# Introduction and Overview of Phase Transitions

In this lecture we try to motivate the study of phase transitions and identify the most important questions we address in this course.

### What's there to be done - and how?

Most objects in the World - big and small - consist of many elementary particles or degrees of freedom. The fundamental physics laws describing these are known: we have to solve a Newton's or Schrödinger equation for 10<sup>23</sup> atoms. Given today's ultra fast computers, what could be easier? Is there anything "fundamental" to learn about large bodies such as an ice cube in your Coke, or a gas bubble in your Pilsner beer? From the "**atomistic**" point of view the answer seems - NOT!

#### Problems with "brute force" approach

- It takes too much time, and the results are **too complicated** (no hard disk can store positions of 10<sup>23</sup> atoms)!
- Have to calculate over and over again for **every** material, chemical composition, lattice structure. So boring and hard!

## SEARCH FOR SIMPLICITY

But is the task of understanding macroscopic bodies in a simple way indeed so hopeless? Surely **NOT**! We know from everyday experience that general, rough features of most microscopic objects are quite similar. There seem to be only a **few** basic states of matter **phases**, that are **qualitatively different**.

Some phases that we will discuss include: solids, liquids, gases, plasmas, ferromagnets, antiferromagnets, superconductors, superfluids,...the list is long. The material properties of matter in each phase is different, since the atoms (or other particles and degrees of freedom involved) are **ordered** in a different fashion.

As we vary parameters such as the temperature, pressure, external magnetic or electric fields the system can experience sudden change from one phase to another - a **phase transition**. In this course our goal will be to understand what gives rise to phase transitions, and describe the behavior in their vicinity.

#### PREDICTIVE POWER OF THEORY

Laziness and doing stupid things can have a great virtue

Lao-Tseu, Ancient Chinese Philosopher, 570-490 B.C.

If one looks at a material in great detail with many experimental probes, one always finds differences. For example, the detailed temperature dependence of response functions such as the specific heat or the magnetic susceptibility will depend on many material details, if one considers a broad parameter range. Since our knowledge of many details, as well as our computational ability are limited, it is generally a hopeless task to attempt a theoretical understanding of every little feature. Estimates can be made, but the predictive power of theory in such cases is limited.

The situation is more under control if one asks simpler questions, such as the qualitative forms of physics laws. For example, if one is interested in quantifying the ordering of local degrees of freedom, one tries to measure (experiments) or calculate (theory) some correlation function. For example, in a magnetic system we consider a spin-spin correlator

$$\chi(\mathbf{r} - \mathbf{r}') = \left\langle S(\mathbf{r}) S(\mathbf{r}') \right\rangle,\,$$

where the brackets  $\langle ... \rangle$  indicate thermal (or time) averages over all different configurations of the local magnetic moments (spins)  $S(\mathbf{r})$  at site  $\mathbf{r}$ . In a high temperature (paramagnetic, i.e. thermally disordered) state, the correlations decay rapidly with distance  $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ 

$$\chi(\mathbf{R}, T > T_c) \sim \exp\{-\mathbf{R}/\xi\}.$$

The correlation length  $\xi$  grows in a powerlaw fashion as the phase transition is approached

$$\xi(T) \sim \left(T - T_c\right)^{-\nu}.$$

In this expression, the **critical exponent**  $\nu$  describes the divergence of  $\xi$  near the critical temperature  $T_c$ . Another example is the "anomalous dimension"  $\eta$  describing the spatial

correlations at criticality  $(\xi=\infty)$ 

$$\chi(\mathbf{R}, T=T_c) \sim \mathbf{R}^{-(d-2+\eta)}$$

Some quantities, like the value of  $T_c$  typically depend on the microscopic details of each experimental system, and as such are difficult to calculate with accuracy.

Remarkably, other quantities, such as the **critical exponents**  $\nu$  and  $\eta$  are **identical** for **many** different materials (so-called "**universality classes**"). Such quantities, which describe the approach to the critical point display **universality**, and prove to depend only on the symmetry properties of the problem and the spatial dimensionality of the material. Such quantities can be accurately calculated by simple theory, since they do not depend on knowing many material properties and details.

### CRITICAL SYSTEMS LIVE IN A FRACTAL WORLD

What are the values of the critical exponents? Simple theories based on dimensional analysis typically predict simple rational values for the exponents. For example, the Landau mean-field theory predicts  $\nu = 1/2$  and  $\eta = 0$ . Careful experiments, however, reveal strange irrational values for these exponents; e.g. for a d = 3 anisotropic (Ising) ferromagnet,  $\nu = 0.63$  and  $\eta = 0.05$ .



What does this mean? To get a glimpse at the complexity of the problem we face, and get a hint OF what may be going on, we take a look at some "snapshots" of spins in a ferromagnet, above, at, and below the phase transition.

This picture shows results of a simulation for an Ising ferromagnet, where spins can point "up" (shown as black) or "down" (while). In the ferromagnetic state ( $T < T_c$ ; left panel) most spins are "up" (black), while in the paramagnetic phase ( $T > T_c$ , right panel), the

spins are randomly oriented (gray). Here, only small clusters of aligned spins exist on scales shorter than the correlation length  $\xi \ll L$  (*L* is the systems size). Precisely **at the critical point** ( $T = T_c$ , center panel), an infinite cluster of "up" spins emerges ("percolates"); the system is at the brink of ordering.

