Fundamental Aspects of Magnetism
Preface

The Lecture on “Fundamental Aspects of Magnetism” is an introduction to the basic concepts in magnetism. It consists of two parts: the first one (by D. Pescia) deals with magnetic effects in atoms (diamagnetism, paramagnetism, formation of magnetic moments in atoms) and with the occurrence of magnetic order in the ground state of a solid in virtue of the exchange interaction. The second part (by A. Vindigni) treats the occurrence of magnetism at finite temperatures, the role of small interactions such as the dipolar interaction, and presents the essential facts about the statistical physics of magnetism. A final chapter on nanoscale magnetism will conclude the course. A very extended introduction in modern magnetism can be found in the book by J. Stöhr and H.C. Siegmann “Magnetism: from fundamentals to the Nanoscale dynamics”, Springer-Verlag, Berlin Heidelberg 2006.

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Contents

Preface ii

1 Quantum theory of atomic magnetism 1

2 Magnetism in solids: the ground state 50

3 Magnetic order at finite temperature 78
   3.1 Coupled effective spins: an N-body problem . . . . . . . . . . 79
   3.2 Mean-field approximation (MFA) . . . . . . . . . . . . . . . . 81
   3.3 Mean-field universality class . . . . . . . . . . . . . . . . . . 84
   3.4 Classical spin models . . . . . . . . . . . . . . . . . . . . . . 86
   3.5 Correlation functions . . . . . . . . . . . . . . . . . . . . . . 95
   3.6 Beyond the Mean-Field Approximation . . . . . . . . . . . . 100
   3.A Averages and thermodynamic potentials . . . . . . . . . . . 110
   3.B Functional approach and Landau theory . . . . . . . . . . . . 113
   3.C Landau theory of correlations . . . . . . . . . . . . . . . . . 118

4 Magnetic domains and domain walls 121
   4.1 Magnetic anisotropy . . . . . . . . . . . . . . . . . . . . . . . 121
   4.2 Finite size and superparamagnetic limit . . . . . . . . . . . . 124
   4.3 Domain walls in the classical Heisenberg model . . . . . . . . 125
   4.4 Continuum formalism . . . . . . . . . . . . . . . . . . . . . . 128
   4.5 Dipolar interaction . . . . . . . . . . . . . . . . . . . . . . . 133
   4.6 Dipolar interaction in extended systems . . . . . . . . . . . . 137
   4.7 Dipolar interaction in low-dimensional systems . . . . . . . . 145
   4.8 Ferromagnetism and magnetic domains . . . . . . . . . . . . 149

5 Nanoscale magnetism 154
   5.1 Landau-Lifshitz dynamics . . . . . . . . . . . . . . . . . . . 155
   5.2 Landau-Lifshitz-Gilbert equation . . . . . . . . . . . . . . . . 157
   5.3 Systems of coupled spins . . . . . . . . . . . . . . . . . . . . 160
5.3.1 Spin waves ................................. 161
5.3.2 A simple model for domain-wall dynamics ........... 164
5.4 Stochastic dynamics .................................. 168
  5.4.1 Nanoparticles with uniaxial anisotropy .............. 169
  5.4.2 High-energy barrier .............................. 171
5.A Micromagnetic limit ................................. 177
Part I
Chapter 1

Quantum theory of atomic magnetism
Chapter 2

Magnetism in solids: the ground state
CHAPTER 2. MAGNETISM IN SOLIDS: THE GROUND STATE

Part II
Chapter 3

Magnetic order at finite temperature

In the first two chapters

- we have shown how magnetic moments are created at the atomic level according to the Hund’s rules (intra-atomic exchange interaction);

- we commented on how atomic magnetic moments, deduced assuming spherically symmetric surrounding (Hund’s rules), generally reduce when the atom is “put” in a crystal and, consequently, in contact with the sea of itinerant electrons (Stoner-Wohlfahrt model);

- we have shown how an interatomic exchange interaction can arise in a metal by means of the RKKY interaction;

- we defined the conditions under which a metal may show ferromagnetic coupling between different magnetic moments.

Already at that level, it was clear that ferromagnetism is not the rule but rather an exception, in the sense that many factors that are encountered in ordinary materials usually prevent the formation of magnetic moments or that of a ferromagnetic interatomic coupling. All the above-mentioned properties\(^1\) have been deduced neglecting thermal fluctuations or, in other words, they are ground-state properties. In this chapter we discuss the consequences of introducing temperature. The general trend is that thermal fluctuations destroy the ground-state ferromagnetism (when present). In the same line as before, we will define some conditions under which ferromagnetism can “survive” at finite temperatures as well.

\(^1\)apart from the Brillouin function.


3.1 Coupled effective spins: an N-body problem

In the previous chapters we have considered the conditions under which an isolated atom possesses a finite magnetic moment. Hund’s rules allow computing the ground-state multiplet, characterized by the total angular momentum (orbital plus spin contribution) which results from all the unpaired electrons. When dealing with coupled magnetic moments, we will indicate the atomic total angular momentum with $S_i$ in order to avoid confusion with the exchange interaction ($J$) and ii) because – in this context – people often speak about “spin” or “effective spin” to indicate the total single-atom angular momentum. As far as a single isolated atom is concerned, its magnetic moment at finite temperature is well described by the Brillouin function:

$$m = -g\mu_B \langle \hat{S}_z \rangle = g\mu_B S B_S \left[ \frac{g\mu_B S B}{k_B T} \right], \quad (3.1)$$

with

$$B_S(\alpha) = \frac{2S + 1}{2S} \coth \left( \frac{2S + 1}{2S} \alpha \right) - \frac{1}{2S} \coth \left( \frac{\alpha}{2S} \right) \quad \text{and} \quad \alpha = \frac{g\mu_B S B}{k_B T}. \quad (3.2)$$

In the derivation of this function, we have implicitly used the knowledge of i) the eigenstates of the atom in the presence of an external, applied field and ii) the way of performing thermal averages for a quantum system (see Appendix). Note that the intra-atomic and the Zeeman interaction have been treated on a different ground: we have considered only the ground-state multiplet (which minimizes the intra-atomic exchange interaction) but we have applied Boltzmann statistics to the levels of this multiplet in case they have been split by an external field (Zeeman interaction). The reason for such a different treatment resides in the characteristic energy scales of the two interactions in relationship with the thermal energy $k_B T$. In fact, the intra-atomic exchange energy is of the order of $4 - 10$ eV $\sim 10^5$ Kelvin, while the Zeeman splitting is roughly $0.1$ meV $\sim 1$ Kelvin for one-Tesla applied field. Further on, we have seen how a ferromagnetic interatomic exchange interaction is necessary for the occurrence of ferromagnetism in a solid. Under specific and relatively strict conditions, this goal is attained by means of the RKKY interaction$^2$. The order of magnitude of the RKKY interaction is $10 - 50$ meV $\sim 100 - 500$ Kelvin. Thus, depending on the material and the

$^2$Other mechanisms are responsible for exchange interaction, e.g. super-exchange or direct exchange, in insulators.
Typical exchange energies and magnetic moments

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<tr>
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</thead>
<tbody>
<tr>
<td>Fe</td>
<td>1043</td>
<td>2.22</td>
<td>2.22</td>
<td>0.012</td>
<td>139</td>
<td>1746</td>
</tr>
<tr>
<td>Co</td>
<td>1395</td>
<td>2.24</td>
<td>1.71</td>
<td>0.015</td>
<td>174</td>
<td>1446</td>
</tr>
<tr>
<td>Ni</td>
<td>629</td>
<td>0.588</td>
<td>0.605</td>
<td>0.013</td>
<td>151</td>
<td>0.510</td>
</tr>
<tr>
<td>Gd</td>
<td>289</td>
<td>7.1</td>
<td>0.00025</td>
<td>2.9</td>
<td>2.060</td>
<td></td>
</tr>
<tr>
<td>Dy</td>
<td>87</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2920</td>
</tr>
<tr>
<td>EuO</td>
<td>69.4</td>
<td>4.68</td>
<td></td>
<td></td>
<td></td>
<td>1930</td>
</tr>
<tr>
<td>EuS</td>
<td>16.5</td>
<td>3.06</td>
<td></td>
<td></td>
<td></td>
<td>1240</td>
</tr>
</tbody>
</table>

Table 3.1: Some typical values for the energy scales, Curie temperature, Curie constant and saturation magnetization $M_s = g \mu_B S/a^3$ ($a$ lattice constant). Often it turns useful to express the exchange interaction in Kelvin units: 1 eV $\approx 1.16 \times 10^4$ K.

temperature range of interest, a statistical-mechanics treatment is required for the RKKY interaction as well. The competition between this interatomic exchange interaction and thermal fluctuations is indeed responsible for the loss of ferromagnetism above a certain temperature, called Curie temperature $T_C$. Table 3.1 reports the values of the Curie temperature, the exchange interaction and other relevant parameters for few typical magnetic materials. Let us come back to the formal treatment of magnetism at finite temperatures, restricting ourselves to ferromagnetic exchange interactions. A system of coupled magnetic moments arranged in a lattice can then be described by the Hamiltonian

$$
\mathcal{H} = -\frac{1}{2} J \sum_{|\mathbf{r} - \mathbf{r}'| = 1} \hat{S}(\mathbf{r}) \cdot \hat{S}(\mathbf{r}') + g \mu_B B \sum_\mathbf{r} \hat{S}^z(\mathbf{r}).
$$

(3.3)

The dimension of the Hilbert space associated with this quantum many-body problem scales as $(2S + 1)^N$, $N$ being the number of magnetic moments (spins) in the lattice. Due to such an exponential dependence on $N$, the exact treatment of a system of many coupled spins becomes intractable – even numerically – as far as the number of spins approaches that of realistic extended systems\(^3\). In practice, one can try to circumvent this problem in several ways:

\(\text{\(^3\)Some effective zero-dimensional structures (magnetic clusters or nanoparticles) are also studied in the context of nanomagnetism. For some of these systems, exact diagonalization of the associated quantum problem is still feasible numerically and makes it possible to describe their magnetic behavior at any temperature.}\)
1. Reduce the many-body problem to a single-particle problem. This corresponds to the mean-field approximation (MFA).

2. Simplify the problem replacing the quantum-spin operators by classical vectors.

3. Take advantage of specific symmetries in the problem under investigation and use a Hamiltonian which can easily be diagonalized.

4. Consider only a selected family of excitations of the ground state, which can have either local (domain walls) or non-local (spin waves) character.

### 3.2 Mean-field approximation (MFA)

The goal of the Mean-Field Approximation (MFA) is to reduce the many-body problem (3.3) to the a single-particle problem. This means to get rid – somehow – of terms which directly involve two-spin operators such as \( \hat{S}(n) \cdot \hat{S}(n') \). In this context, we understand a paramagnet as the reference single-particle problem. We will first make use of the Brillouin function (3.1) to write down the MF equation of state heuristically and discuss its relevant implications. Within the more rigorous Landau approach (see Appendix 3.B for more details), it can be shown that the MFA is actually the best approximation of Hamiltonian (3.3) in terms of a single-particle Hamiltonian.

Figure 3.1: Sketch of the idea behind the mean-field approximation.

to write down the MF equation of state heuristically and discuss its relevant implications. Within the more rigorous Landau approach (see Appendix 3.B for more details), it can be shown that the MFA is actually the best approximation of Hamiltonian (3.3) in terms of a single-particle Hamiltonian.

