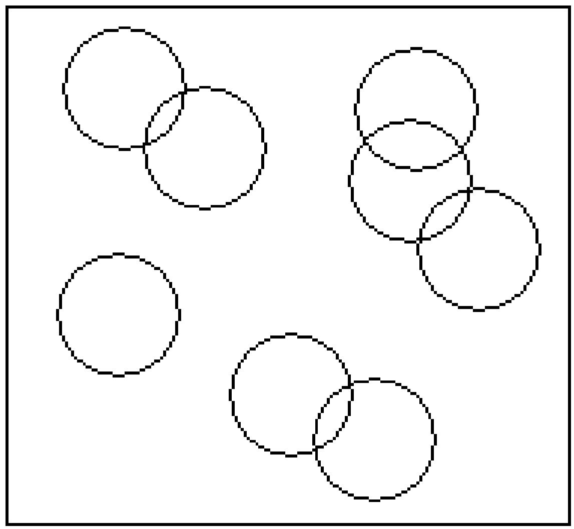
	0.45	0.99	6	0.84	0.12
	3	4	5	0.81	0.77
	2	0.75	0.91	0.58	0.35
	1	0.81	0.50	0.78	0.60
	0.91	0.98	0.53	0.72	0.70

After 6 steps

Other types of percolation

- Continuum

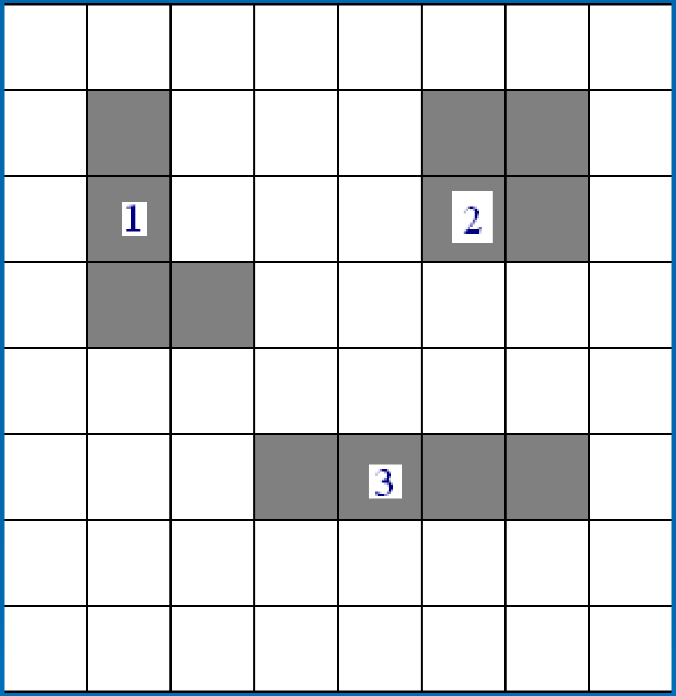
We fill the “continuum” with N identical discs, representing a predefined concentration of “mass”. The discs are randomly distributed in the medium.



They form a cluster if they overlap

Percolation theory (I)

For site percolation



$$n_s(p) = \sum_t g_{st} p^s (1-p)^t$$

Here we have s=4, but 3 different realizations (depending on t – the number of surrounding sites)

Cluster 1: t = 9

Cluster 2: t = 8

Cluster 3: t = 10

Percolation theory (II)

Percolating cluster

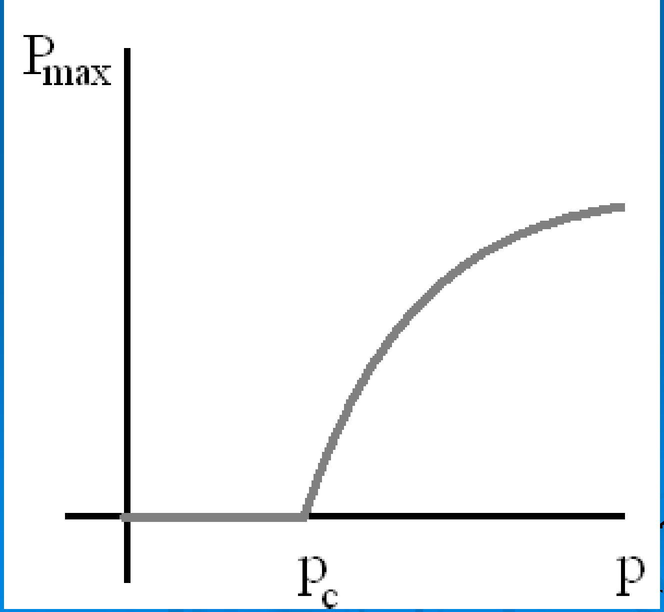
$$P_\infty = \begin{cases} 0, & p < p_c \\ P, & p > p_c \end{cases}$$

$$P_\infty + \sum_{s<s_{max}} s n_s = p$$

Mean cluster size

$$\langle s \rangle = \sum_s \frac{s^2 n_s}{\sum_s s n_s}$$

Typical transition



Percolation theory – Scaling relations (I)

