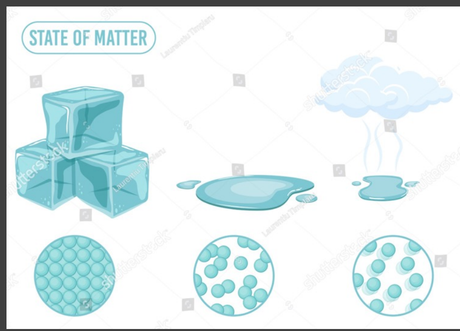

Introduction to Phase Transitions & Critical Phenomena

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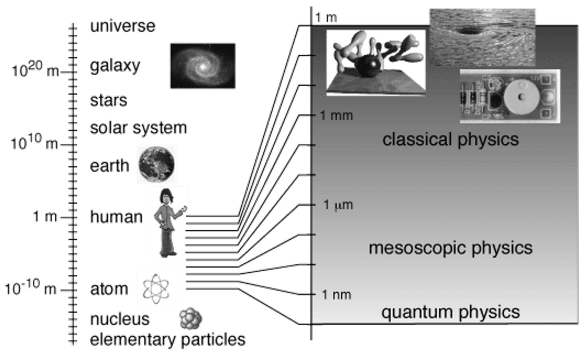


Physics

A Physicist observes and imagines theories to describe phenomena at all length scales (Feynman).

The infinitely small and the infinitely large are beyond the reach of everyday experience and require massive teams, and formidable equipment.

2

Condensed matter physics

The understanding of phenomena at our scale is the challenge of condensed matter Physics, where the balance between order and disorder determines the structure and the properties of all phases of matter, including living matter.

3

Program

The macroscopic properties of condensed matter may be studied by looking at its microscopic constituents and their interactions and determining how these produce observable effects at much larger length scales.

Large numbers of particles (electrons, atoms or even colloids) are moving and interacting with one another. The proper dynamics (e.g., quantum or classical) with the appropriate interactions (e.g., Coulomb between the electrons in solids or effective interactions between colloids) can give an "exact" description of the macroscopic properties.

4

Problem & Solution

These equations are generally intractable.

Therefore, in condensed matter Physics a coarse-grained description is often sought through the methods of statistical physics, where the macroscopic properties **emerge** from the interactions among the microscopic constituents or degrees of freedom.

5

Emerging properties

Condensed matter is characterized by a large number of interacting particles and emerging properties.

For example, the rigidity of solids and the fluidity of liquids are emerging properties. The values of these properties may differ, but solids are rigid while fluids flow. The rigidity is thus a robust property of solids. It depends on the order of the particles in the solid rather than on their specific interactions. The same could be said about the fluidity of liquids.

6

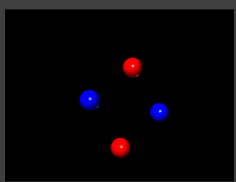
Solids are rigid

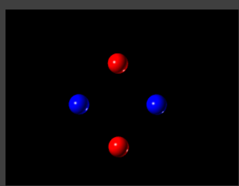
The rigidity depends on the order of the particles in the solid rather than on their specific interactions.

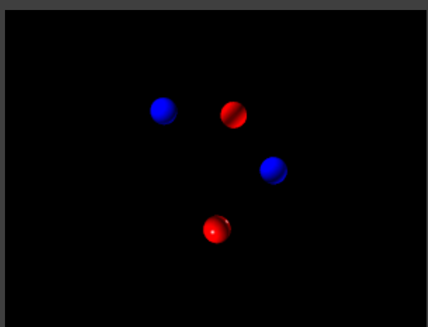
One defect does not destroy the global order.

Rigidity is an emerging property.

7







Phases of matter

Solids and liquids are different states or phases of matter, corresponding to different types of order of their constituents.

In this sense the states or phases of condensed matter are also emerging properties.

The interactions are responsible for the emergence of new states, which are **different from combinations of states of the individual components**.

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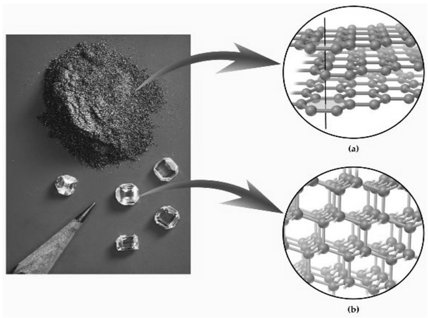

Crystalline order(s)

Different states have different physical properties and these are essentially determined by the order or molecular arrangement of each state (symmetry).