### Equation of state

Referring to the sketch in Fig. 3.1, we may think that the actual field experienced by each spin in a ferromagnetic sample contains a contribution
arising from the interaction with its neighbors, besides the typical Zeeman term (due to the interaction with the external, applied field). More explicitly, we assume that the physics of each spin can be described by a single-particle Hamiltonian of the form

\[ \mathcal{H}_{\text{sp}}(n) = g_\mu B (B + B_W) \hat{S}_z(n) \]  \hspace{1cm} (3.4)

where \( g_\mu B W = -\bar{z} J \langle \hat{S}_z(n) \rangle_{\mathcal{H}_{\text{sp}}} \). The origin of the Weiss field \( B_W \) is the interatomic exchange interaction, whose effect is taken into account only as an average and not rigorously. Such an average is performed using the Hamiltonian (3.4) itself and \( \bar{z} \) indicates the number of nearest neighbors of each spin. As anticipated, the Hamiltonian \( \mathcal{H}_{\text{sp}} \) is equivalent to the one of a paramagnetic atom in a magnetic field \( B^t = B + B_W \) so that the thermal average of the \( \hat{S}_z(n) \) projection is given by the Brillouin function:

\[ \langle \hat{S}_z(n) \rangle_{\mathcal{H}_{\text{sp}}} = -SB_S(\alpha) \]  \hspace{1cm} (3.5)

with

\[ \alpha = \frac{g_\mu B S B^t}{k_B T} = \frac{g_\mu B S B - \bar{z} JS \langle \hat{S}_z(n) \rangle_{\mathcal{H}_{\text{sp}}}}{k_B T} . \]  \hspace{1cm} (3.6)

Since the average \( \langle \hat{S}_z(n) \rangle_{\mathcal{H}_{\text{sp}}} \) is also contained in \( \alpha \), i.e. the argument of the Brillouin function, Eq. (3.5) is actually a self-consistent equation. To write Eq. (3.5) in a more transparent way, we exploit the relation between the average of the spin component along the field and the associated magnetic moment \( m = -g_\mu B \langle \hat{S}_z(n) \rangle_{\mathcal{H}_{\text{sp}}} \). The MF equation of state finally reads:

\[ m = g_\mu B S B_S \left[ \frac{g_\mu B S B}{k_B T} + \frac{\bar{z} JS m}{g_\mu B k_B T} \right] . \]  \hspace{1cm} (3.7)

In order to visualize the solution of Eq. (3.7) graphically, it is convenient to set

\[ \left\{ \begin{array}{l} \sigma = \frac{m}{g_\mu B S} = B_S(\alpha) \\ \sigma = \frac{k_B T}{\bar{z} JS^2} \alpha - \frac{g_\mu B}{\bar{z} JS} . \end{array} \right. \]  \hspace{1cm} (3.8)

Let us list the most remarkable facts arising from the graphical analysis of solutions depending on the external parameters \( T \) and \( B \).

1. When \( B = 0 \), there exists a non-trivial solution with \( \sigma \neq 0 \) only if the slope of the Brillouin function exceeds that of the straight line (the
second one of Eqs. (3.8)). In particular, expanding the former around \( \alpha \simeq 0 \) yields

\[
B_S(\alpha) \simeq \frac{S + 1}{3S} \alpha + \ldots
\]

so that a spontaneous magnetization \( (\sigma \neq 0) \) only arises for \( T < T_C \) with

\[
T_C = \frac{S + 1}{3S} \frac{\bar{z}JS^2}{k_B}.
\]

One can show that if solutions with \( \sigma \neq 0 \) exist, they have a lower free energy than the solution corresponding to \( \sigma = 0 \).

2. For \( T < T_C \), the system of Eqs. (3.8) admits two graphical solutions of opposite sign in the region \( B \in [-B_c, B_c] \). Outside of this interval the solution is unique and with \( \sigma > 0 \) \((\sigma < 0)\) for \( B > 0 \) \((B < 0)\).

3. For \( T > T_C \) and small \( \alpha \) the Brillouin function can again be linearized and the system of Eqs. (3.8) takes the simplified form

\[
\begin{align*}
\sigma &= \frac{S + 1}{3S} \alpha \\
\sigma &= \frac{k_B T}{\bar{z}JS^2} \alpha - \frac{g\mu_B B}{\bar{z}JS};
\end{align*}
\]

by using the definition of \( T_C \) given in Eq. (3.10), the solution of the previous set of equations can be written as

\[
\left(1 - \frac{T}{T_C}\right) \sigma = -\frac{g\mu_B}{\bar{z}JS} B
\]

or equivalently (using again Eq. (3.10))

\[
m = g\mu_B S\sigma = \frac{(g\mu_B)^2}{\bar{z}J} \frac{T_C}{T - T_C} B = \frac{(g\mu_B)^2 S(S + 1)}{3k_B} \frac{1}{T - T_C} B.
\]

The pre-factor of \( B \) on the right-hand side is proportional to the magnetic susceptibility \( \chi = \mu_0 \partial M/\partial B \) (computed in \( B = 0 \))

\[
\chi = \frac{\mu_0}{a^3} \frac{C}{T - T_C}
\]

which is the well-known Curie-Weiss law with

\[
C = \frac{(g\mu_B)^2 S(S + 1)}{3k_B}
\]

being the Curie constant (already encountered when discussing paramagnetism).
Equation (3.14), together with other MF predictions, is not expected to hold true in the vicinity of $T_C$. In fact, in this critical region the neglected terms (fluctuations) play a major role. This statement should sound clearer at the end of this chapter. Keeping in mind the limitations of the MFA, it is still interesting to investigate how different observables should behave according to the MFA as a reference framework for introducing critical phenomena.

3.3 Mean-field universality class

Now we will discuss some consequences of the equation of state (3.7) in the vicinity of $T_C$. Since the results presented in this section (3.3) do not depend on the value of the effective spin $S$, we will deduce some scaling relations for the simplest case: $S = 1/2$. For this particular case, $B_S(\alpha) = \tanh(\alpha)$ and $T_C = \bar{z}J/4k_B$. Additionally, we assume that $S = 1/2$ refers to the spin of an electron\(^4\) so that $g = 2$. Under these hypotheses, Eqs. (3.8) can be written in the compact form

$$\sigma = \tanh \left( \frac{\mu_B B}{k_BT} + \frac{T_c}{T}\sigma \right).$$

(3.16)

By using the fact that $\tanh(\alpha) \simeq \alpha - \frac{1}{3}\alpha^3$ for $\alpha \simeq 0$, Eq. (3.16) can be expanded for small $\sigma$ and $B$ as follows:

$$\sigma = \left( \frac{\mu_B B}{k_BT} + \frac{T_c}{T}\sigma \right) - \frac{1}{3}\sigma^3 + \mathcal{O}(B\sigma^2)$$

(3.17)

which, for $T \simeq T_C$ and neglecting higher infinitesimal than $\sigma^3$, becomes a polynomial of the reduced temperature $\tau = (T - T_C)/T_C$:

$$\frac{\mu_B B}{k_BT} = \left( \frac{T - T_C}{T_C} \right) \sigma + \frac{1}{3}\sigma^3 = \tau\sigma + \frac{1}{3}\sigma^3.$$

(3.18)

Equation (3.18) is suitable for deriving some critical exponents.

Mean-field critical exponents

1. Setting $B = 0$, one has

$$\left( \frac{T - T_c}{T_c} \right) \sigma + \frac{1}{3}\sigma^3 = 0$$

---

\(^4\)In fact, any system whose ground state is two-fold degenerate with a degeneration that can be removed by the application of an external field can be thought of as possessing an effective spin 1/2, with $g \neq 2$ in general.
whose solutions are
\[
\begin{cases}
\sigma = 0 & \text{for } T \geq T_c \\
\sigma \simeq \sqrt{3} \left(1 - \frac{T}{T_c}\right) \beta \propto (-\tau)^\frac{1}{2} & \text{for } T < T_c.
\end{cases}
\]

This result provides the value of the critical exponent $\beta$ within the mean-field approximation: $\beta_{\text{MF}} = 1/2$.

2. Now we want to evaluate the behavior of the susceptibility around $T_c$. First, let us recall the proportionality relation

\[
\chi(T, B = 0) = \mu_0 \left( \frac{\partial M}{\partial B} \right) \bigg|_{B=0} \sim \frac{\partial \sigma}{\partial B}.
\]

Then the derivative $\partial \sigma / \partial B$ can easily be put in relationship with the reduced temperature and $\sigma$ by differentiating both sides of Eq. (3.18):

\[
\frac{\mu_B}{k_B T_C} \sim - \left(1 - \frac{T}{T_C}\right) \frac{\partial \sigma}{\partial B} + \sigma^2 \frac{\partial \sigma}{\partial B}.
\]

Since the relevant infinitesimal quantity is the reduced temperature $\tau$, we have identified $T = T_C$ on the left-hand side of the equation above. For $T > T_C$, we can further neglect the term containing $\sigma^2$ so that

\[
\frac{\partial \sigma}{\partial B} \sim \frac{\mu_B}{T - T_C} \quad \Rightarrow \quad \chi(T) \simeq \frac{\mu_0 C}{a^3 (T - T_C)} \quad \text{for } T > T_C.(3.19)
\]

This is nothing but the Curie-Weiss law deduced in an alternative way in Eq. (3.14). For $T > T_C$, instead, we have to take into account that $\sigma^2 \simeq -3\tau$. In this case one has

\[
\frac{\partial \sigma}{\partial B} \sim \frac{\mu_B}{2} \frac{1}{T_C - T} \quad \Rightarrow \quad \chi(T) \simeq \frac{\mu_0 C}{a^3} \frac{1}{2} \frac{1}{T_C - T} \quad \text{for } T < T_C(3.20)
\]

The Eqs. (3.19) and (3.20) give the mean-field prediction for another critical exponent: $\gamma = 1$.

**Critical exponents in general**

The fact that these observables behave like powers of the reduced temperature $\tau$ close to the transition point is not an artifact of the MFA. On the
contrary, this feature defines the condition of \textit{criticality}. Other critical exponents can be deduced similarly to $\beta$ and $\gamma$. Below we recall the definition of some of them. Letting $\tau = (T - T_C)/T_C$ be the reduced temperature, $\alpha$, $\beta$, $\gamma$ and $\delta$ critical exponents are defined as follows:

$$
C(\tau, B = 0) \sim |\tau|^{-\alpha}
$$
$$
M(\tau, B = 0) \sim (-\tau)^{\beta}, \quad \tau < 0
$$
$$
\chi(B = 0, \tau) \sim |\tau|^{-\gamma}
$$
$$
|M(\tau = 0, B)| \sim |B|^{1/\delta}.
$$

Another important feature captured by the MFA is that critical exponents do not depend on the details of the model, e.g., on $J$ and the details of the lattice (dimensionality or $\tilde{z}$). However, this \textit{universality} of mean-field critical exponents is somewhat exaggerated: for instance, the correct critical exponents do depend on the dimensionality of the lattice.

In the following table the critical exponents obtained within the MFA (classical values of the critical exponents) are compared with the exact values obtained for the 2d Ising model and with numerical values obtained for the 3d Ising and Heisenberg model\textsuperscript{5} (see following section):

<table>
<thead>
<tr>
<th></th>
<th>MFA</th>
<th>2d-Ising</th>
<th>3d-Ising</th>
<th>3d-Heisenberg (sc)</th>
</tr>
</thead>
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<tr>
<td>$\alpha$</td>
<td>0 (Jump)</td>
<td>0</td>
<td>0.110(1)</td>
<td>-0.1108(7)</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$1/2$</td>
<td>$1/8$</td>
<td>0.3265(3)</td>
<td>0.3606(2)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1</td>
<td>$7/4$</td>
<td>1.2372(5)</td>
<td>1.3896(70)</td>
</tr>
<tr>
<td>$\delta$</td>
<td>3</td>
<td>15</td>
<td>4.789(2)</td>
<td>4.853</td>
</tr>
</tbody>
</table>

Experimentally, critical exponents are independent of the values of $M_s$, $S$, $g$, $T_C$, $J$, etc. which are specific of a given magnetic material. They rather depend on more general symmetries of the experimental system under investigation. The concept of \textit{universality class} is associated with this property.

### 3.4 Classical spin models

If the conditions to have magnetic moments coupled ferromagnetically among them are fulfilled in the ground state, MF theory predicts that magnetic order is retained up to some finite temperature $T_C$. Above this temperature ferromagnetism is lost. This scenario describes a phase transition which is indeed observed in real ferromagnets. However, the Curie temperature given by formula (3.10) is almost always an overestimate compared to the values

\textsuperscript{5}Taken from \textit{Phys. Rev. B} 48, 3249 (1993).
computed with more sophisticated methods or observed in experiment. This is because fluctuations, neglected in MF theory, tend to have a disordering effect, and therefore suppress the true $T_C$ value. In sufficiently low dimensions, this suppression can lead to total loss of magnetic order at any temperature. We will discuss this phenomenon for the simplest collective spin model: the Ising model.

From what discussed about the MF critical exponents in Appendix 3.B, it should be clear that they only depend on the powers of the order parameter appearing in the Landau free-energy functional of Eq. (3.107). More generally, MF critical exponents depend on the symmetry of the considered problem but not, e.g., on the dimensionality of the lattice. The fact that such exponents are independent of the dimensionality is another artifact of the MF approximation. On the contrary, two facts remain true beyond the MF approximation: 

1) critical exponents do not depend on some details of the system such as the strength of interactions while 

2) they do depend on the symmetry of the considered problem.