Near p_c $n_s \sim s^{-\tau} f_{\pm}(|p-p_c|^{1/\sigma} s) \quad (s \to \infty, p \to p_c)$

Using

$$p = \sum_s s n_s(p) = P_\infty + \sum_s s n_s(p_c)$$
$$\Rightarrow P_\infty = \sum_s s[n_s(p) - n_s(p_c)]$$

and $z = (p-p_c)s^{\sigma}$

we arrive at

$$P_\infty = \frac{1}{\sigma} |p-p_c|^{(\tau-2)/\sigma} \int |z|^{-1-(\tau-2)/\sigma} \left[f(z) - f(0)\right] dz$$

Recalling

$$P_\infty = \begin{cases} 0, & p < p_c \\ P, & p > p_c \end{cases} \quad \Longrightarrow \quad \int |z|^{-1-(\tau-2)/\sigma}[f(z) - f(0)]dz = 0 \quad for\ p < p_c$$

Thus $P_\infty \sim (p-p_c)^{\beta} \Rightarrow \beta = (\tau-2)/\sigma$

Percolation theory – Scaling relations (II)

Mean cluster mass

$$\langle s \rangle = \sum_s \frac{s^2 n_s}{\sum_s s n_s}$$

At p_c

$$\langle s \rangle = \frac{1}{p_c} \sum_s s^2 n_s \propto \frac{1}{\sigma} |p - p_c|^{(\tau-3)/\sigma} \int |z|^{1-(\tau-3)/\sigma} f(z) dz$$

Thus

$$\langle s \rangle \propto |p - p_c|^{-\gamma} \Rightarrow \gamma = (3 - \tau)/\sigma$$

Generally

$$M_k = \sum_{s=1}^{\infty} s^k n_s(p)$$

It can be proved [BH91] that

$$M_k \sim |p - p_c|^{(\tau-k-1)/\sigma}$$

E.g.

$$M_0 \sim |p - p_c|^{2-\alpha} \Rightarrow 2 - \alpha = \frac{\tau - 1}{\sigma}$$

Percolation theory – Scaling relations (III)

Correlation length ξ : represents the average cluster radius

It is given by the relation: $\xi^2 = \sum_{s=1}^{\infty} R_s^2 s^2 n_s / \sum_{s=1}^{\infty} s^2 n_s$

Near p_c, large clusters dominate the sum, thus, taking $R_s \sim s^{1/d_f}$

and following the derivation of [BH91], it can be shown that the correlation length ξ is given by

$$\xi^2 \sim |p - p_c|^{-2/d_f\sigma}$$

Using $\xi \sim |p - p_c|^{-\nu}$ $\longrightarrow$ $\nu = \frac{1}{d_f\sigma} = \frac{\tau - 1}{d\sigma}$

Percolation theory – Scaling relations (IV)

Summarizing the critical exponent relations

$$\beta = \frac{\tau - 2}{\sigma} \qquad \gamma = \frac{3 - \tau}{\sigma} \qquad 2 - \alpha = \frac{\tau - 1}{\sigma}$$

$$\nu = \frac{1}{d_f \sigma} = \frac{\tau - 1}{d\sigma} \qquad d\nu = 2\beta + \gamma$$

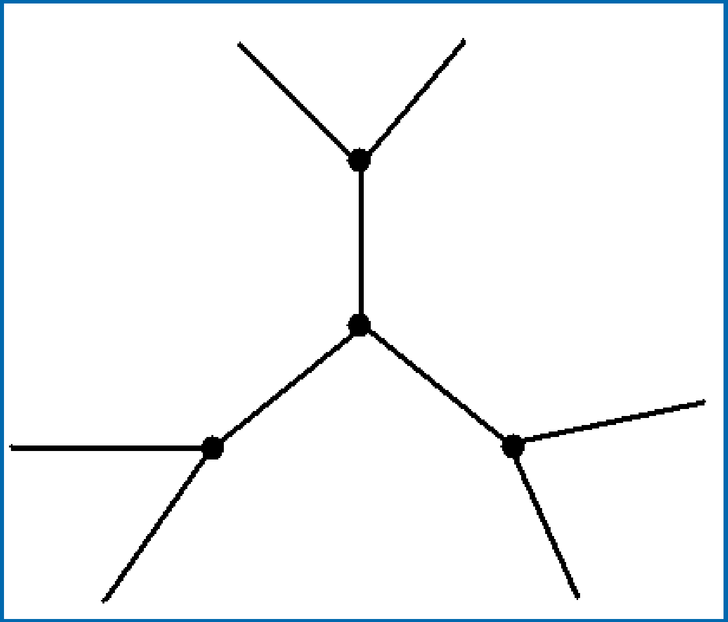
It was shown in [S85] that

$$\log n_s \sim s^{\zeta}\ , s \to \infty \ and\ \zeta = \begin{cases} 1, & p < p_c \\ 1 - 1/d, & p > p_c \end{cases}$$