Diamond and graphite are both solid at room temperature and have the same chemical composition (carbon), but have different physical properties, which are due **exclusively to a different molecular arrangement (or symmetry).**

9

Crystalline state

The interactions between atoms and molecules are electrostatic and can be quite complicated. However, the effects of these interactions on the organization of a large number of particles are surprisingly simple.

Isolated systems with many interacting atoms or molecules exhibit equilibrium states that are more orderly the lower the temperature.

The crystalline state results from breaking the balance between order and disorder and it exhibits properties that are not the properties of the individual atoms, e.g., phonons.

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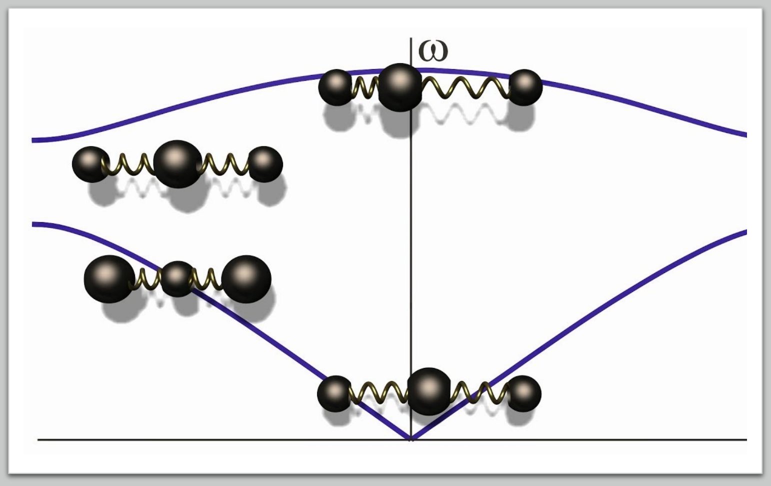

Phonons are collective vibrational states

Acoustical phonons excited by heat or sound and optical phonons excited by light

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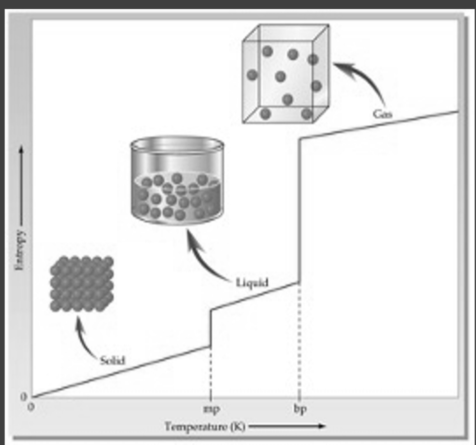
Thermodynamics



A macroscopic system is composed by 10^{23} particles. The particles interact, bond and collide. The number of interactions at play, at any one time, is unimaginable. How can we predict the structure and the properties of this system?

Macroscopic systems at thermal equilibrium have an extremely simple behavior described by the laws of thermodynamics.

For example, the second law, or the principle of maximum entropy, *S*, tells us that the stable state of a system with constant volume, at temperature *T*, is determined by the state that minimizes free energy *F*,

$$F = E - TS$$

where *E* is the energy (sum of the kinetic and potential energy) of the system. The stability of the solid or gas derives from this principle and the fact that matter is made up of atoms.

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Stability of solids & gases

The crystalline solid is the stable state at low temperatures and high densities, since energy is minimized by the molecular order - the interatomic potential has a minimum, for a well-defined distance, and the crystal is constituted by the periodic spatial arrangement that minimizes the potential energy of the system.

In a similar way, it is concluded that the gas is stable at high temperatures and low densities, where the interaction energy is negligeable and the entropy is maximized by the molecular disorder.

13

Phase Transitions

The argument is general and can be used to show the existence of phase transitions. The two phases, in this case the crystalline solid and the gas, have different symmetries.