In the following some of these issues will be clarified in the context of classical spin models.

**Spins with continuous symmetry**

The substitution of the quantum-spin operators in Hamiltonian (3.3) by classical spins is somewhat justified in the limit $S \rightarrow \infty$, that is when the relative spacing between levels inside each multiplet $S(n)$ becomes smaller and smaller. Moreover, when correlations among spins develop, cooperative effects create a sort of collective large spin which behaves classically. Then, one has:

$$\hat{S}(n) \rightarrow \vec{S}(n) \equiv S_0 (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$$  \hspace{1cm} (3.21)

where $S_0^2 = S(S+1)$ (more often $S_0 = 1$ is assumed and the term $S_0^2 = S(S+1)$ is re-absorbed into the definition of the other constants, $J$ and $g$, in Eq. (3.3)). The Hamiltonian given in Eq. (3.3) is modified into

$$\mathcal{H} = -\frac{1}{2} J \sum_{|n-n'|=1} \vec{S}(n) \cdot \vec{S}(n') + g\mu_B B \sum_n S^z(n).$$  \hspace{1cm} (3.22)

and, accordingly, the partition function becomes

$$Z = \int d\Omega_1 \int d\Omega_2 \ldots \int d\Omega_N e^{-\beta \mathcal{H}(\{\vec{S}(\Omega)\})},$$  \hspace{1cm} (3.23)

with $d\Omega_n = \sin \theta_n d\theta_n d\varphi_n$ being the solid-angle element of the spin located at the site $n$. 
In some cases, due to the symmetry of the problem, it is more realistic to describe each spin with a two-component vector (in-plane), which can thus be parameterized with just one angle

\[ \vec{S}(n) \equiv S_0 (\cos \varphi, \sin \varphi) . \]  

Vocabulary of classical models with continuous symmetry:

- three-component \( \vec{S}(n) \equiv S_0 (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \): classical Heisenberg model

- two-component \( \vec{S}(n) \equiv S_0 (\cos \varphi, \sin \varphi) \): classical planar or XY model.

Referring again the reader to Appendix 3.B for details, let us mention that the Landau free-energy functionals associated with these two types of classical spins are generally different, between them and from the one given in Eq. (3.107) for the Ising model (see below). This means that the number of components of the order parameter determines the Landau free-energy functional and eventually the critical behavior of a system. This is one of the features characterizing a specific universality class.

**Spins with discrete symmetry: the Ising model**

When consistent with the symmetry of the problem, two-value classical spins, \( S^z \), can be assumed:

\[ \mathcal{H} \{ S^z(n) \} = -\frac{1}{2} J \sum_{|n-n'|=1} S^z(n) S^z(n') + g \mu_B B \sum_n S^z(n) . \]  

The configurations of the classical Hamiltonian (3.25) correspond to the spectrum of eigenvalues of the quantum Hamiltonian

\[ \mathcal{H} = -\frac{1}{2} J \sum_{|n-n'|=1} \hat{S}^z(n) \hat{S}^z(n') + g \mu_B B \sum_n \hat{S}^z(n) , \]  

which is, indeed, diagonal on the basis

\[ |\varphi^i\rangle \equiv |\sigma_1 \sigma_2 \ldots \sigma_N\rangle \]

with

\[ \hat{S}^z |\sigma_\pm\rangle = \frac{1}{2} |\sigma_\pm\rangle \] and \( \sigma_\pm = \pm 1 \).
CHAPTER 3. MAGNETIC ORDER AT FINITE TEMPERATURE

More often, the Ising model is introduced directly assuming the Hamiltonian

$$\mathcal{H} \{\sigma_n\} = -\frac{1}{2} J' \sum_{|n-n'|=1} \sigma_n \sigma_{n'} - h' \sum_n \sigma_n$$  \hspace{1cm} (3.28)

with classical variables $\sigma_n = \pm 1$. Note that the Hamiltonian (3.28) is equivalent to the one given in Eq. (3.93) in which the nearest-neighbor coupling is expressed in a matrix form. The model (3.28) corresponds to the exact spectrum of eigenvalues relative to the Hamiltonian of coupled quantum spins one-half given in Eq. (3.26) provided that:

$$\begin{cases} 
J' &= \frac{1}{4} J \\
N h' &= -\frac{1}{2} g\mu_B B.
\end{cases} \hspace{1cm} (3.29)$$

However, the Ising model is applied in many different contexts rather than magnetism, ranging from biophysics to social sciences.

**Magnetic order and lattice dimensionality**

Probably one of the most striking failures of MF theory is the prediction of a magnetic phase transition for $d=1$. In fact, for one-dimensional systems rigorous proofs exist which forbid the occurrence of a magnetically ordered phase at finite temperature in the sole presence of short-range coupling between spins. But let us clarify first what is meant by lattice dimension in this specific context. The dimension $d$ corresponds to the number of directions along which the exchange coupling propagates indefinitely. In practice, this dimension may also be different from the actual dimensionality of the considered solid. If the latter is $D$, in general one has $d \leq D$.

The lattice dimensionality $d$ is another fundamental feature characterizing a specific universality class.

Limiting ourselves – for now – to the Ising model, we start considering the case $d=1$.

**$d=1$**

An Ising chain composed of $N$ spins $1/2$ can be represented schematically as in Fig. 3.2. Following an argument presented in the Landau–Lifshitz series, we evaluate the variation of the free energy associated with the creation of a domain wall in a configuration with all the spins parallel to each other. Creating a domain wall increases the exchange energy by a factor $E_2 - E_1 = J/2$. However, such a domain wall may occupy $N$ different positions in the spin chain, so that this set of configurations has an entropy
$S_2 \simeq k_B \ln(N)$. The entropy of the ground state vanishes if we assume that the two spins at the boundaries have been forced to point upward (otherwise one has $S_1 = k_B \ln(2)$). Therefore, the free-energy difference between the two configurations sketched in Fig. 3.2 is roughly given by

$$\Delta G = \frac{J}{2} - k_B T \ln(N). \quad (3.30)$$

As a consequence, splitting the ground state into domains is

$$\begin{cases} \text{convenient} & \text{if } \ln(N) > J/(2k_B T) \Rightarrow N > e^{J/2k_B T} \\ \text{inconvenient} & \text{if } \ln(N) < J/(2k_B T) \Rightarrow N < e^{J/2k_B T}. \end{cases} \quad (3.31)$$

The inequalities written above suggest an estimate of how many consecutive aligned spins can be found at finite temperature in an Ising chain. In particular, when the thermodynamic limit $N \to \infty$ is taken, one immediately realizes that it is always convenient to split the system into groups of parallel spins (magnetic domains), i.e., ferromagnetism is destroyed at any finite temperature.

$d=2$

A similar, but more rough argument can be given for $d=2$ as well. In this case we should refer to the possibility of reversing a cluster of spins enclosed in a perimeter of $l$ lattice sites and embedded in a region of spins all pointing in the same direction. We consider for simplicity a square lattice. The total cost in terms of exchange energy is of the order $\sim l J/2$. To estimate the entropy we can think of a self-avoiding random walk: at each step the walker has at most three choices of which way to go, since it has to avoid itself. Thus, we expect the number of closed loops corresponding to the perimeter $l$ to be of the order $p^l$, with $p < 3$. As a result, the free-energy variation associated with the flip of a cluster delimited by a perimeter $l$ is roughly
$\Delta G = lJ/2 - k_B T \ln p$. Therefore, for $T < J/(2k_B \ln p)$ the ordered phase should be stable against the formation of large domains of reversed spins. This argument for the existence of a phase transition in the 2d Ising model was first given, in more precise terms, by Peierls.

**Rigorous results**

The Ising model represents a particularly lucky case in which the heuristic arguments given above can be checked by solving the problem analytically. Even if we will not derive these results, it is useful to recall which crucial steps should be followed to prove rigorously whether a model is consistent with a phase with **spontaneous** magnetization (finite magnetization in zero external field) for $T \neq 0$ or not. To this end, one has to compute:

1. the partition function
   \[ Z = Tr \left\{ e^{-\beta H(S(z))} \right\} \] (3.32)
   where the trace is obtained by letting each discrete variable take the two possible values $S^z(n) = \pm 1/2$ ($Z$ is a sum with $2^N$ terms!)

2. the average magnetic moment
   \[ m(T, B) = -\frac{1}{N} \frac{\partial G}{\partial B} = \frac{1}{N} \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} \] (3.33)

3. the limit
   \[ m(T, 0) = \lim_{B \to 0^+} m(T, B) \] (3.34)
   and evaluate if there exists a temperature $T_C$ below which the limit (3.34) takes a non-zero value.

This procedure can be carried out analytically for $d=1$ or $d=2$ only, producing different results:

- for $d=1$, no spontaneous magnetization is possible at finite temperatures
- for $d=2$, a spontaneous magnetization appears for $T < T_C \approx 2.27J/(4k_B)$.

Indeed these exact results show that the MF approximation overlooks some important features as it predicts the occurrence of a phase with spontaneous magnetization **independently** of the dimension $d$. 
**d=1:** spin chains with uniaxial anisotropy

To fix the ideas, we take $S = 1/2$. As anticipated, in this case

$$m(T, 0) = \lim_{B \to 0^+} m(T, B) = -g\mu_B \lim_{B \to 0^+} \lim_{N \to \infty} \left[ \frac{1}{N} \sum_2 \langle S_z(n) \rangle \right] = 0. \quad (3.35)$$

For the 1d case, two-spin correlations can also be computed:

$$\langle S_i^z S_{i+r}^z \rangle = \frac{1}{4} \tanh \left[ \left( \frac{\beta J}{4} \right) \right] = \frac{1}{4} e^{-r/\xi} \quad (3.36)$$

with

$$\xi = -\frac{1}{\ln \left[ \tanh \left( \frac{\beta J}{4} \right) \right]}. \quad (3.37)$$

$\xi$ is called correlation length and it is a fundamental quantity in the study of critical phenomena. The correlation length of the 1d Ising model is characterized by an exponential divergence at low temperatures:

$$\xi \sim e^{J/(2k_B T)}. \quad (3.38)$$

By comparing the inequalities in Eq. (3.31) with the formula for the correlation length it is clear that $\xi$ gives the order of magnitude of the average size of groups of correlated spins. The existence of such a correlation, marks a major difference between a 1d system of coupled spins and a paramagnet. This is evidenced by the differential susceptibility at $B = 0$:

$$\chi(T, B = 0) = \frac{\mu_0}{a^3} \frac{\partial m}{\partial B} \sim \frac{\xi}{T}. \quad (3.39)$$

In practical cases

- the plot of $1/\chi$ versus $T$ highlights deviations from the paramagnetic behavior (Curie-Weiss law)

- the plot of $\ln \chi T$ versus $1/T$ highlights an 1d Ising-like behavior (when experimental points at low temperature lie on a line).

The behavior of two-spin correlations for the 1d Ising model is plotted in Fig. 3.4.

**d=2:** ultrathin magnetic films with uniaxial anisotropy
Figure 3.3: Example of a molecular spin chain with uniaxial anisotropy which – in a proper range of temperature – behaves as a 1d Ising chain (taken from C. Coulon et al., Phys. Rev. B 69, 132408 (2004)). At low temperature, $\chi T$ saturates because of the presence of non-magnetic impurities and 3d interactions with the other spin chains in the crystal.

The 2d Ising model was solved for the first time by Lars Onsager in 1944. Such a solution is a “veritable mathematical tour de force” (with the words of M. Le Bellac). To our purposes, it is enough to recall the formula which
CHAPTER 3. MAGNETIC ORDER AT FINITE TEMPERATURE

gives the spontaneous magnetization\(^0\) for \(T < T_C\):

\[
m(T, 0) = \lim_{B \to 0^+} m(T, B) = -g\mu_B \lim_{B \to 0^+} \lim_{N \to \infty} \frac{1}{N} \left[ \sum_n \langle S^n_z(n) \rangle \right]
\]

\[
= g\mu_B \left[ 1 - \sinh^{-4} \left( \frac{\beta J}{2} \right) \right]^{\frac{1}{8}}
\]

and the definition of \(T_C\) itself

\[
\sinh \left( \frac{J}{2k_B T_C} \right) = 1 \quad \Rightarrow \quad T_C = \frac{2}{1 + \sqrt{2} \frac{J}{4k_B}} \approx 2.27 \frac{J}{4k_B}.
\]

As anticipated at the beginning of this chapter, MF theory typically overestimates the transition temperature. The specific value reported in Eq. (3.41) has to be compared with the MF Curie temperature given by Eq. (3.10) for a spin one-half and for \(\bar{z} = 4\) (square lattice): \(T_{C}^{MF} = \frac{J}{k_B}\).

