

Chapter 1: Introduction

Thermodynamics tells us about the macroscopic properties of a system with a large number of particles while taking into account only a very small number of relevant quantities such as energy, temperature, volume, etc. However, as we know from many examples such as an entire lake freezing in cold weather, the macroscopic behavior can change dramatically when one of the relevant quantities changes only very slightly. If such a behavior is observed, we speak of a “phase transition”, as the state of matter of the system (also called the “thermodynamic phase”) has changed.

The investigation of phase transition is interesting mainly for two reasons. First of all, phase transitions are interesting from a fundamental point of view. A phase transition is a prime example for how systems with relatively simple dynamics on the microscopic level display highly complex behavior that emerges on much larger scales. As a result, concepts and methods first developed for the understanding of phase transitions have found applications in other areas such as particle physics, but even in fields beyond physics such as biology or economics. The other reason while phase transitions are interesting is that certain phases have important technological applications. For instance, a ferromagnet is an excellent permanent memory device used in many computer hard disks. Other examples include liquid crystals used in displays or smart glasses that change its transparency upon a change in temperature or when applying an external voltage.

I. WHAT IS A PHASE TRANSITION?

While we are familiar with the melting of ice from our daily lives, this is less so for the microscopic details of the underlying phase transition. To get a better understanding, it is helpful to first make some very general considerations. During many (but not all) phase transitions, the symmetry of the system will change. For example, a liquid exhibits translational invariance, i.e., the probability to find an atom at some point in space is the same everywhere. However, if the liquid is frozen into a crystalline solid, this is no longer the case, as a crystal has atoms only at certain fixed positions. In this case, we speak of a symmetry-breaking phase transition. Another important example is the ferromagnet-paramagnet transition at the Curie temperature of a magnetic material.

For such phase transitions, it is evident that the symmetry-broken phase exhibits a higher degree of order than the symmetric phase. We can quantify this order in terms of an order parameter, which is the magnetization m for the ferromagnet-paramagnet transition. In the paramagnetic phase, m is exactly zero, whereas it is finite in the ferromagnetic phase [1]. While this last statement looks pretty harmless, it actually has pretty dramatic consequences for how a phase transition works. Remarkably, an analytic function (i.e., representable by a power series) that is zero on a finite interval is zero everywhere. This immediately implies that the free energy of a system undergoing a phase transition cannot be analytic everywhere, as the order parameter is some derivative of the free energy. However, we can always find locally valid analytic functions for each of the phases, meaning that the analyticity is broken exactly at the phase transition. This brings us to a definition of a phase transition which actually goes beyond the notion of symmetry-breaking transitions: A phase transition occurs whenever the free energy exhibits nonanalytic behavior.

A consequence of this definition is that phase transitions can only occur in the thermodynamic limit of infinite system sizes. For finite systems, the partition function

$$Z = \sum_i \exp(-\beta E_i) \quad (1)$$

of a system at inverse temperature β with energy levels E_i is always analytic, as the sum contains only a finite number of terms. Hence, the free energy $F = -\beta^{-1} \log Z$ is always analytic for finite systems.

II. CLASSIFICATION

While any phase transition, classical or quantum, is accompanied by non-analytic behavior of the free energy F , there are important aspects where the nature of phase transitions can differ in a substantial way. Considering a system with generalized couplings $\{K_i\}$, then F is always a continuous function of all K_i . Phase transitions can be categorized into two different classes related to the nature of the non-analyticity of F [2]:

1. One or more $\partial F / \partial K_i$ is discontinuous across the phase boundary. Then the transition is called a “first-order phase transition”.
2. When all $\partial F / \partial K_i$ are continuous across the phase boundary the transition is referred to as a “continuous phase transition”. Often one or more of the second derivatives

$\partial^2 F / \partial K_i^2$ is discontinuous, but this is not necessarily the case. Sometimes these transitions are also called “second order phase transitions” if such a discontinuity in the second derivative is present.

Interestingly, it is even possible that the free energy is non-analytic although all its derivatives are continuous. Such transitions are called “infinite-order transitions”, with the Kosterlitz-Thouless transitions in two dimensions being the most prominent example.