At the macroscopic scale, the gas is characterized by **continuous translation symmetry** (all points are equivalent from the point of view of their physical properties), while the crystalline solid has **discrete translation symmetry** (the equivalent points are those related by a discrete translation group: the Bravais lattice).

Since the solid is stable at low temperatures and the gas is stable at high temperatures, the system must necessarily exhibit at least one phase transition.

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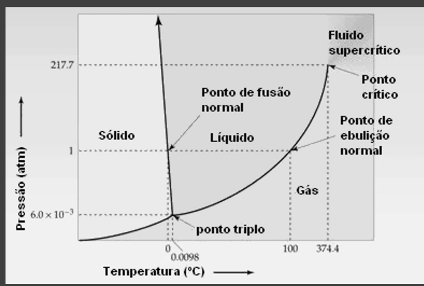
The liquid state

Unlike the solid and the gas, the liquid is stable over a temperature range limited by the triple point (where the solid, the liquid and the gas coexist) and the critical point, where the condensation line ends, along which liquid and gas coexist.

The critical point between the liquid and the gas is an example of a **continuous phase transition**, that is, a transition that does not involve latent heat.



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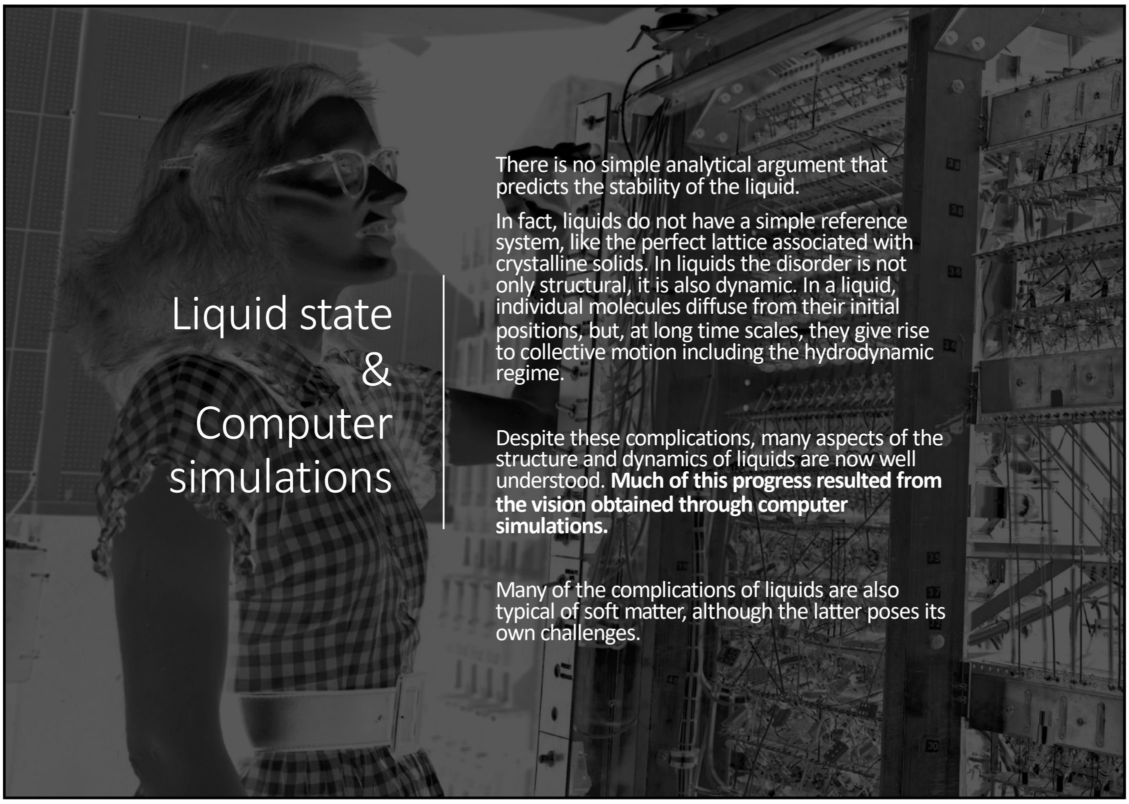


Liquid state & Computer simulations

There is no simple analytical argument that predicts the stability of the liquid.