Expanding the spontaneous magnetization \(m(0)\) close to \(T_C\) yields

\[
m(T, 0) \sim (T_C - T)^{\frac{1}{8}}.
\]

Thus, for the 2d Ising model \(\beta = 1/8\) at odds with the MF value \(\beta^{MF} = 1/2\).

---

6We identify the magnetization with the average magnetic moment per magnetic atom (or molecule), while in the SI (Système international d’unités) it is the average magnetic moment per unit volume.
3.5 Correlation functions

Figure 3.5: Group of people in the “paramagnetic” (a) and in the “ferromagnetic” (b) phase. (Taken from L. J. de Jongh and A. R. Miedema Adv. Phys. 50 p. 947-1170 (2001)).

In the following sections we will try to render more quantitative the effect of neglecting fluctuations in the mean-field approximation. A pictorial idea of what happens when a system passes from the paramagnetic phase to the ferromagnetic phase is sketched in Fig. 3.5. In the picture on the left-hand side, people walk in the street without conditioning each other, like magnetic moments do in the paramagnetic phase. In the picture on the right-hand side, instead, a strong feed-back mechanism is present so that if one of the individuals is attracted, e.g., by a window all the others are conditioned and end up staring at the same thing. This situation can be assimilated to spontaneous symmetry breaking occurring in a magnet below $T_C$. However, everyday experience offers also intermediate degrees of correlation in which such a feed-back mechanism involves a limited number of people. Think, for instance, of a road artist playing music in a subway station: the majority of people will be more concerned of not missing their train rather than listening to his/her performance. Nevertheless, there will still be a sort of short-range correlation among the people whose train is not departing soon and whose attention is captured by the musician. This last situation resembles short-range correlations in magnetic systems.
Figure 3.6: Magnetic specific heats of the S=1/2 Ising model for d=1,2,3 and within the MF approximation. d=2 is given by the Onsager solution for the square lattice while d=3 is obtained by high-temperature series expansion for a simple cubic lattice. All temperatures are expressed in units of the corresponding MF transition temperature, $\theta$, with $\bar{z} = 2, 4, 6$ for the d=1,2,3 respectively. (Taken from L. J. de Jongh and A. R. Miedema Adv. Phys. 50 p. 947-1170 (2001)).

Specific heat tail
As already noticed, the mean-field theory predicts a finite discontinuity in the specific heat at the critical temperature. On the contrary, in experimental systems showing a magnetic phase transition the specific heat diverges at $T_C$. This behavior is reproduced by more sophisticated models. In Fig. 3.6, the behavior of the specific heat is plotted for the Ising model. There the MF prediction is compared with exact results for d=1,2 and high-temperature series expansion for d=3 (no exact solution is available in this case yet).

First, we notice that the true $T_C$ is lower than the MF value in each case. In particular, $T_C$ shifts at lower temperature as the lattice dimensionality is reduced, down to $T_C = 0$ for the Ising spin chain (d=1). This is an indication that the effect of thermal fluctuations becomes progressively more dramatic as the lattice dimensionality is reduced.

Second, apart from the MF calculation, all the models show a high-temperature tail in the specific heat. Also this feature is more enhanced the lower the lattice dimensionality is. Such tail is due to the presence of
short-range correlations above $T_C$ that are not taken into account in the MF theory. Both calculations for $d=2$ and $d=3$ show the expected singularity at $T_C$, while the specific heat does not diverge at any temperature for $d=1$, not even at $T = 0$.

The most natural way to characterize short-range correlations is by studying the behavior of the correlation function.

### The fluctuation-response theorem

Here we show how two-spin correlations are related to the susceptibility. From the definition of the magnetization itself, it follows that

$$m(T, B) = -\frac{1}{N} \frac{\partial G}{\partial B} = \frac{1}{N} \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} = \frac{1}{\beta} \frac{1}{N} \sum \langle S^z(n) \rangle e^{-\beta H} = -g\mu_B \frac{1}{N} \sum \langle S^z(n) \rangle$$

(3.43)

where the trace is taken over all the possible values of the $N$ variables $\tilde{S}(n)$. With the definition of Eq. (3.43), the magnetization equals the average magnetic moment. This value can be converted to any other unit to compare with experiments (Bohr magneton per atom, emu/mol, A/m, etc.). The susceptibility is the derivative of the magnetization with respect to the applied field

$$\chi(T, B) = \frac{\mu_0}{a^3} \frac{\partial m(T, B)}{\partial B} = \frac{\mu_0}{a^3} \frac{1}{N} \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} \left\{ \beta (g\mu_B)^2 \sum \frac{S^z(n) \cdot S^z(n')} e^{-\beta H} \right\}$$

$$= \frac{\mu_0}{a^3} \frac{\beta (g\mu_B)^2}{N} \left\{ \left( \sum \langle S^z(n) \rangle \right)^2 - \sum \langle S^z(n) \rangle^2 \right\},$$

(3.44)

where we have used the fact that $\left( \sum \langle S^z(n) \rangle \right)^2 = \sum \langle S^z(n) \rangle ^2$.

Defining the correlation function as

$$G_{nn'} = \langle S^z(n) S^z(n') \rangle - \langle S^z(n) \rangle \langle S^z(n') \rangle,$$

(3.45)
a relation between $G_{nn'}$ (not to be confused with the Gibbs free energy $G$!) and the magnetic susceptibility can be deduced

$$\chi(T, B) = \mu_0 a^3 \beta (g\mu_B)^2 \sum_{nn'} G_{nn'} ,$$

(3.46)

also known as fluctuation-response theorem.

Remarkably, according to the definition of the correlation function given in

Figure 3.7: Qualitative behavior of the correlation function for $T > T_C$ (left) and $T < T_C$ (right) assuming an exponential decay $G_{ij} \sim \exp(-r_{ij}/\xi)$ (taken from Quantum and Statistical Field Theory, M. Le Bellac).

Eq. (3.45), when $\langle S_z(n') \rangle \neq 0$ (i.e. for $T < T_C$ or for $B \neq 0$) the assertion that “two spins are uncorrelated” means $\langle S_z(n) S_z(n') \rangle = \langle S_z(n) \rangle \langle S_z(n') \rangle \propto m^2$. In other words, the correlation function $G_{nn'}$ only measures the degree of short-range correlation. The term relating to long-range order has been eliminated by subtracting $\langle S_z(n) \rangle \langle S_z(n') \rangle$ (see Eq. (3.45)).

Susceptibility for the different magnetic phases at $B = 0$

<table>
<thead>
<tr>
<th>$\chi(T, 0)$</th>
<th>2d-3d systems $T \simeq T_C$</th>
<th>1d-system</th>
<th>Paramagnet</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi$</td>
<td>$\chi \sim \frac{r_+}{</td>
<td>T-T_C</td>
<td>}$</td>
</tr>
</tbody>
</table>

From the previous table and from the theorem (3.46), it is clear that the differential susceptibility is strictly related to the degree of correlation of fluctuations at the considered temperature:

$$\chi(T, B) = \frac{\mu_0}{a^3} \beta (g\mu_B)^2 \sum_{nn'} G_{nn'} .$$

(3.47)
Note that even for the ordered phase (occurring for \(d \geq 2\)) the susceptibility diverges \textit{only} at \(T = T_C\) and tends to zero as \(T \to 0\) (in a perfectly ordered system fluctuations are not allowed).

**Fourier transform of correlations**

The Fourier transform \((\tilde{G})\) of the correlation function can be accessed experimentally, for instance through neutron scattering. At \(T = T_C\), \(\tilde{G}(q)\) is found to behave as

\[
\tilde{G}(q) \sim \frac{1}{q^{2-\eta}}. \tag{3.48}
\]

A simple argument based on dimensional analysis suggests that

\[
G(r) \simeq \int \tilde{G}(q) d^d q \quad \Rightarrow \quad G(r) \sim \frac{1}{r^{d-2+\eta}} \quad \text{at} \quad T = T_C. \tag{3.49}
\]

From Eq. (3.49) we learn that at the critical point spatial correlations decay with a power law. In other words, the system is not characterized by any typical length scale and possesses the property of being self-similar at different spatial scales\(^7\). Such a \textit{scale invariance} is the key ingredient of the theory of critical phenomena and it is, indeed, strictly related to the divergence of the correlation length for \(T \to T_C\). Notice that the fluctuation-response theorem may also be written as

\[
\chi(T, B) \sim \tilde{G}(0). \tag{3.50}
\]

Since in practice \(\eta < 2\) always, Eq. (3.48) implies that \(\tilde{G}(q = 0)\) diverges for \(T \to T_C\) and so does the susceptibility.

In Appendix 3.B it is shown that within the Landau theory of critical phenomena the Fourier transform of the correlation function is given by

\[
\tilde{G}(q) \sim \frac{1}{q^2 + \xi^{-2}}. \tag{3.51}
\]

The inverse Fourier transform of Eq. (3.51) gives the asymptotic behavior

\[
G(r) \sim \frac{e^{-r/\xi}}{r^{(d-1)/2}} \quad \text{for} \ T \ \text{far away from} \ T_C. \tag{3.52}
\]

In this case the decay of the correlation function is characterized by the typical length scale \(\xi\), the correlation length. The different behavior of the

\(^7\)See the paper C. H. Back, \textit{et al.}, Nature 378, p. 597. The authors report on the experimental check of the scaling hypothesis on a Fe film which behaves as the 2d Ising model.
correlation function above and below $T_C$ and both in real and reciprocal space is sketched in Figs. 3.7 and 3.8. It is worth remarking that we are considering short-range correlations as the unique source of broadening of the quasi-elastic peaks. Of course, experimentally this is not true and the correlation length can be deduced only after removing the other sources of broadening such as experimental resolution, etc.

Figure 3.8: Qualitative behavior of the correlation function in the real space (b) and in the Fourier space (a). (Taken from Quantum and Statistical Field Theory, M. Le Bellac).

3.6 Beyond the Mean-Field Approximation

The argument sketched in Fig. 3.2 to state that the Ising model does not show a magnetically ordered phase at finite temperature for $d=1$ holds also for the Heisenberg chain with uniaxial anisotropy, provided that the appropriate domain-wall energy is considered (see next chapter). Similarly, one concludes that the same model can sustain ferromagnetism at finite temperatures in $d=2$. Different arguments are, instead, needed to provide a conclusive statement about the existence or not of magnetic order at finite temperature in systems with continuous symmetry. For the last ones, it will turn out that linear excitations are able to destroy ferromagnetism both in $d=1$ and $d=2$. For the Heisenberg model, these linear excitations can be identified with spin waves. Spin waves are usually introduced as linear solutions to the Landau-Lifshitz equation of motion (see chapter 5). However, the capability of these type of excitations to destroy magnetic ordering for
d ≤ 2 in systems with continuous symmetry can be evidenced without introducing dynamics. We prefer to follow this way because it is straightforward to apply a unique argument to both the XY and the Heisenberg model.

**Linear excitations in models with continuous symmetry**

With the classical spin Hamiltonian (3.22), the minimal energy is obtained by aligning all the magnetic moments along the direction of the applied field (spins along negative $z$ direction). We consider how the energy increases due to small deviations from this configuration. Our goal is to simplify the original problem by means of an effective Hamiltonian that is formally equivalent to the one describing a system of coupled harmonic oscillators. To this end, we may write

$$S^z(n) = -\sqrt{1 - \sum_{\alpha=x,y} (S^\alpha(n))^2} \simeq -1 + \frac{1}{2} \sum_{\alpha=x,y} (S^\alpha(n))^2$$

with the hypothesis $(S^\alpha(n))^2 \ll (S^z(n))^2$.