Note that the ordered cluster has a funny "fractal" shape, with shape fluctuations on all length scales. This fractal geometry of the ordered cluster is directly reflected in strange, irrational values of the critical exponents. Clearly, simplistic theories cannot come to grips with the description of such fractal objects or their properties. Physically, the emergence of such shape fluctuations on all scales reflect the extreme lack of stability in the system at the critical point. Can we ever hope to understand this complex behavior?

### CLASSICAL OR QUANTUM MECHANICS?

When we entered kindergarten, our teachers demanded that we chant: "Laws of quantum mechanics determine the fundamental behavior of all elementary particles that make up matter". And to this day no one has proved them wrong!



Newton or Schrodinger?

At the same time, most ordered phases can be destroyed as we raise the temperature, hence the phase transitions are often driven by **thermal fluctuations**. In such cases, the critical behavior can be described using purely classical models! This is great, since classical theories are **much simpler** than quantum mechanical ones.

In other cases, the phase transitions can be driven even at strictly zero temperature, by experimentally tuning the "quantum fluctuations". For these "quantum phase transitions" the classical models are of little use, but the full theory yet remains to be completed.

#### THEORETICAL FRAMEWORK

In this course we will limit our attention to **equilibrium** statistical mechanics and phase transitions. This is sufficient in many systems, since the relaxation time (time to return to equilibrium) is very short, i.e. most systems are in equilibrium (or quasi-equilibrium). Our task will be simple: calculate the partition function of the system

$$Z(T,H,\ldots) = \sum_{n} e^{-E_n/T}$$

From this, we can calculate the free energy

$$F = -k_B T \ln Z,$$

as a function of temperature and other control parameters (pressure, external fields); from this we can calculate all thermodynamic quantities.

But how do we obtain a phase transition from this? After all, a phase transition is a **sudden** change of behavior of the system at the critical temperature. On the other hand, Z is just a sum of exponentials (Boltzmann factors  $e^{-E_n/T}$ ), which are smooth, analytic functions of temperature, external fields...We will show that not all systems can undergo sharp phase transitions, only "large", (macroscopic) systems, i.e. in the **thermodynamic** limit.

### MANY QUESTIONS TO ADDRESS...

When I arrived at FSU as a young assistant professor, I walked into the office of a very distinguished senior colleague (can you guess who?) and politely said: "Excuse me, can I ask you a physics question? Here is the answer I got:

#### "Many have tried,... but few have obtained answers!"

In this course I plan to do precisely the opposite: to answer all possible questions that students (or walkers by from the street) may want to answer.

Some important questions that we will address in technical detail, even if everyone in class is silent (I promise to tell jokes so you stay awake) include the following.

• How do we experimentally identify a critical point using scaling ideas and approaches (even if the theory is not available!).

- What quantities are universal and which ones are not? What is the origin of universality of critical phenomena?
- How are the phase transitions modified in finite systems (e.g. nuclei, nano-scale samples...)?
- How do we calculate (predict) the critical behavior? Can we understand the fractal geometry of critical objects?
- How does the critical behavior depend on the internal symmetries and dimensionality of space?
- Why is quantum mechanics unimportant in most finite temperature phase transitions, but not at T = 0?

We will start from simplest theoretical approaches using Landau mean-field theories and phenomenological scaling to gradually more sophisticated theoretical tools borrowing mathematical tricks from quantum field theory. We will develop a renormalization-group (RG) language that at present permeates the scientific jargon, and without which it becomes hard to follow and understand the results at the cutting edge of discovery.

Since this course is not intended only for theorists, but should be of interest and be accessible to a general physicist, the class presentation will not emphasize technical details, but will instead focus on physical pictures and qualitative interpretation. In order to save time in class from lengthy and boring derivations, many technical steps will be assigned as homework problems or will be left for extra-credit work.

Traditionally, courses on critical phenomena are geared towards condensed matter students. However, in recent years, active study of phase transitions has emerged in many other research areas ranging from nuclear to high energy physics. Recognizing that many of these topics represent fairly advanced material, effort will nevertheless be made to at least introduce the physical framework where phase transition ideas play a key role.

### SYNOPSIS

In this class, we hope to cover a number of topics which will include (time permitting) the following

- Experimental systems showing classical and quantum critical phenomena.
- Thermodynamic potentials. Heat capacity. Magnetic susceptibility.
- Phases. Phenomenology of 1st order phase transitions. Continuous transitions.
- Landau theory. Order parameters. Spontaneous symmetry breaking.
- Critical behavior. Scaling. Critical exponents. Relations between critical exponents.
- Kadanoff scaling. Universality conjecture.
- Calculation of critical exponents: Real space RG methods.
- RG of Wilson and Fisher,  $\phi^4$  theory,  $4 \varepsilon$  expansion.
- Continuous symmetry: Mermin-Wagner theorem.
- Non-linear sigma-model;  $2 + \varepsilon$  expansion.
- Scaling theory of localization. Asymptotic freedom in QCD.
- Topological order. Kosterlitz-Thouless phase transition. Dissipative quantum tunneling.
- Quantum critical phenomena.