In fact, liquids do not have a simple reference system, like the perfect lattice associated with crystalline solids. In liquids the disorder is not only structural, it is also dynamic. In a liquid, individual molecules diffuse from their initial positions, but, at long time scales, they give rise to collective motion including the hydrodynamic regime.

Despite these complications, many aspects of the structure and dynamics of liquids are now well understood. **Much of this progress resulted from the vision obtained through computer simulations.**

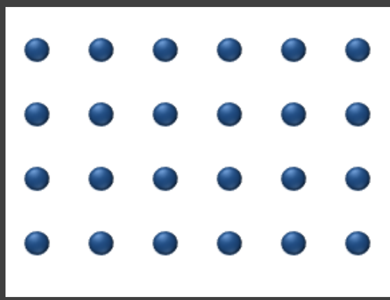
Many of the complications of liquids are also typical of soft matter, although the latter poses its own challenges.

16

Thermal fluctualtions

Thermal fluctuations are random deviations of a system from its average state, that occur in a system at equilibrium. All thermal fluctuations become larger and more frequent as the temperature increases, and likewise they decrease as temperature approaches absolute zero.

Thermal fluctuations are a basic manifestation of the temperature of systems: A system at nonzero temperature does not stay in its equilibrium microscopic state, but instead randomly samples all possible states, with probabilities given by the Boltzmann distribution.



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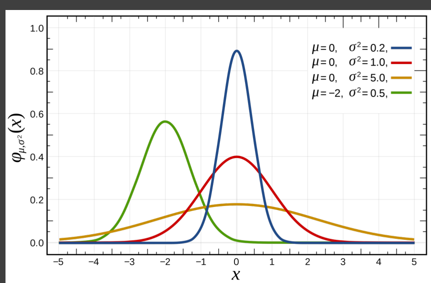
Gaussian distribution

Thermodynamic variables, such as pressure, temperature, or entropy, undergo thermal fluctuations. For example, for a system that has an equilibrium pressure, the system pressure fluctuates to some extent about the equilibrium value.

Only the 'control variables' of statistical ensembles (such as the number of particles N, the volume V and the internal energy E in the microcanonical ensemble) do not fluctuate.

For large systems at equilibrium the central limit theorem aplies and the distribution of the thermal fluctuations is a sharply peaked Gaussian.



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$T > T_c$ $T = T_c$ $T < T_c$

Critical fluctuations

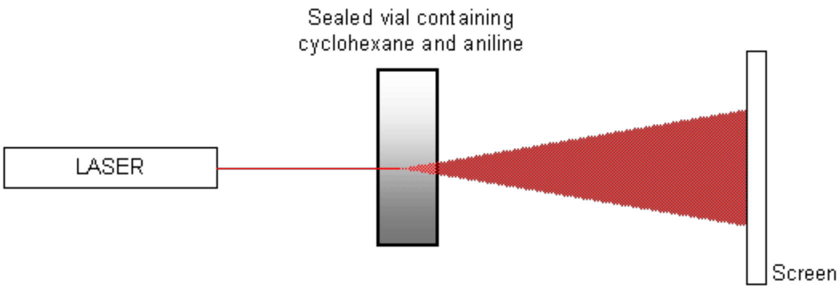
Thermal fluctuations play a major role in continuous phase transitions. The understanding that the fluctuations become non-Gaussian had enormous impact in condensed matter Physics, where new paradigms were introduced.

The understanding of fluctuations at all length scales in critical phenomena led to the development of a profound theory, the renormalisation group theory. The theory provides a microscopic understanding of **scaling and universality**, observed experimentally, and established the concepts of **broken symmetry and order parameters** as unifying theoretical concepts to describe condensed matter phases ranging from periodic solids to disordered systems, including simple fluids, liquid crystals and polymers.

19

Critical Opalescence

Image of the vial and image on the screen as the laser beam passes through the vial when the mixture is cooled through the critical point.



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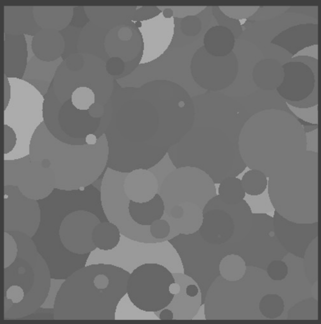
Scaling & Scale invariance

Close to the critical point of a fluid, matter fluctuates on every scale. Bubbles and droplets, some as small as a few atoms, others as large as the container, appear and disappear, coalesce and separate.