Note that for the planar (or XY) model $\alpha$ takes just one value and two values for the Heisenberg model. From now on, we will not specify the number of extra components but $z$ represented by the index $\alpha$; while doing so, we are going to derive results that apply to both models. The approximation in Eq. (3.53) reflects in the Hamiltonian as follows:

$$\mathcal{H} \simeq -\frac{1}{2} J \sum_{|n-n'|=1} \left[ 1 - \frac{1}{2} \sum_{\alpha} (S^\alpha(n))^2 \right] \times \left[ 1 - \frac{1}{2} \sum_{\alpha'} (S^{\alpha'}(n'))^2 \right]$$

$$- \frac{1}{2} J \sum_{|n-n'|=1} \sum_{\alpha} S^\alpha(n) S^{\alpha'}(n') - g\mu_B B \sum_{n} \left[ 1 - \frac{1}{2} \sum_{\alpha} (S^\alpha(n))^2 \right]$$

$$= -\frac{1}{2} \varepsilon NJ - g\mu_B BN + \frac{1}{2} \varepsilon J \frac{1}{2} \left[ \sum_{n} (S^\alpha(n))^2 + \sum_{n'} (S^{\alpha'}(n'))^2 \right]$$

$$- \frac{1}{2} J \sum_{|n-n'|=1} \sum_{\alpha} S^\alpha(n) S^{\alpha'}(n') + \frac{1}{2} g\mu_B B \sum_{n} \sum_{\alpha} (S^\alpha(n))^2 + \mathcal{O} ((S^\alpha)^4)$$

$$\simeq E_{g.s.} + \mathcal{H}_{h.o.}$$

(3.54)
where, by nothing that the double summations $\sum_n \sum \alpha$ and $\sum_{n'} \sum_{\alpha'}$ are actually the same, we have defined

$$H_{h.o.} = \frac{1}{2} \bar{z} J \sum_n \sum_{\alpha} (S^\alpha(n))^2 - \frac{1}{2} J \sum_{|n-n'|=1} \sum_{\alpha} S^\alpha(n)S^\alpha(n')$$

$$+ \frac{1}{2} g\mu_B B \sum_n \sum_{\alpha} (S^\alpha(n))^2$$

and the constant ground-state energy

$$E_{g.s.} = -\frac{1}{2} \bar{z} N J - g\mu_B BN.$$  

(3.55)

The Hamiltonian $H_{h.o.}$, written in Eq. (3.55), is equivalent to the Hamiltonian of $N$ coupled harmonic oscillators which can be decoupled by the usual Fourier transform in the discrete space:

$$\begin{cases} 
S^\alpha(n) = \frac{1}{\sqrt{N}} \sum_q \tilde{S}^\alpha(q) e^{-iq\cdot n} \\
\tilde{S}^\alpha(q) = \frac{1}{\sqrt{N}} \sum_n S^\alpha(n) e^{iq\cdot n}
\end{cases}$$

with orthogonality relation

$$\sum_n e^{i(q-q')\cdot n} = N \delta_{q,q'}.$$  

(3.57)

For simplicity we assume unitary lattice constant. It is convenient to evaluate the two relevant summations appearing in the Hamiltonian of Eq. (3.55) separately. The first summation reads

$$\sum_n (S^\alpha(n))^2 = \frac{1}{N} \sum_n \sum_{q>q'} \tilde{S}^\alpha(q)\tilde{S}^\alpha(q') e^{-i(q+q')\cdot n} = \sum_q |\tilde{S}^\alpha(q)|^2.$$  

(3.59)

This is nothing but the Parseval’s formula for the discrete-lattice Fourier transform. For what concerns the second summation on the right-hand side of Eq. (3.55), we first rewrite it as

$$\sum_{|n-n'|=1} S^\alpha(n)S^\alpha(n') = \sum_n \sum_{\delta} S^\alpha(n)S^\alpha(n+\delta)$$

(3.60)

where $\delta$ is a vector connecting the site $n$ with its nearest neighbors. For simplicity, we will consider just a linear, square and simple-cubic lattice for $d=1, 2$ and 3, respectively. Passing to the Fourier space one finds

$$\sum_n \sum_{\delta} S^\alpha(n)S^\alpha(n+\delta) = \sum_n \sum_{\delta} \frac{1}{N} \sum_{q,q'} \tilde{S}^\alpha(q)\tilde{S}^\alpha(q') e^{-i(q+q')\cdot n} e^{-iq\cdot \delta}$$

$$= \sum_{\delta} \sum_q |\tilde{S}^\alpha(q)|^2 e^{-i\delta\cdot \delta} = \sum_q |\tilde{S}^\alpha(q)|^2 \sum_{\{\delta>\delta\}} 2 \cos(q \cdot \delta);$$

(3.61)
the notation \(\{\delta > 0\}\) means that the summation extends over half of the nearest neighbors of the spin located at site \(n\): it consists of \(\bar{\ell}/2\) terms. Eqs. (3.59) and (3.61) enable us to decouple the elastic Hamiltonian given in Eq. (3.55), which then reads

\[
\mathcal{H}_{h.o.} = \frac{1}{2} J \sum_q \sum_\alpha \left( \bar{\ell} - \sum_{\{\delta > 0\}} 2 \cos(q \cdot \delta) \right) |\tilde{S}^\alpha(q)|^2 + \frac{1}{2} g\mu_B B \sum_q \sum_\alpha |\tilde{S}^\alpha(q)|^2 \tag{3.62}
\]

\[
= \frac{1}{2} \sum_\alpha \sum_q \Gamma(q) |\tilde{S}^\alpha(q)|^2,
\]

with

\[
\Gamma(q) = J[\bar{\ell} - \sum_{\{\delta > 0\}} 2 \cos(q \cdot \delta)] + g\mu_B B. \tag{3.63}
\]

Figure 3.9: Sketch of a spin-wave excitation in a Heisenberg ferromagnetic spin chain.

Indeed, for the Heisenberg model, the linear excitations associated with the quadratic Hamiltonian in Eq. (3.55) are spin waves with dispersion relation \(\hbar\omega(q) = \Gamma(q)\). Spin waves are collective excitations analogous to phonons. Similarly to phonons, spin waves are also quantized and the specific dependence of \(\Gamma(q)\) on the wave vector (especially for \(q \approx 0\)) determines the behavior of the magnetization at low temperature (in the absence of anisotropy). The dispersion curve \(\Gamma(q)\) can be measured, e.g., by inelastic neutron scattering.

Coming back to our goal, we proceed by evaluating the average of fluctuations, namely those terms in Eq. (3.53) that we have assumed to be
small for linearizing the Hamiltonian (3.22). The approximated Hamiltonian, Eq. (3.62), consists of \( N \) independent quadratic degrees of freedom so that the equipartition theorem applies:

\[
\frac{1}{2} \Gamma(q) \langle |\bar{S}^{\alpha}(q)|^2 \rangle_{th} = \frac{1}{2} k_B T \quad \Rightarrow \quad \langle |\bar{S}^{\alpha}(q)|^2 \rangle_{th} = \frac{k_B T}{\Gamma(q)} ;
\]

where \( \langle \ldots \rangle_{th} \) denotes thermal average performed using the Hamiltonian \( \mathcal{H}_{h.o.} \) in Eq. (3.62). Thermal averages of the squared transverse components in real space read

\[
\langle (S^{\alpha}(n))^2 \rangle_{th} = \frac{1}{N} \sum_{q,q'} \langle \bar{S}^{\alpha}(q) \bar{S}^{\alpha}(q') \rangle_{th} e^{-i(q+q') \cdot n} = \frac{1}{N} \sum_q \langle |\bar{S}^{\alpha}(q)|^2 \rangle_{th} ,
\]

where we have used the fact that transverse components fluctuate randomly so that \( \langle \bar{S}^{\alpha}(q) \bar{S}^{\alpha}(q') \rangle_{th} = \delta_{q,q'} \langle |\bar{S}^{\alpha}(q)|^2 \rangle_{th} \). Note that the right-hand side of Eq. (3.65) is independent of the lattice site, thus the label \( n \) will be dropped henceforth from \( \langle (S^{\alpha}(n))^2 \rangle_{th} \). In order to evaluate whether the considered linear excitations are able or not to destroy ferromagnetism, we shall let the field \( B \to 0^+ \). First, we approximate the summation on the right-hand side of Eq. (3.65) with an integral

\[
\langle (S^{\alpha})^2 \rangle \approx \frac{k_B T}{(2\pi)^d} \int \frac{d^d q}{\Gamma(q)} .
\]

Since what matters is the behavior for small values of \( q \) (i.e., the effect of fluctuations at large spatial scales), the denominator of the integral can be linearized as

\[
\Gamma(q) \simeq J \bar{z} - 2J \sum_{\mu} (1 - \frac{1}{2} q^2_\mu) + g\mu_B B = J \bar{z} - 2J \left( \frac{\bar{z}}{2} - \frac{1}{2} q^2 \right) + g\mu_B B = J q^2 + g\mu_B B
\]

with \( \mu=1\ldots d \) and \( q^2 = \sum_\mu q^2_\mu \), which yields

\[
\langle (S^{\alpha})^2 \rangle \approx \frac{k_B T}{(2\pi)^d} \int \frac{d^d q}{J q^2 + g\mu_B B} .
\]

When taking the limit \( B \to 0^+ \), the integral in Eq. (3.68) has an infrared divergence\(^8\) for \( d \leq 2 \). The consequences of such a divergence can be appreciated more effectively by setting a lower bond to the integral: \( q_{min} = \pi/N_\alpha \).

\(^8\)A possible ultraviolet divergence does not matter \( i \) because the lattice unit sets a physical upper limit to large values of \( q \) \( ii \) because we are interested in fluctuations acting on large spatial scales corresponding to \( q \sim 0 \).
with $N_\alpha$ being of the order of the linear size of the system in lattice units. Depending on the dimensionality of the lattice we have

$$\langle (S^\alpha)^2 \rangle \sim \frac{k_B T}{J} \int_{q_{\text{min}}} q^{d-1} \frac{dq}{q^2} \Rightarrow \begin{cases} 
\text{d}=1 & \langle (S^\alpha)^2 \rangle \sim \frac{k_B T}{J} N_\alpha \\
\text{d}=2 & \langle (S^\alpha)^2 \rangle \sim \frac{k_B T}{J} \ln(N_\alpha) \\
\text{d}=3 & \langle (S^\alpha)^2 \rangle < \infty
\end{cases} \quad (3.69)$$

In order to understand what a divergence with increasing $N_\alpha$ means, it is convenient to rephrase the mathematical steps that we followed according to their physical sense:

- We assumed the system to be in a ferromagnetic state at $T = 0$, namely, with all the spins aligned along the same direction.
- We let each spin deviate by a small amount from its direction of alignment, $z$.
- We built an effective linear Hamiltonian, describing this family of small excitations, that can easily be decoupled passing to the Fourier space.
- We calculated thermal averages of such small excitations (transverse spin components) in the Fourier space.
- We transformed those averages back to the real space.
- We evaluated if the initial hypothesis stated in Eq. (3.53) remains valid at finite temperature.

The set of Eqs. (3.69) allows stating that in the thermodynamic limit, $N_\alpha \to \infty$, the hypothesis of small deviations fails for $d=1, 2$ at any finite $T$. This fact suggests that spontaneous magnetization is not stable against thermal fluctuations for $d \leq 2$. On the contrary, according to Eqs. (3.69), it seems possible to have ferromagnetism up to some finite temperature for $d=3$. This scenario is indeed confirmed by more rigorous proofs such as the Mermin-Wagner theorem\(^9\).

At this point we are in the position to state that for both the isotropic ($D = 0$) Heisenberg and XY classical model with short-range interactions the lower critical dimension is $d=2$ (the highest dimensionality for which magnetic order cannot occur at any finite temperature). This result marks a major difference between the universality class of classical spin models with continuous or discrete symmetry (Ising). As already noticed, in systems with continuous symmetry the effects of thermal fluctuations are more severe and manage to destroy ferromagnetism more easily.

