Spin bosons and spin glasses

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1 Phase transitions and critical phenomena

In this chapter we introduce fundamental concepts of phase transitions and critical phenomena. There are many good text books on critical phenomena where the reader can find an extensive treatment of the problem. In order to write this chapter the author has mainly benefited from Refs. [Ma82, Bel91, Sac99, NO98, ID89, BGZJ76] to which the reader is referred for further reading.

When describing a piece of material, we are mainly interested in quantities such as, the energy, the mass, the total magnetic moment, or the corresponding intensive counterparts, the energy density, mass density, magnetization. These are referred to as mechanical variables [Ma82]. In most cases they are properly defined once we characterize the environment of the material of interest, say, we know the external fields applied to it, the temperature, magnetic field, pressure, etc. These external fields define the parameter space, and the response or state of the system in each of the points of this parameter space define the phase diagram. At some points or lines of the different external field variables, the system undergoes a phase transition. At this stage, one of the mechanical variables, or a combination of them, will define an order parameter. The order parameter is a variable which is zero in one phase and non-zero in the other. At the transition it starts to grow. Most studies in critical phenomena are devoted to find the order parameter or to understand how it evolves. Examples of order parameters are for a ferromagnet: the magnetization, for a liquid gas transition: the relative density with respect to the one at the critical point, for superconductors: the complex field density amplitude of “Cooper pair bosons”.

Since in this thesis we study the critical phenomena of magnetic systems, we proceed using them as the example for defining the critical exponents.

The different critical exponents are defined as:

$\alpha$: Specific heat divergence [BGZJ76]:

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At zero field $h = 0$, the specific heat diverges at $T_c$ as a power law

$$C = \begin{cases} A(T - T_c)^{-\alpha} + B & \text{for } T > T_c, \\ A'(T_c - T)^{-\alpha} + B' & \text{for } T < T_c. \end{cases} \quad (1.1)$$

3: Order parameter $m$ as a function of temperature $T$:

For zero external magnetic field, $h = 0$, the magnetization is a decreasing function of $T$ and vanishes at $T_c$

$$m \propto (T_c - T)^3 \quad \text{for } T < T_c. \quad (1.2)$$

γ: Magnetic susceptibility divergence:

The magnetic field susceptibility $\chi = \frac{\partial m}{\partial h} |_T$ diverges at $h = 0$ at the transition temperature

$$\chi = \begin{cases} C(T - T_c)^{-\gamma} & \text{for } T > T_c, \\ C'(T_c - T)^{-\gamma} & \text{for } T < T_c. \end{cases} \quad (1.3)$$

δ: Order parameter $m$ as a function of the external magnetic field $h$:

At the transition temperature $T_c$, the magnetic field follows a power law with the external magnetic field, vanishing for vanishing field

$$m \propto |h|^{1/\delta} \quad \text{for } T = T_c. \quad (1.4)$$

η: Spatial dependence of the correlation function $G_{ij}$

Near the transition temperature $T_c$ the correlation function

$$G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle. \quad (1.5)$$

can be expressed for long enough distances $r_{ij} = r_i - r_j$

$$G(r) = \frac{g(r/\xi)}{r^{D+\eta-2}} , \quad \hat{G}(q) \sim q^{-2+\eta}. \quad (1.6)$$

where $\hat{G}$ is the correlation function in Fourier space, $D$ corresponds to the dimension of the system, $g$ is a function that at $r \to \infty$ decays exponentially $g(r/\xi) \sim \exp(-r/\xi)$, and $\xi$ is the correlation length.

ν: Divergence of the correlation length $\xi$

At the transition temperature $T = T_c$ and for vanishing field $h = 0$, the correlation length diverges

$$\xi = \begin{cases} D(T - T_c)^{-\nu} & \text{for } T > T_c, \\ D'(T_c - T)^{-\nu'} & \text{for } T < T_c. \end{cases} \quad (1.7)$$
z: Divergence of the correlation time $\tau$

At the transition temperature $T = T_c$ and for vanishing field $h = 0$, the correlation time diverges

$$\tau \propto \xi^2 \propto |T - T_c|^{-2\nu}; \quad \Delta \propto |T - T_c|^{2\nu}.$$  \hspace{1cm} (1.8)

where $\Delta$ corresponds to the characteristic energy fluctuation.