At exactly the critical point, the scale of the largest fluctuations diverges, but the effect of fluctuations on smaller scales is not negligible. The standard deviation of the equilibrium Gaussian distribution diverges (we say that the correlation length, which is a measure of the extent of correlated fluctuations, diverges) and the distribution of the fluctuations becomes non-Gaussian.

This critical distribution lacks a characteristic scale and as a result the distribution function is invariant for scale transformations. This implies, in turn, that the theory is scale invariant.



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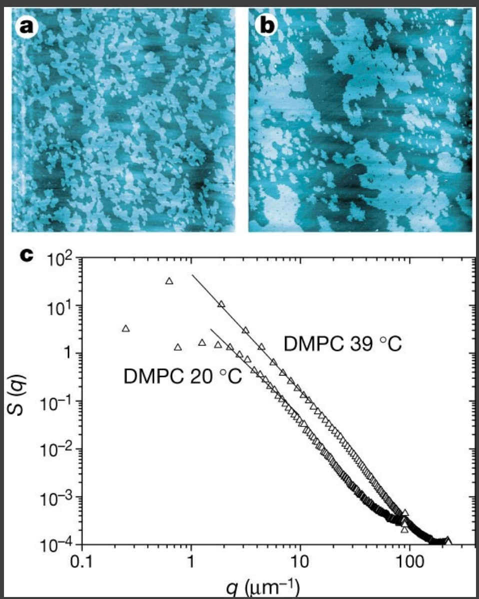


Power law behaviour of the Structure factor, S(q)

S(q) relates the observed diffracted intensity per atom to that produced by a single scattering unit.

For fluids, it is the Fourier Transform of the radial distribution function, g(r).

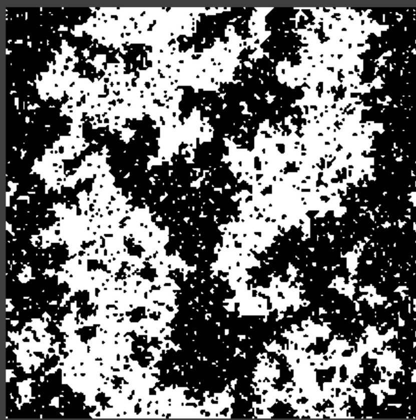
22

Universality

In the early 1970s, K. Wilson proposed a theory for critical phenomena called the renormalization group theory.

The theory that earned Wilson the Nobel Prize in Physics in 1982 allowed the description of the behavior of systems close to the critical point, including the calculation of the critical exponents.

One of the most important results of the theory is the prediction of **the existence of universal classes that do not depend on the details of microscopic interactions, but only on their symmetry.**



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Ferro to paramagnetic phase transition

The paradigm of continuous phase transitions is the transition from the paramagnetic state of iron to the ferromagnetic state, at the Curie temperature, T_c = 1043 K.

The spin of each iron atom has a particular orientation, corresponding to the direction of its local magnetic field.

Above T_c, the spins point in different directions and their magnetic fields are canceled. This disordered configuration is caused by the random thermal movement of the spins. The higher the temperature, the more difficult it is for any orderly arrangement of spins to be maintained.

However, when the temperature drops, the spins align spontaneously. Instead of canceling each other out, the individual magnetic fields are added, producing a macroscopic magnetic field.

At T_c critical fluctuations lead to scaling and universality, i.e., the same power laws describe different ferromagnets.

24

Universality class

Results of the RG studies showed that when the scale changes, the equations that describe the system change in such a way, that in the thermodynamic limit only some aspects of the system are relevant.

The discovery of this universality implies the existence of deep mechanisms, generally simple, responsible for the behavior of critical systems.

In particular, the theory predicts that both fluids and (uniaxial) magnets have the same critical behavior.

Universality is also observed in soft matter and other systems even out of equilibrium.