\(^9\text{Phys. Rev. Lett. 17, 1133 (1966).}\)
The effect of uniaxial anisotropy

The presence of uniaxial anisotropy (see next chapter) stabilizes a system against the linear excitations considered above. Due to this interaction an additional term like

$$H_{m.a.} = -D \sum_n (S^z(n))^2$$

appears in the Hamiltonian in Eq. (3.22). The anisotropy energy indeed favors configurations in which spins lie along a specific axis regardless of the sign of their projections. In this case we choose the same axis as the one along which the field is applied. Because of the equality $$\sum_{\alpha} (S^\alpha(n))^2 + (S^z(n))^2 = 1$$, the Hamiltonian (3.70) may also be written as

$$H_{m.a.} = -D + D \sum_n \sum_{\alpha} (S^\alpha(n))^2.$$  

The summation appearing above transforms into the Fourier space according to the Parseval’s formula in Eq. (3.59). Finally, the uniaxial anisotropy provides a term into the energy spectrum $$\Gamma(q)$$ formally equivalent to the magnetic field:

$$\Gamma(q) = J[z - \sum_{\{\delta \rangle > 0\}} 2 \cos(q \cdot \delta)] + g\mu_B B + 2D.$$  

For small values of $$q$$ and $$B = 0$$, we get

$$\Gamma(q) \simeq Jq^2 + 2D.$$  

The average of transverse fluctuations is modified as follows

$$\langle (S^\alpha)^2 \rangle \simeq \frac{k_BT}{(2\pi)^d} \int \frac{d^dq}{Jq^2 + 2D} \sim k_BT \int \frac{q^{d-1} dq}{Jq^2 + 2D}.$$  

Henceforth, let us refer only to the thermodynamic limit $$N_a \to \infty$$, consistent with $$q_{\text{min}} = 0$$. Clearly, the introduction of uniaxial anisotropy removes the infrared divergence$^8$ from the average of fluctuations independently of the lattice dimensionality. The consequences of this result have to be understood as follows: “The considered linear excitations alone are not able to destroy ferromagnetism at any finite temperature”. This statement does not exclude:

1. that ferromagnetism may be destroyed by some other type of excitations

2. that these linear excitations play any role in the “suppression” of ferromagnetism at finite temperature.
An obvious counterexample, supporting the comment 1., is represented by the 1d Ising model. The latter can be considered as a limit case of the Heisenberg model with uniaxial anisotropy (the one that is discussed here) for $D \gg J$. For $d=1$, as for any $d$, the integral in Eq. (3.74) is convergent so that linear excitations are not able to destroy ferromagnetism for every $T \neq 0$. However, the argument sketched in Fig. 3.2 can be repeated for the Heisenberg model with uniaxial anisotropy, in which domain walls possibly extend over more than one lattice unit (see next chapter). This means that domain-wall excitations are responsible for the loss of ferromagnetism at any temperature in 1d spin systems with uniaxial anisotropy. In conclusion, even if the absence of an infrared divergence in the integral on the right-hand side of Eq. (3.74) would allow for ferromagnetism at finite $T$, we know that a phase with spontaneous magnetization does not occur.

**Limitations of the mean-field approximation**

To conclude this part about the critical aspects of magnetism at finite temperature we summarize the artifacts produced by the MFA around the critical region, $T \simeq T_C$.

1. The MFA predicts a the occurrence of a magnetic phase transition at finite temperature independently of the lattice dimensionality, $d$. However, a phase with spontaneous magnetization is not encountered in the 1d Ising model. The Mermin-Wagner theorem forbids the occurrence of spontaneous magnetization (spontaneous symmetry breaking) in classical models with short-range interactions and with continuous symmetry for $d \leq 2$. This fundamental theorem applies to both the Heisenberg and the XY model.

2. The transition temperature is generally overestimated within the MFA.

3. The classical values of the critical exponents, i.e., those given by the MFA, are generally not correct even when a phase with spontaneous magnetization exists at finite temperature. Depending on the model, classical critical exponents are wrong for $d$ larger than the lower critical dimension, $d_l$, and smaller that the upper critical dimension ($d_u=4$ for systems with short-range interactions). For the Ising model $d_l=1$, while it is $d_l=2$ for the Heisenberg and XY models.

4. The classical critical exponents turn out to be exact for $d \geq 4$ in systems with short-range interactions (Ginzburg criterion). Strictly speaking, only the critical exponents are exact for $d \geq 4$. However, the MFA
is expected to give a more appropriate description of finite-temperature properties for a given model when the number of spins with which each spin interacts increases. This number increases with increasing $d$ or with increasing range of the involved interactions. The best realization of the MFA is an ideal case in which every spin interacts with any other one with the same intensity. This is – of course – unrealistic when magnetic systems are considered. For the model

$$
\mathcal{H} = -\frac{J}{N} \sum_{n \neq n'} \hat{S}^z (n) \cdot \hat{S}^z (n'),
$$

with the summation extended over all the different couples, the Mean Field Approximation is exact. The model described by the Hamiltonian in Eq. (3.75) is called Curie-Weiss model but sometimes also “mean-field” model. However, one should not confuse this model with the Mean Field Approximation which does not assume from the very beginning an all-to-all interaction, like in the Hamiltonian of Eq. (3.75)\textsuperscript{10}.

The type of ordering that can occur in different magnetic systems is summarized schematically in Table 3.2. Systems are classified according to their magnetic-lattice dimensionality ($d$) and to the symmetry of the order parameter (classical spin). Both features specify a certain universality class. The table has to be understood as the maximum degree of order or bistability that can be sustained at finite temperature.

**“Truth” table of magnetic ordering**

<table>
<thead>
<tr>
<th>symmetry</th>
<th>0d</th>
<th>1d</th>
<th>2d</th>
<th>3d</th>
</tr>
</thead>
<tbody>
<tr>
<td>continuous</td>
<td>paramagnet</td>
<td>SR order</td>
<td>SR order</td>
<td>LR order</td>
</tr>
<tr>
<td>discrete</td>
<td>superparamagnet</td>
<td>SR order</td>
<td>LR order</td>
<td>LR order</td>
</tr>
</tbody>
</table>

Table 3.2: Fields refer to the maximum degree of order/bistability that can be achieved in a given system. SR (LR) stands for short-range (long-range).

\textsuperscript{10}The exchange interaction is divided by $N$ to guarantee *extensivity* of the energy.
CHAPTER 3. MAGNETIC ORDER AT FINITE TEMPERATURE

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Appendices

3.A Averages and thermodynamic potentials

Classical models

In the canonical ensemble, the partition function is given by

\[ Z = \int \frac{d^{3N} q d^{3N} p}{(2\pi \hbar)^{3N}} e^{-\beta \mathcal{H}(p,q)}, \quad (3.76) \]

\( \mathcal{H} \) being the Hamiltonian of the system and \( \beta = 1/(k_B T) \). \( Z \) is related to a thermodynamic potential, \( \mathcal{F} \), via the general relation

\[ \mathcal{F} = -\frac{1}{\beta} \ln Z. \quad (3.77) \]

The average of any observable \( \mathcal{O}(p,q) \) can be computed as

\[ \langle \mathcal{O} \rangle = \frac{1}{Z} \int \frac{d^{3N} q d^{3N} p}{(2\pi \hbar)^{3N}} \mathcal{O}(p,q) e^{-\beta \mathcal{H}(p,q)}. \quad (3.78) \]

Classically, the trace operator is defined as

\[ \mathcal{T}_r = \int \cdots \frac{d^{3N} q d^{3N} p}{(2\pi \hbar)^{3N}}, \quad (3.79) \]

which allows defining

\[ Z = \mathcal{T}_r \{ e^{-\beta \mathcal{H}(p,q)} \} \quad \text{and} \quad \langle \mathcal{O} \rangle = \frac{1}{Z} \mathcal{T}_r \{ \mathcal{O}(p,q) e^{-\beta \mathcal{H}(p,q)} \}. \quad (3.80) \]
Quantum models
Assume that $|\psi_\alpha\rangle$ be a complete basis of the Hilbert space on which the Hamiltonian of the model is defined. Quantum-mechanically, the trace is then given by
\[ \text{Tr} = \sum_\alpha \langle \psi_\alpha | \cdots | \psi_\alpha \rangle . \] (3.81)
By analogy with (3.80), the partition function and thermal averages are accordingly defined
\[ Z = \text{Tr} \{ e^{-\beta H} \} = \sum_\alpha \langle \psi_\alpha | e^{-\beta H} | \psi_\alpha \rangle \]
(3.82)
\[ \langle O \rangle = \frac{1}{Z} \text{Tr} \{ O e^{-\beta H} \} = \frac{1}{Z} \sum_\alpha \langle \psi_\alpha | O e^{-\beta H} | \psi_\alpha \rangle . \]
In few advanced computations one stops at this level. Generally, the trace is evaluated on a complete basis of eigenstates of $H$:
\[ H|\varphi^i\rangle = E^i|\varphi^i\rangle . \] (3.83)
The computation of (3.82) is, consequently, simplified:
\[ Z = \sum_i \langle \varphi^i | e^{-\beta H} | \varphi^i \rangle = \sum_i e^{-\beta E^i} \]
\[ \langle O \rangle = \frac{1}{Z} \text{Tr} \{ O e^{-\beta H} \} = \frac{1}{Z} \sum_i \langle \varphi^i | O | \varphi^i \rangle e^{-\beta E^i} . \] (3.84)
Spin models
Limiting ourself to a Hamiltonian of the type
\[ H = -\frac{1}{2} J \sum_{|\mathbf{n}-\mathbf{n}'|=1} \hat{S}(\mathbf{n}) \cdot \hat{S}(\mathbf{n}') + g\mu_B B^{\text{ext}} \sum_\mathbf{n} \hat{S}^z(\mathbf{n}) \] (3.85)
one possible choice for the basis of the Hilbert space is the following one: $|\psi_\alpha\rangle=|M_1, M_2, \ldots M_N\rangle=|M_1 \otimes M_2 \cdots \otimes M_N\rangle$ with $\hat{S}^z(\mathbf{n})|M_n\rangle=M_n|M_n\rangle$ and $\mathbf{n}$ label for the lattice site. Note that the Hamiltonian in Eq. (3.85) is not diagonal on this basis. After having diagonalized it, thermal averages can be computed according to Eqs. (3.84).
For many problems in magnetism, substituting the quantum-mechanical operators $\hat{S}(\mathbf{n})$ by classical vectors is legitimate:
\[ \hat{S}(\mathbf{n}) \rightarrow \vec{S}(\mathbf{n}) \equiv S_0 (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \] (3.86)
where $S_0^2 = S(S+1)$ (more often $S_0 = 1$). The partition function then reads

$$Z = \int d\Omega_1 \int d\Omega_2 \ldots \int d\Omega_N e^{-\beta H(\{\vec{s}(\Omega)\})}, \quad (3.87)$$

with $d\Omega_n = \sin \theta_n d\theta_n d\varphi_n$ being the solid-angle element of the spin located at the site $n$.

Both in the quantum and the classical case $Z$ depends on $T$ and on the external applied field $B^{\text{ext}}$. As a useful (heuristic) trick to remember to which thermodynamic potential is proportional the logarithm of this $Z$ function (see Eq. (3.77)), one may start from the combined first and second laws of thermodynamics:

$$dU = TdS + dW \quad (3.88)$$

where $dU$ represents an infinitesimal variation of the internal energy, $TdS$ the exchanged heat and $dW$ the external work done on the system. It can be shown that $dW = NB^{\text{ext}} dm$, where $m$ is the average magnetic moment per (magnetic) atom and $N$ the total number of spins. The internal energy is thus a function of $S$ and $m$, namely $U(S,m)$. Two successive Legendre transformations are necessary to obtain a thermodynamic potential which is a function of $B^{\text{ext}}$ and $T$: a first one yielding the Helmholtz free energy

$$F(T,m) = U - TS \quad (3.89)$$

and a second one giving the Gibbs free energy

$$G(T,B^{\text{ext}}) = F - NB^{\text{ext}} m = U - TS - NB^{\text{ext}} m. \quad (3.90)$$

Therefore, the thermodynamic potential associated with the partition function of a generic spin Hamiltonian in the canonical ensemble is the Gibbs free energy of macroscopic thermodynamics:

$$G(B^{\text{ext}}, T) = -\frac{1}{\beta} \ln [Z(B^{\text{ext}}, T)]. \quad (3.91)$$

Some confusion may arise from the fact that the letter $F$ is sometimes used to indicate the thermodynamic potential obtained in this way, even though it is actually a function of $B^{\text{ext}}$ and $T$.

In the main document the superscript “ext” is dropped from $B^{\text{ext}}$, but it is implicitly assumed that relevant for thermodynamic averages is the external $B$ field, which does not contain the contribution due to the spins in the system. This point will be clarified in the next chapter while discussing the dipolar interaction.
CHAPTER 3. MAGNETIC ORDER AT FINITE TEMPERATURE

3.B Functional approach and Landau theory

There is no univocal way of introducing it nor the literature is consistent in what it is meant by Landau approach to critical phenomena. The procedure proposed here aims at highlighting how the MFA is a drastic simplification of the more general theoretical-field approach based on functional integrals. We will try to avoid confusion between the Landau free-energy functional and the MF (Gibbs) free energy. Finally, we should be able to discuss some qualitative arguments whose validity goes beyond the mean-field approach.