Each system has its own critical exponents. However, although being very different, many systems share the same critical exponents. Such systems are said to belong to the same universality class. At the critical point and in nearby surroundings, the scaling limit can be taken. The scaling limit of an observable is defined as its value when all corrections involving the ratio of small to large lengths are neglected. In the case of magnetic spins on a lattice, the small length would be the lattice spacing $a$, while the large ones would be the correlation length $\xi$ and the system size. The assertion of universality is that the results of the scaling limit are not sensitive to the precise microscopic model used. This can be seen as a formal consequence of the physically reasonable requirement that correlations at the scale of large $\xi$ should not depend upon the details of the interactions on the scale of the lattice spacing, $a$. In this situation, we can map our Hamiltonian onto a continuum field theory that represents the universality class. Typically, only essential qualitative features, such as the symmetry of the order parameter, the dimensionality of the space, and constraints placed by conservation laws, survive the continuum limit, and the structure of the quantum field theory is severely constrained by these restrictions.

The critical exponents depend strongly on the spatial dimension of the system. In next chapter we will solve analytically the critical phenomena of the quantum spherical model for arbitrary spatial dimension. We will see there that below a certain dimension the phase transition does not occur anymore, which is a general phenomenon. The dimension where this happens is called lower critical dimension. Qualitatively this can be understood because cooperative effects are not strong enough to overcome the disorder created by temperature. On the contrary, above a certain dimension, the cooperative effects are so strong that fluctuations can be ignored and the mean field approximation turns out to be valid. This dimension is called upper critical dimension. The system then has the mean field critical exponents, see table 1.1. Between the upper and the lower critical dimension, there are the hyperscaling relations, i.e. the critical exponents are functions of the space dimension and relations among them can be found in terms of this dimension $d$. Some examples can be

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$\delta$</th>
<th>$\eta$</th>
<th>$\nu$</th>
</tr>
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<td>0</td>
<td>1/2</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Table 1.1: The mean field critical exponents
1.1. Phase transitions and critical phenomena

\[ \nu = \frac{\gamma}{2 - \eta}. \quad (1.9) \]

\[ \alpha = 2 - \nu d. \quad (1.10) \]

\[ \beta = \frac{1}{2} \nu(d - 2 + \eta). \quad (1.11) \]

\[ \delta = \frac{d + 2 - \eta}{d - 2 + \eta}. \quad (1.12) \]

So far in these definitions we were considering classical critical points. Classical critical points occur at finite temperature. In such situations, all fluctuations have a thermal origin. No matter how quantum the system behaves, for instance the transition to a superconductor phase, as long as the transition occurs at a finite temperature, thermal fluctuations are responsible for the transition and the transition is classical. On the contrary, quantum phase transitions occur at zero temperature, \( T = 0 \). [Sac99, Voj00a, Voj00b]. Classical systems at zero temperature usually freeze into a fluctuationless ground state. In contrast, quantum systems have fluctuations driven by the Heisenberg uncertainty principle even in the ground state. These are responsible for the quantum phase transitions since in such situations, temperature and the corresponding thermal fluctuations cannot play a role, and the only possible source of fluctuations is quantum mechanical. A simple model that exhibits a quantum phase transition is the Ising model with transversal field. This model reproduces the main ideas of quantum phase transitions. We will reproduce it qualitatively here not only for pedagogical reasons, but also because it was a source of inspiration for the work described in the following chapter.

The Ising model is one of the simplest models to study magnetism. It consists of pairwise interactions among the Ising spins. Ising spins can only take 2 values, \(+1\) and \(-1\). Physically, they describe strongly anisotropic magnetic moments on which the typical 3 directions available to the microscopic magnetic moment, only one is available leaving as the only degree of freedom the orientation, whether positive or negative. A physical realization of such model are the low-lying excitations of the insulator LiHoF\(_4\) which consist of fluctuations of the Ho ions between two spin states that are aligned parallel or antiparallel to a particular crystalline axis [Sac99]. Dipolar interactions among these ions at low temperatures align all spins parallel forming thus a ferromagnet. We will simplify these interactions to only nearest neighbours. For this study of quantum phase transitions the relevant situation is having a transversal field, say in the \(x\)-direction. The Hamiltonian reads

\[ \mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - g \sum_i \hat{\sigma}_i^x, \quad (1.13) \]

where \( J \) is the coupling constant, positive for ferromagnetic couplings, i.e. when the spins tend to align with respect to each other, \( g > 0 \) is a coupling proportional to the external magnetic field, and \( \hat{\sigma}_i^a \) are the Pauli matrices \( (a = x, y, z) \) that correspond to the spin on the lattice site \( i \) with \( \hat{\sigma}^z = \text{diag}(1, -1) \). The transversal field induces
quantum tunneling between the two states of each Ho ion, and a sufficiently strong tunneling rate can eventually destroy the long range order.