25

Universality classes

class	dimension	Symmetry	α	β	γ	δ	ν	η
3-state Potts	2	S3	1/3	1/9	13/9	14	5/6	4/15
Ashkin-Teller (4-state Potts)	2	S4	2/3	1/12	7/6	15	2/3	1/4
Ordinary percolation	1	1	1	0	1	∞	1	1
	2	1	−2/3	5/36	43/18	91/5	4/3	5/24
	3	1	−0.625(3)	0.4181(8)	1.793(3)	5.29(6)	0.87619(12)	0.46(8) or 0.59(9)
	4	1	−0.756(40)	0.657(9)	1.422(16)	3.9 or 3.198(6)	0.689(10)	−0.0944(28)
	5	1	≈ −0.85	0.830(10)	1.185(5)	3.0	0.569(5)	−0.075(20) or −0.0565
	6+	1	−1	1	1	2	1/2	0
Directed percolation	1	1	0.159464(6)	0.276486(8)	2.277730(5)	0.159464(6)	1.096854(4)	0.313686(8)
	2	1	0.451	0.536(3)	1.60	0.451	0.733(8)	0.230
	3	1	0.73	0.813(9)	1.25	0.73	0.584(5)	0.12
	4+	1	−1	1	1	2	1/2	0
Ising	2	Z2	0	1/8	7/4	15	1	1/4
	3	Z2	0.11008(1)	0.326419(3)	1.237075(10)	4.78984(1)	0.629971(4)	0.036298(2)
XY	3	O(2)	-0.01526(30)	0.34869(7)	1.3179(2)	4.77937(25)	0.67175(10)	0.038176(44)
Heisenberg	3	O(3)	−0.12(1)	0.366(2)	1.395(5)		0.707(3)	0.035(2)
Mean field	all	any	0	1/2	1	3	1/2	0

26

Collective behaviour

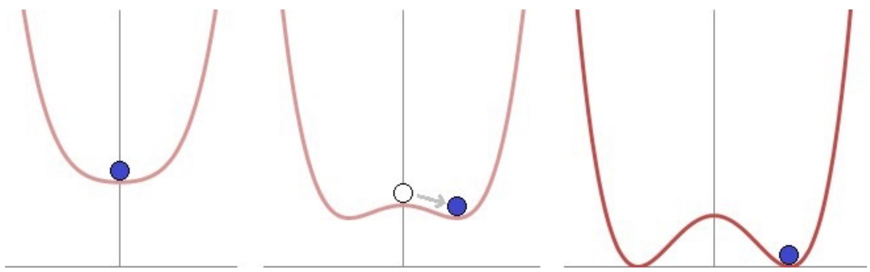
Discoveries made in the context of critical phenomena are applied in areas of the natural sciences, where collective effects play a decisive role: **polymer physics uses ideas and methods from the theory of critical phenomena, the theory of percolation (geometric critical phenomena) is applied to the description of gel transitions, and there are striking analogies between phase transitions at equilibrium and processes of self-organization out of equilibrium (including in active systems).**

The world around us is full of phenomena where the language of thermodynamic, dynamic or geometric phase transitions seems to be the most appropriate.

27

Spontaneous symmetry breaking

On the left the ball settles in the center, and the result is symmetric. On the right, the symmetric potential enforces an asymmetric outcome, since eventually the ball must rest at some random spot on the bottom, "spontaneously," and not at the other.



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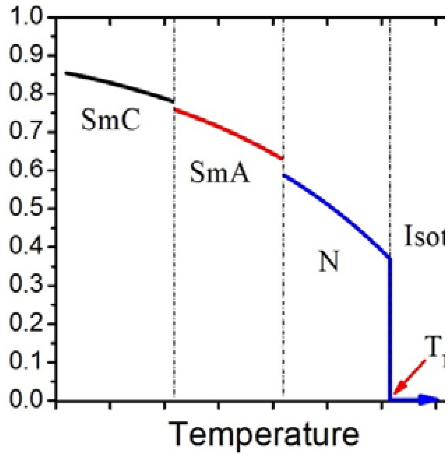
Order parameter

Phases of matter, such as crystals and magnets can be described by spontaneous symmetry breaking.

For ferromagnets, the laws are invariant under spatial rotations. Here, the order parameter is the magnetization. Above the Curie temperature, the order parameter is zero, which is spatially invariant, and there is no symmetry breaking. Below the Curie temperature, however, the magnetization acquires a constant nonvanishing value, which points in a certain direction. The rotation which does not leave this state invariant is spontaneously broken.

The laws describing a solid are invariant under the full Euclidean group, but the solid spontaneously breaks this group down to a space group. The displacement and the orientation are the order parameters.