To avoid useless complications, we refer to $S = 1/2$ operators and assume that only their $z$ component enters the spin Hamiltonian:

$$H = -\frac{1}{2} J \sum_{|n-n'|=1} \hat{S}^z(n) \hat{S}^z(n') + g\mu_B B \sum_n \hat{S}^z(n). \quad (3.92)$$

Later on, we will discuss the Ising Hamiltonian (3.92) in some more details. For now we use only the fact that the corresponding energy levels can be written in terms of two-valued classical variables $\sigma = \pm 1$:

$$H[\{\sigma\}] = -\frac{1}{2} \sum_{i,j} \sigma_i J_{i,j} \sigma_j + \frac{1}{2} g\mu_B B \sum_i \sigma_i, \quad (3.93)$$

where $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ and $J_{i,j}$ is a symmetric matrix describing the (exchange) coupling among different spins in the lattice\(^{11}\). The partition function associated with the Ising Hamiltonian reads

$$Z(B, T) = \mathcal{T} \{\sigma\} \left\{ \exp \left[ \frac{1}{2} \beta \sum_{i,j} \sigma_i J_{i,j} \sigma_j - h \sum_i \sigma_i \right] \right\} \quad (3.94)$$

with $\beta = 1/k_B T$ and $h = \beta g\mu_B B/2$. The summation over all the configurations $\{\sigma\}$ can be performed analytically only for the one-dimensional lattice (Ising chain) and in 2d for $B = 0$. Before proceeding, it is useful to make a mathematical digression and recall the well-known Gaussian identity

$$\int_{\mathbb{R}} e^{-\frac{1}{2} \eta^2 - s \eta} d\eta = \sqrt{\frac{2\pi}{k}} e^{s^2/2k} \quad (3.95)$$

which can easily be obtained from the integral of a Gaussian by completing the square at the exponent. With some more efforts, the above result can be

\(^{11}\)Referring to Hamiltonian (3.92) the non-zero terms of $J_{i,j}$ equal $J/4$. However, the matrix $J_{i,j}$ can describe a more general coupling among spins.
generalized to $N$ variables $\eta = (\eta_1, \eta_2, \ldots, \eta_N) \in \mathbb{R}^N$:

$$\int d\eta_1, d\eta_2 \ldots \exp \left(-\frac{1}{2} \eta^T \mathbf{M} \eta - \mathbf{s} \cdot \eta \right) d\eta_N = \sqrt{\frac{(2\pi)^N}{\det(M)}} \exp \left(\frac{1}{2} \mathbf{s}^T \mathbf{M}^{-1} \mathbf{s} \right).$$

(3.96)

Apart from a constant pre-factor, the right-hand side of Eq. (3.96) becomes equal to the term involving spin pairs in Eq. (3.94) when $M^{-1}_{ij} = \beta J_{i,j}$ and $\mathbf{s} = \mathbf{\sigma}$ are chosen. The partition function of the Ising model (in any dimension) can, thus, be written as

$$Z(B, T) = N T \mathcal{T}_r \left\{ \int d\eta_1, d\eta_2 \ldots e^{-\eta^T M^{-1} \eta / 2} e^{-\mathbf{s} \cdot \eta} d\eta_N \right\} \prod_i \cosh(h + \beta \sum_j J_{i,j} \phi_j).$$

(3.97)

where $\mathbf{h} = (h, h, \ldots, h)$ and $N$ is a constant irrelevant for magnetic observables. The trace over the variables $\{\mathbf{\sigma}\}$ appearing in Eq. (3.97) can now be performed analytically

$$\mathcal{T}_r \left\{ e^{-\sum_i (h + \eta_i) \sigma_i} \right\} = \prod_i \left\{ \sum_{\sigma_i=\pm 1} e^{-(h + \eta_i) \sigma_i} \right\} = 2^N \prod_i \cosh(h + \eta_i).$$

(3.98)

In order to write the partition function in (3.97) in a more transparent way, we make the linear change of variables $\eta = \beta J \phi$:

$$Z(B, T) = N \int d\phi_1 \ldots \exp \left(-\frac{1}{2} \beta \phi^T J \phi \right) 2^N \prod_i \cosh(h + \beta \sum_j J_{i,j} \phi_j) \ d\phi_N.$$

(3.99)

The latter is usually expressed in a more compact form

$$Z(B, T) = \int \mathcal{D}[\phi] \ e^{-\beta \mathcal{L}[\{\phi\}]}$$

(3.100)

where the symbol $\int \mathcal{D}[\phi] \propto \int \prod_i d\phi_i$ stands for the functional integral and

$$\mathcal{L}[\{\phi\}] = \frac{1}{2} \sum_{i,j} \phi_i J_{i,j} \phi_j - \beta^{-1} \sum_i \ln \left[ \cosh \left( h + \beta \sum_j J_{i,j} \phi_j \right) \right] - \beta^{-1} N \ln(2)$$

(3.101)

for the Landau free-energy functional. In this representation $Z$ has been rewritten as an average over the auxiliary fields $\phi$ of the partition function

---

*The vector $h$ has this simple form because a uniform $B$ has been assumed but – in principle – different sites could experience different external fields.*
of a paramagnet, experiencing the external field plus the auxiliary fields themselves. By doing this, we have somehow “traded” the original spin-spin interaction with the coupling (in principle site-dependent) of each spin with a set of auxiliary fields $\phi_j$. Note that no assumption has been made on such fields which can, thus, span all over $\mathbb{R}^N$.

From Eqs. (3.100) and (3.101) an implicit form for the averaged spin projections $\langle \sigma_i \rangle$ can be deduced. This is obtained straightforwardly if we let the field $h$ be site dependent:

$$
\langle \sigma_i \rangle = -\frac{1}{Z} \frac{\partial}{\partial h_i} \ln(Z) = -\langle \tanh \left( h + \beta \sum_j J_{i,j} \phi_j \right) \rangle_{\{\phi\}}, 
$$

(3.102)

where $\langle \ldots \rangle_{\{\phi\}}$ stands for average over the auxiliary fields. We will come back to this result in the following. Generally, performing the functional integral in Eq. (3.100), i.e. tracing over the auxiliary fields $\{\phi\}$, is far from being trivial. The simplest approximation which can be made to evaluate $Z$ is replacing the functional integral by the maximum value of the integrand, namely

$$
Z (B, T) = \int D[\phi] \, e^{-\beta L[\{\phi\}]} \overset{\text{MFA}}{=} \max_{\{\phi\}} \left\{ e^{-\beta L[\{\phi\}]} \right\} = \exp \left\{ -\beta \min_{\{\phi\}} \left( L[\{\phi\}] \right) \right\}
$$

(3.103)

which is known as saddle-point approximation. This is equivalent to the mean-field approximation. In fact, by requiring $\partial L/\partial \phi_i = 0$ for $\phi_i = \bar{\phi}_i$, the following equation is obtained

$$
\bar{\phi}_i = \tanh \left( h + \beta \sum_j J_{i,j} \bar{\phi}_j \right).
$$

(3.104)

As we are considering nearest-neighbor ferromagnetic exchange coupling, the solution to the previous equation turns out to be independent of the site index $i$, meaning that the field which minimizes the Landau free-energy functional is spatially homogeneous. Consequently, Eq. (3.104) is equivalent to the MF equation of state (3.16). It is worth remarking that, within this framework, only when it is evaluated in its minimum the Landau free-energy functional $L[\{\phi\}]$ acquires the meaning of Gibbs free energy:

$$
G(B, T) = -\beta^{-1} \ln(Z) \overset{\text{MFA}}{=} \min_{\{\phi\}} \left( L[\{\phi\}] \right) = L[\{\bar{\phi}\}].
$$

(3.105)

The equivalence between the MFA and the saddle-point approximation of the functional integral (3.103) allows establishing that the average of the
auxiliary fields $\phi$ is proportional to local magnetic moments. In other words, the average $\bar{\phi}$ plays the role of the Weiss field $B_W$ (apart from constant factors). As far as the critical behavior ($T \simeq T_C$) is concerned, it makes sense to expand the Landau free-energy functional for small values of the fields $\phi$. To this aim we make use of the Taylor expansion

$$\ln \cosh(x) = \frac{1}{2} x^2 - \frac{1}{12} x^4 + O(x^6) \quad \text{for} \quad x \simeq 0.$$  \hfill (3.106)

After some algebra and taking the continuum limit $\phi_i \to \phi(x)$ one obtains

$$\mathcal{L}_{\text{GL}}[\phi] = \int \left[ \frac{1}{2} J (\nabla \phi)^2 + \frac{b}{2} \phi^2 + \frac{\lambda}{4} \phi^4 \right] d^4x - \beta^{-1} N \ln(2)$$ \hfill (3.107)

with

$$\left\{ \begin{array}{l}
    b = \bar{z} J \left( 1 - \frac{1}{8} \beta \bar{z} J \right) = \bar{z} J \left( 1 - \frac{T}{T_C} \right) \simeq \bar{z} J \tau \\
    \lambda = \frac{1}{3} \beta^3 \left( \frac{1}{2} \bar{z} J \right)^4 = \frac{16}{3} \left( \frac{T}{T_C} \right)^3 k_B T_C \simeq \frac{16}{3} k_B T_C
\end{array} \right.$$ \hfill (3.108)

where we have used the fact that the MF Curie temperature is $T_C = \bar{z} J/4k_B$ for a system of spins one-half (see Eq. (3.10)). (The subscript in $\mathcal{L}_{\text{GL}}$ stands for Ginzburg-Landau). Note that in both Eqs. (3.101) and (3.107) the paramagnetic limit $\mathcal{L} = -k_B T N \ln(2)$ is recovered at high temperature, when $\beta J \to 0$ and $\phi \to 0$ ($k_B \ln(2)$ being the entropy of an isolated spin one-half).

Limiting – for the time being – ourselves to homogeneous fields $\phi(x)$, we can set the gradient term to zero. First, we remark that $\lambda$ appearing in Eq. (3.107) is always positive. On the contrary, $\tau$ can change its sign originating two different free-energy landscapes. For $\tau > 0$, the Landau functional $\mathcal{L}_{\text{GL}}$ has a minimum for $\phi = 0$ only, which clearly corresponds to the magnetically disordered phase. For $\tau < 0$, the Landau functional displays the typical Mexican-hat shape with two minima occurring at some finite $\phi = \pm \bar{\phi}$ (see Fig. 3.10). These minima are degenerate in the absence of an external field and correspond to the non-trivial solution of the MF equation of state for $T < T_C$. When $\phi = \bar{\phi}$, $\mathcal{L}_{\text{GL}}[\{\bar{\phi}\}]$ acquires the meaning of Gibbs free energy. Then, from the knowledge of the Landau free-energy functional the MF critical exponent $\alpha$ related to the specific heat can be deduced. For $T > T_C$ ($\tau > 0$), we have $\mathcal{L}_{\text{GL}}[\{\bar{\phi}\}] = -k_B T N \ln(2)$ so that the specific heat $C = -T \partial^2 \mathcal{L}_{\text{GL}}/\partial T^2 = 0$. For $T < T_C$ ($\tau < 0$), instead, $\mathcal{L}_{\text{GL}}[\{\bar{\phi}\}] = -k_B T N \ln(2) + \bar{z} J O(\tau^2)$. Therefore the specific heat is finite when $T_C$ is approached from lower temperatures. This discontinuity implies that $\alpha = 0$ within the MF theory.

Note that only even powers of $\phi$ appear in the functional $\mathcal{L}_{\text{GL}}$ in Eq. (3.107). This fact is not accidental and reflects the symmetry $\sigma_n \leftrightarrow -\sigma_n$. 
intrinsic to the problem. Landau developed his theory of phase transitions starting from the idea that the effective free energy should be an analytic function of the order parameter (which needs to be identified with $\phi$ in our approach), consistently with the requirements of symmetry of the considered problem. In fact, all the critical properties (critical exponents, etc.) derived previously in this chapter could have been obtained just postulating the form of Eq. (3.107) for the Landau free-energy functional. For the Ising model discussed here, postulating a form for $L_{GL}$ was not necessary since we could carry out the calculation from first principles (i.e., starting from Hamiltonian (3.93)). For problems characterized by less trivial symmetries and, e.g., vectorial order parameters, being able to write the Landau free-energy functional on the basis of symmetry arguments alone is often very useful. Then, performing a saddle-point approximation analogous to Eq. (3.103) one can normally deduce MF critical exponents with little mathematical efforts. Such exponents are named classical, or mean-field, critical exponents and depend only on the symmetry of the problem reflected in the functional $L_{GL}$. However, a functional built with the same symmetry criteria
can be used as a starting point for more sophisticated mathematical treatments, like the renormalization-group approach. A successful example is the theory of critical phenomena for which Kenneth G. Wilson was awarded the Nobel Prize in 1982.