Percolation theory – results at infinity (I)

Cayley tree

$$p_c = \frac{1}{z-1}$$



It can be shown that [BH91]

$$\xi_l \sim |p - p_c|^{-1} \Rightarrow \nu = 1$$

Using $n_s(p) \sim n_s(p_c) f_s(p), \quad p \to p_c$ **and** $f_s(p) \sim exp(-cs), \quad s \to \infty$

with $c \sim (p - p_c)^2 \sim (p - p_c)^{1/\sigma}$ → $\sigma = 1/2$

Also $\langle s \rangle \sim (p_c - p)^{-1}$ → $\gamma = 1$

Percolation theory – results at infinity (II)

Using the previous scaling relations we get for the rest of the critical exponents

$$\gamma = \frac{3-\tau}{\sigma} \Rightarrow \tau = 3 - \sigma\gamma \quad \Longrightarrow \quad \tau = 5/2$$

$$\beta = \frac{\tau - 2}{\sigma} \quad \Longrightarrow \quad \beta = 1$$

$$2 - \alpha = \frac{\tau - 1}{\sigma} \quad \Longrightarrow \quad \alpha = -1$$

These exponents are valid for all lattices in d > d_c=6 dimensions

Percolation theory – general properties of critical exponents

For two different 2-D configurations, it is proven that

$$p_{c_{site}}^{square} = 0.5927$$

$$p_{c_{site}}^{trianglular} = 0.5$$

Also, for <u>site</u> and <u>bond</u> percolation on a square 2-D lattice, we have:

$$p_c^{site} = 0.5927$$

$$p_c^{bond} = 0.5$$

However, for the critical exponents, we have

d	*β*	*γ*	*ν*
2	5/36	43/18	4/3
3	0.41	1.796	0.88
≥ 6	1	1	1/2

Exponents α, σ and τ can be calculated by the previous scaling relations

Percolation theory – results for the networks (I)

The critical exponents of Erdos Renyi Networks are the same as those of a Cayley tree (or generally, of an infinite dimensional lattice)

Using generating functions formalism, the following relations can be proven for Scale Free Networks (γ,m) [CH10]

<u>Be careful</u>: only valid when there is no degree – degree correlations

$$P_\infty \sim (p-p_c)^\beta \quad \Longrightarrow \quad \beta = \begin{cases} \frac{1}{3-\gamma} & ,2<\gamma<3 \\ \frac{1}{\gamma-3} & ,3<\gamma<4 \\ 1 & ,\gamma>4 \end{cases}$$

$$P_\infty = a(\gamma)(p-p_c)^\beta = \begin{cases} a(\gamma)\to const \quad as\ \gamma\to 4 \\ \\ a(\gamma)\to\infty \quad as\ \gamma\to 4 \end{cases}$$

Note that $p_c = 0$ for γ<3

Percolation theory – results for the networks (II)

$$n_s \sim s^{-\tau} \exp\left(-s/s^*\right), \quad s^* \sim |p - p_c|^{-\sigma}$$

$$\tau = \begin{cases} 3, & 2 < \gamma < 3 \\ 2 + \frac{1}{\gamma - 2}, & 3 < \gamma < 4 \\ \frac{5}{2}, & \gamma > 4 \end{cases}$$

$$\sigma = \begin{cases} \frac{3-\gamma}{\gamma-2}, & 2 < \gamma < 3 \\ \frac{\gamma-3}{\gamma-2}, & 3 < \gamma < 4 \\ \frac{1}{2}, & \gamma > 4 \end{cases}$$

Giant component

$$S \sim N^{\frac{1}{\tau}-1} = N^{\frac{\gamma-2}{\gamma-1}}$$

$$S \sim \begin{cases} N^{2/3}, & \gamma = 4 \\ N^{1/2}, & \gamma \to 3 \end{cases}$$

No meaningful interpretation for γ<3

Percolation theory – general comments

In general, the critical exponents for ordinary random percolation depend on the dimensionality (d) and NOT on the lattice structure

Universality means that we can investigate the simplest of a collection of systems that has the same critical properties

Percolation theory – finite size effects

For a finite system *L x L*, every quantity which scales like

$$X \sim |p - p_c|^x$$

near p_C, can be written as

$$X = L^{x/\nu} F[L^{1/\nu}(p - p_c)]$$

For example [TMKA10]

$$P_{max} = L^{-\beta/\nu} F[L^{1/\nu}(p - p_c)] \qquad \langle s \rangle = L^{-\gamma/\nu} F_1[L^{1/\nu}(p - p_c)]$$

Thus, calculating the values of X at p_c for different values of L, one can numerically estimate the critical exponents

[more about this in the mid level programming course]

Bibliography for percolation theory

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