In the limit of zero temperature and zero external field, \( T \to 0, g \to 0 \), the system finds itself in its ground state: all spins point parallel or antiparallel to the \( z \) direction. Conversely, at zero temperature but in the limit of very large magnetic transversal field, \( T \to 0, g \to \infty \) the ground state consists of having all spins pointing in the \( x \) direction. Then by tuning the transversal field \( g \), one is able to go from a phase where all spins are ordered in the \( z \) direction towards one where the spins are pointing mostly to the \( x \) direction. In between these two limiting situations there must be a critical value of the external field \( g = g_c \) where the transition takes place since the system cannot analytically go from one situation to the other.

In this quantum critical point, all definitions of critical exponents made above must be reformulated. In this situation, the temperature plays the role the transversal magnetic field was playing in the classical critical point. Figure 1.1 a typical phase diagram is sketched. One can see how temperature pulls the system away from the critical point in the same manner the transversal magnetic field \( g \) does in the classical critical point. The role played before by temperature is now played by the control parameter of quantum fluctuations, which drive the phase transition. In this case it is the transversal magnetic field \( g \). Then, in all critical exponent definitions above, temperature has to be changed by transversal field, \( T \to g \) and \( T_c \to g_c \). On the contrary, since the longitudinal magnetic field \( h \) always helps the transition in the same way, its role is unchanged.

Using renormalization group arguments, Hertz [Her76] proved that the critical exponents in the quantum critical point are related with their counterparts in the classical critical point. The relation is set by the dynamical critical exponent \( z \). The quantum critical point behaves as the classical one for dimensions \( D = d + z \). So the upper and lower critical dimensions are shifted down in the critical point by \( z \) and the hyperscaling relations in between these two dimensions are found by changing \( d \) by \( D \).

1.1 Path Integrals

In this section we give a brief introduction on how to compute the partition function of a quantum system using Feynman path integrals [FH65]. To find the partition function, using one technique or another, is usually the starting point of any calculation in statistical mechanics. Here, we will only focus on finding the partition function of a system of bosons in their coherent state representation. This tech-
technique will be exploited and extended in the following chapter. The reader is referred to e.g. [NO98] or [Sto] for a review of path integrals and coherent states and to e.g. [KS85] for a complete study of coherent states. These books served as source and inspiration for the elaboration of this section.

1.1.1 Bosonic coherent state representation for a single oscillator

Fock space is the Hilbert space of states labeled by the number of oscillator quanta. Coherent states are defined as the eigenstates of the annihilation operator $\hat{a}$. Then it can be proven that for a system with many particles

$$|\phi\rangle = e^{\sum_n \phi_n \hat{a}_n^\dagger} |0\rangle = \prod_n \left( \sum_{n_\alpha} \frac{(\phi_n \hat{a}_n^\dagger)^{n_\alpha}}{n_\alpha!} \right) |0\rangle,$$

(1.14)

is a coherent state, where $|0\rangle$ is the vacuum representation in Fock's space, and $\alpha$ stands for an index of a mode of the system. Indeed, because of the identity $\hat{a}_\alpha (\hat{a}_n^\dagger)^{n_\alpha} = n_\alpha (\hat{a}_n^\dagger)^{n_\alpha-1} + (\hat{a}_n^\dagger)^{n_\alpha} \hat{a}_\alpha$, it holds that $\hat{a}_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle$. The scalar product of two coherent states gives

$$\langle \phi | \phi' \rangle = e^{\sum_n \phi_n^* \phi'_n}.$$

(1.15)

A crucial property of the coherent states is that they form an overcomplete set of states. Any vector in Fock space can then be expanded in terms of coherent states. This is expressed by the closure relation [NO98]

$$\int \prod_\alpha d\Im(\phi_\alpha) d\Re(\phi_\alpha) e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} |\phi\rangle \langle \phi| = 1.$$