III. UNIVERSALITY CLASSES

As we will see later, near the critical point of a continuous transition the system becomes scale invariant. This means that microscopic details of the system become irrelevant, and the macroscopic behavior is dominated by its long-range physics, associated with a diverging length scale ξ . Mathematically, a function $f(s)$ is called scale-invariant, if it satisfies the equation

$$f(\lambda s) = c(\lambda)f(s). \quad (2)$$

Performing a series expansion around $\lambda = 1$ given by

$$f(\lambda s) = f(s) + \frac{df}{ds}s(\lambda - 1) + O([\lambda - 1]^2) = c(\lambda)f(s), \quad (3)$$

one can see that the resulting differential equation has solutions in terms of power laws $f \sim s^\kappa$ with $c(\lambda) = \lambda^\kappa$. Hence, near the critical point all observables can be described by power laws of the diverging scale ξ . Since ξ itself depends on the generalized couplings K_i , we may equally express the scaling of an observable O as

$$O = O_0|K - K_c|^\kappa. \quad (4)$$

The critical exponent κ does not need to be a simple rational number. However, it was discovered that critical exponents are identical for systems completely different at the microscopic level. For example, the scaling with temperature of both the magnetization near the ferromagnetic transition and the density difference between the liquid and gas phases near the critical point of a fluid have the same highly nontrivial exponent [3]. This equivalence allows for the classification of phase transitions into universality classes with identical critical exponents.

IV. THE ISING MODEL

The two-dimensional Ising model on the square lattice is a paradigmatic model for a phase transition. Its microscopic description is quite simple, yet its properties translate to many other phase transitions as well. Each lattice site of the model carries a spin degree of freedom S_i which may take the value -1 or $+1$. Neighboring spins interact with each other according to the Hamiltonian $H_{int} = -J \sum_{\langle ij \rangle} S_i S_j$, where the negative sign indicates a ferromagnetic interaction. Then, the partition function of the Ising model is given by

$$Z = \sum_{\{S_i\}} \exp \left(K \sum_{\langle ij \rangle} S_i S_j \right), \quad (5)$$

where we have introduced the dimensionless coupling constant $K = \beta J$.

At zero temperature, the Ising model has two degenerate ground states, which are the fully polarized ferromagnetic states with all spins pointing either up or down. Importantly, the fully polarized states are examples of a symmetry-broken states, as the Hamiltonian of the Ising model does not differentiate between up and down spins (a \mathbb{Z}_2 symmetry), while the two ferromagnetic states certainly do. Does this mean we have already found a phase transition? Not quite, as the central question is what happens when the temperature is nonzero, which we shall see in a moment.

In order to see that the finite temperature properties can be vastly different from the zero temperature behavior, let us consider first the one-dimensional Ising model. The first excited state above the ground state is a domain wall excitation, i.e., a configuration of the form $\dots \uparrow\uparrow\downarrow\downarrow \dots$. A domain wall costs an energy of $2J$, as one bond of the lattice changes from $S_i S_j = -1$ to $S_i S_j = +1$. However, since there are $N - 1$ positions to place the domain wall, putting a single domain wall into the system increases the entropy by $\Delta S = k_B \log(N - 1)$. Consequently, the free energy will change by

$$\Delta F = J - \beta^{-1} \log(N - 1), \quad (6)$$

which is negative for $N \rightarrow \infty$ and $\beta < \infty$. This means that at finite temperature, the system will be filled up with domain walls until the spontaneous magnetization vanishes completely, i.e., the system is always paramagnetic at finite temperature. Note that this argument is only valid for the one-dimensional Ising model, as in higher dimensions, the energy cost of

the domain wall will depend on its size. As a consequence, there is indeed a phase transition at finite temperature in spatial dimensions larger than one [3].

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- [1] P. M. Chaikin and T. C. Lubensky, *Principles of condensed matter physics* (Cambridge University Press, Cambridge, 1995).
 - [2] N. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Perseus Books, Reading, 1992).
 - [3] K. Huang, *Statistical Mechanics* (John Wiley and Sons, New York, 1987).