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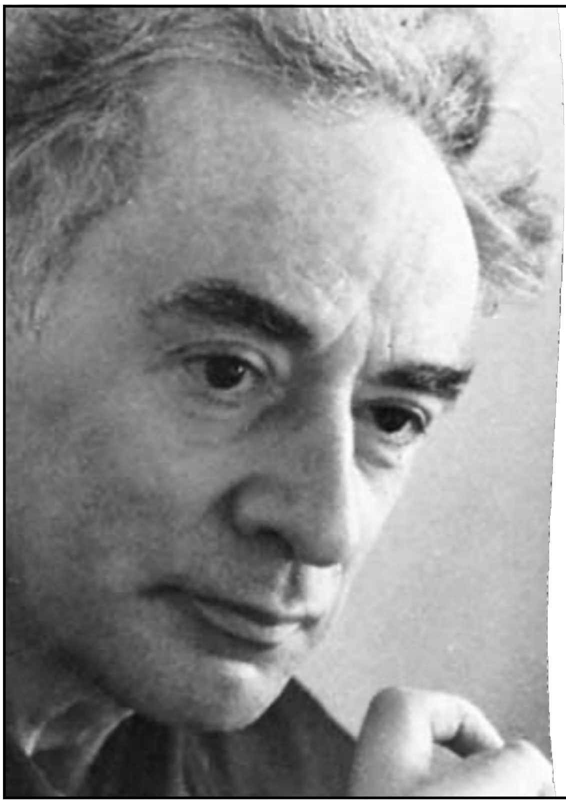

Landau Theory

Most phases can be understood through the lens of spontaneous symmetry breaking. For example, crystals are periodic arrays of atoms that are not invariant under all translations (only under a small subset of translations by a lattice vector). Magnets have north and south poles that are oriented in a specific direction, breaking rotational symmetry. In addition to these examples, there are a whole host of other symmetry-breaking phases of matter — including nematic phases of liquid crystals, and many others in soft matter and beyond.

Lev Landau introduced a framework in an attempt to formulate a general theory of continuous (i.e., second-order) phase transitions. This theory can be extended to systems under externally-applied fields and used as a quantitative model for discontinuous (i.e., first-order) transitions.

Other generalizations include vector and tensor order parameters, appropriate to describe polar and nematic ordered phases. More complicated ordered phases, with two or more coupled order parameters may also be considered, and the generalized Landau theory is a useful tool to understand the structure of complex soft matter phases.

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Objetivos

Fornecer aos alunos os conceitos e os métodos de análise das transições de fase contínuas. A aprendizagem baseia-se na resolução de problemas e na simulação computacional de modelos de percolação e de modelos de Ising e termina com uma introdução aos modelos de criticalidade auto-organizada.

Programa

- Percolação
  - Introdução
  - Percolação em d=1
  - Percolação na rede de Bethe
  - Percolação em d=2
  - Distribuição de agregados: Escalamento
  - Propriedades geométricas dos agregados
  - Efeitos de tamanho finito
  - Universalidade
  - Renormalização no espaço real
- Modelo de Ising
  - Introduçao
  - Spins independentes
  - Modelo de Ising em d=1
  - Teoria de campo médio
  - Teoria de Landau
  - Escalamento de Widom
  - Universalidade
  - Renormalização no espaço real
  - Grupo de renormalização de Wilson
- Criticalidade auto-organizada

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Nuno Araújo

e

Margarida Telo da Gama

Sala 8.2.04

- **Avaliação**

50%: 5 conjuntos de exercícios (2 de Percolação e 3 de Transições de Fase térmicas).

Submetidos de duas em duas semanas.

Os exercícios devem ser discutidos com o docente ou avaliados nas TPs.

Para cada conjunto de exercícios a avaliação tem em conta a resolução escrita e a sua discussão.

50%: projeto de Transições de Fase

- **Bibliografia**

Principal

Complexity and Criticality, de K Christensen e N R Moloney (World Scientific) 2005: K Christensen e N R Moloney 2005

- **Horário**

Quarta 15h00-16h00 (T)   Sexta 11h00-13h00 (T&TP)

Ou de preferência tutoriais na Quarta das 15h00-18h00, no meu gabinete.

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