(1.16)

where the measure in the integral comes from gaussian integration with complex variables ($\Im$ stands for imaginary part and $\Re$ for real part and these parts are integrated from $-\infty$ to $\infty$) and the exponential term is due to the fact that coherent states are not normalized. Let us check that eq. (1.16) is indeed a representation of the identity of Fock space. We insert it in the left hand side of eq. (1.15) and we get

$$\langle \phi | 1 | \phi' \rangle = \int \prod_\alpha d\Im(v_\alpha) d\Re(v_\alpha) \frac{1}{\pi} e^{-\sum_\alpha v_\alpha^* v_\alpha} \langle \phi | v \rangle \langle v | \phi' \rangle =$$

$$\int \prod_\alpha d\Im(v_\alpha) d\Re(v_\alpha) \frac{1}{\pi} e^{\sum_\alpha -v_\alpha^* v_\alpha + \phi_\alpha^* v_\alpha + v_\alpha^* \phi'_\alpha} = e^{\sum_\alpha \phi_\alpha^* \phi'_\alpha},$$

(1.17)

which indeed is the right hand side of eq. (1.15).

The partition function of any quantum system $Z = \text{tr} \left[ e^{-\beta H(\hat{a}^\dagger, \hat{a})} \right]$ can be computed by the Trotter approach. The exponential has the same form as a time evolution operator in imaginary time; thus it is possible to create a path integral over
closed paths. The procedure is to split the exponential in a product of \( M \) equal terms. Between each pair of them a representation of the identity, eq. (1.16), is inserted. The partition sum then has the following shape

\[
Z = \text{tr} \left[ \left( e^{-\epsilon H(\hat{a}^\dagger, \hat{a})} \right)^M \right] = \text{tr} \left[ e^{-\epsilon H(\hat{a}^\dagger, \hat{a})} \mathbf{1} e^{-\epsilon H(\hat{a}^\dagger, \hat{a})} \cdots \mathbf{1} e^{-\epsilon H(\hat{a}^\dagger, \hat{a})} \right],
\]

where \( \epsilon = \beta/M \) and each \( \mathbf{1} \) is the above identity operator. Each of these identities is given an index; they represent the steps the system passes through in a discretized path. By using the identity defined in Eq. (1.16) only the following matrix element is needed in the calculation:

\[
\langle \phi_j | e^{-\epsilon H(\hat{a}^\dagger, \hat{a})} | \phi_{j-1} \rangle.
\]

Provided the Hamiltonian is normal ordered, the outcome is [NO98]

\[
\langle \phi_j | e^{-\epsilon H(\hat{a}^\dagger, \hat{a})} | \phi_{j-1} \rangle \approx \langle \phi_j | 1 - \epsilon H(\hat{a}^\dagger, \hat{a}) | \phi_{j-1} \rangle = e^{\phi_j^* \cdot \phi_{j-1} (1 - \epsilon H(\phi_j^*, \phi_{j-1}))} = e^{\phi_j^* \cdot \phi_{j-1} - \epsilon H(\phi_j^*, \phi_{j-1})} + \mathcal{O}(\epsilon^2).
\]

Correction terms can be neglected in the limit \( M \to \infty \) [NO98]. Each identity brings an integral at each time step. These integrals cover any path between its initial and its final state. The trace will finally tie the ends giving a closed path. The partition function finally reads

\[
Z = \int_{\phi_\alpha(\beta) = \phi_\alpha(0)} D(\phi_\alpha^\ast(\tau)\phi_\alpha(\tau)) \exp \left\{ -\sum_{\tau=0}^{\beta} d\tau \left[ \phi^\ast(\tau) \cdot \frac{d\phi(\tau)}{d\tau} + H(\phi^\ast(\tau), \phi(\tau - d\tau)) \right] \right\},
\]

where the subindex of the integral reflects the trace structure of the partition function since it gives a closed path integral; \( \tau \) stands for the imaginary time step, so \( \phi(\tau) = \phi_i \); \( d\tau \) is the imaginary time difference between steps, so \( \phi(\tau - d\tau) = \phi_{i-1} \); and

\[
\frac{d\phi(\tau)}{d\tau} = \frac{\phi(\tau) - \phi(\tau - d\tau)}{d\tau} = \frac{\phi_i - \phi_{i-1}}{\beta/M}.
\]

Despite the fact that the nomenclature used in these formulas suggests a continuous time, it should always be understood as being discrete. The limit \( M \to \infty \) should always be taken at the end of the calculations, otherwise some indeterminacies may arise. Continuous notation is used nevertheless because it is more compact.