3.C Landau theory of correlations

The whole mathematic derivation described above can be summarized as follows. First, we showed that the calculation of the partition function of the Ising model (for any dimension d) can be recasted into the problem

\[ Z(B, T) = \int D[\phi] e^{-\beta L[\phi]} \]  

(3.109)

from which, in principle (but not always in practice!), thermodynamic properties can be deduced. Two possible independent approximations can be made to tackle the problem stated by Eq. (3.109):

1. the saddle-point approximation, which consists in evaluating the partition function only in the minimum of the functional \( L[\phi] \) (see Eq. (3.103));

2. a Taylor expansion of \( L[\phi] \) itself for small auxiliary fields \( \phi \), which holds in the critical region (i.e., for \( T \approx T_C \)) and gives the Ginzburg-Landau functional \( L_{GL}[\phi] \).

The condition 1. requires to set to zero the functional derivative of \( L[\phi] \) with respect to \( \phi \); this leads to a self-consistent equation for the average magnetic moment that turns out to be equivalent to the MF equation of state, for every \( T \). As a consequence, by making both approximations 1. and 2. the MF critical behavior can be studied. More concretely, one can start from the Ginzburg-Landau functional in Eq. (3.107) set the gradient term to zero (because we seek for spatially homogeneous solutions) and minimize the integrand with respect to \( \phi \). This leads to the equation

\[ \bar{\phi} \left( b\bar{\phi} + \lambda \bar{\phi}^3 \right) = 0 \]  

(3.110)

whose solutions are given by

\[
\begin{align*}
\bar{\phi} &= 0 \quad \text{for } \tau > 0 \\
\bar{\phi}^2 &= -\frac{b}{\lambda} \quad \text{for } \tau < 0,
\end{align*}
\]

(3.111)
with \( b \simeq \varepsilon J \tau \) and \( \lambda \simeq 16k_B T_C/3 \).

To evaluate correlation functions we need to go slightly beyond the crude saddle-point approximation (equivalent to the MFA). In practice, we allow the field \( \phi \) to deviate slightly from the MF solution obtained for \( \tau < 0 \) (the treatment for \( \tau > 0 \) is analogous):

\[
\phi = \bar{\phi} + \delta \phi, \tag{3.112}
\]

\( \delta \phi \) being a small, random field. The integrand \( (f_{GL}) \) of the Ginzburg-Landau functional in Eq. (3.107) takes the form

\[
f_{GL}[\bar{\phi} + \delta \phi] = \frac{1}{2} J (\nabla \delta \phi)^2 + \frac{b}{2} (\bar{\phi} + \delta \phi)^2 + \frac{\lambda}{4} (\bar{\phi} + \delta \phi)^4
\]

\[
= \frac{1}{2} J (\nabla \delta \phi)^2 + \left( \frac{b}{2} + \frac{6\lambda}{4} \bar{\phi}^2 \right) \delta \phi^2 + f_{GL}[\bar{\phi}] + (\ldots) \tag{3.113}
\]

where \((\ldots)\) stands for constants, \( \mathcal{O}(\delta \phi^4) \) and odds terms in \( \delta \phi \) which vanish after spatial or thermal averaging. The first two terms in the last line of Eq. (3.113) are associated with fluctuations around the MF solution \( \bar{\phi} \). Thus, at this level of approximation, the partition function reads:

\[
Z(B, T) = e^{-\beta L_{GL}[\bar{\phi}]} + \int \mathcal{D}[\delta \phi] e^{-\beta L_{fl}[\delta \phi]} \tag{3.114}
\]

where the first term on the right-hand side corresponds to the saddle-point approximation while

\[
L_{fl}[\delta \phi] = \int \left[ \frac{1}{2} J (\nabla \delta \phi)^2 - b (\delta \phi)^2 \right] d^d x. \tag{3.115}
\]

is the functional associated with the fluctuation field \( \delta \phi(x) \). The underlying strategy of the mathematical passages described above aims at considering corrections to the saddle-point approximation which are described by a sort of quadratic Hamiltonian with respect to the fluctuation field. In fact, the functional (3.115) is formally equivalent to the potential energy of a set of coupled harmonic oscillators, described in the continuum formalism (remember that \( b < 0 \) for \( \tau < 0 \)): Thermal averages of the fluctuation field \( \delta \phi(x) \) can be computed similarly to average displacements in a system of harmonic oscillators. The gradient term in \( L_{fl}[\delta \phi] \) effectively couples the fluctuation fields \( \delta \phi(x) \) defined at different points in space, at different locations \( x \). However, the functional (3.115) can be decoupled (diagonalized) passing to the
CHAPTER 3. MAGNETIC ORDER AT FINITE TEMPERATURE

Fourier space:

\[ \mathcal{L}_{\delta \phi} = \frac{1}{(2\pi)^d} \int \frac{1}{2} (Jq^2 - 2b) |\tilde{\delta \phi}(q)|^2 d^d q. \] (3.116)

If we forget the parametric\(^{13}\) dependence on temperature of \(b\), Eq. (3.116) has the form of a quadratic Hamiltonian with respect to the independent degrees of freedom \(\tilde{\delta \phi}(q)\). Now, equipartition theorem can be applied to get

\[ \frac{1}{2} (Jq^2 - 2b) \langle |\tilde{\delta \phi}(q)|^2 \rangle_{\mathrm{fl}} = \frac{1}{2} k_B T \Rightarrow \langle |\tilde{\delta \phi}(q)|^2 \rangle_{\mathrm{fl}} = \frac{k_B T}{Jq^2 - 2b}, \] (3.117)

where the subscript reminds that \(\langle \ldots \rangle_{\mathrm{fl}}\) represents an average over the fluctuation field \(\delta \phi\).

Before proceeding, it is useful to establish a contact between the correlation function defined in Eq. (3.45) and the fluctuation field \(\delta \phi\). In the formalism of the present section we shall write the correlation function as

\[ G(x, x') = \langle \sigma(x) \sigma(x') \rangle - \langle \sigma(x) \rangle \langle \sigma(x') \rangle \]
\[ = \langle (\tilde{\phi} + \delta \phi(x)) (\tilde{\phi} + \delta \phi(x')) \rangle_{\mathrm{fl}} - \bar{\phi}^2 \]
\[ = \langle \delta \phi(x) \delta \phi(x') \rangle_{\mathrm{fl}}. \] (3.118)

By comparing Eq. (3.117) with Eq. (3.118) we obtain the following result

\[ \tilde{G}(q) = \frac{k_B T}{Jq^2 - 2b}. \] (3.119)

Note that this result corresponds to the case in which \(\tau < 0\) and hence \(b < 0\). For \(\tau > 0\), the same calculation would yield

\[ \tilde{G}(q) = \frac{k_B T}{Jq^2 + b}. \] (3.120)

Summarizing, within the Landau theory, the correlation function takes the \textit{Ornstein-Zernicke} form:

\[ \tilde{G}(q) = \frac{k_B T}{J} \frac{1}{q^2 + \xi^{-2}}, \] (3.121)

with \(\xi \sim |\tau|^{-1/2}\). As discussed at the end of Section 3.5, \(\xi\) has the meaning of correlation length. The corresponding \textit{classical} critical exponent \(\xi \sim |\tau|^{-\nu}\) is \(\nu_{\mathrm{cl}} = 1/2\).

\(^{13}\)This implicit temperature dependence, which may look strange at first sight, comes from having expanded \(\mathcal{L}_{\mathrm{GL}}[\phi]\) around its minimum: it is reasonable that coefficients of the expansion contain information about the saddle point \(\tilde{\phi}\), corresponding to the minimum.
Chapter 4

Magnetic domains and domain walls

4.1 Magnetic anisotropy

Let us go back to consider a single magnetic center. For the atom embedded in a spherically symmetric environment Hund’s rules generally succeed in predicting the observed magnetic moment. When this scenario holds, the spin “points” with the same probability along any spatial direction in the absence of an external magnetic field. Due to the reduced symmetry of the surrounding, the situation is generally different for an atom in a solid. As already seen in Part I, a first consequence is that magnetic moments are generally smaller in solids with respect to those predicted by Hund’s rules.

![Figure 4.1: Schematic representation of the energy landscape associated with a uniaxial-anisotropy term as a function of the polar coordinate \( \theta \) of a classical spin.](image)
(remember the quenching of the angular momentum). Another implication is that magnetic moments (effective spins) prefer to lie along some crystallographic directions. This tendency is taken into account by introducing a magnetic anisotropy energy which is function of the effective-spin projections along the crystallographic axes. The simplest anisotropy term that can be considered in single-spin Hamiltonian is

\[ \mathcal{H}_A = -D(\hat{S}_z)^2. \]  

(4.1)

Notice that the symmetry \( \hat{S}_z \to -\hat{S}_z \) is not broken by such an anisotropy term. Additional terms which combine higher powers of the single-spin operators may arise according to the symmetry of the lattice in which the magnetic atom is embedded (or according to the symmetry of the substrate for adatoms). For example, in the case of a crystal lattice with cubic symmetry the first non-zero anisotropy term is a fourth-order combination of the spin operators; thus in this case the term in Eq. (4.1) vanishes.

The physical mechanism which couples the spin degrees of freedom with the spatial degrees of freedom is the spin-orbit interaction.

**Magnetic anisotropy away from the bulk**

![Figure 4.2: Ab-initio calculation of the magnetic anisotropy energy, \( DS^2 \), and the magnetic moment per Co atom on Pt(111). Values in brackets have been computed with a different computational method. Remember that 1 meV \( \simeq 11.6 \) K (C. R. Physique 6 p. 75 (2005)).](image)

As stated above, a crucial ingredient for magnetic anisotropy to arise is the reduced symmetry of the surrounding, “seen” by a magnetic atom in a solid, with respect to the spherical symmetry (Hund’s rules). It is not surprising that a further increase of the anisotropy is observed when the symmetry of the environment is further reduced. This happens, e.g., when magnetic atoms are arranged in clusters (0d) or in 1d and 2d nanostructures. In Fig 4.2
CHAPTER 4. MAGNETIC DOMAINS AND DOMAIN WALLS

Figure 4.3: Experimental results: magnetic anisotropy energy $DS^2$ (right, (b)), and magnetic moment per Co atom on Pt(111) (left, (a)) C. R. Physique 6 p. 75 (2005).

Theoretical predictions (from \textit{ab initio} calculations) for different aggregates of Co atoms on a Pt(111) surface are reported. Notice that when passing from a single atom to five atoms the value of the magnetic anisotropy per atom already decreases of one order of magnitude. The magnetic moment per atom also decreases with increasing the number of atoms. This fact is instead associated with the degree of hybridization of magnetic orbitals, which becomes more and more significant when the bulk limit is approached. The theoretical predictions of Fig 4.2 are in qualitative agreement with the experimental results reported in Fig 4.3. Indeed, the fact that the magnetic anisotropy increases up to a factor $10^3$ when approaching the atomic scale is a good trend in view of magnetic-storage applications.

**Classical approximation**

If the operator in Eq. (4.1) is substituted by a classical spin, the anisotropy energy reads

$$
\mathcal{H}_A = -DS^2 \cos^2 \theta.
$$

(4.2)

Depending on the sign of $D$, the energy (4.2) has either one minimum for $\theta = \pi/2$ ($D < 0$) or two minima for $\theta = 0, \pi$ ($D > 0$), which describes the two physical situations

$$
D < 0 \quad \text{easy plane}
$$

$$
D > 0 \quad \text{easy axis / uniaxial}.
$$

(4.3)
For the easy-axis case, $D > 0$ (see Fig. 4.1), only few configurations around $\theta = 0$ or $\theta = \pi$ will be statistically relevant for $k_B T \ll DS^2$. In other words, the spin will spend about half of the time visiting configurations for which $\theta \approx 0$ and half of the time around $\theta \approx \pi$. For $k_B T \ll DS^2$, the escape rate from each one of the two wells is $\nu = \nu_0 e^{-DS^2/k_B T}$, so that the relaxation time diverges exponentially as:

$$\tau_A \sim e^{DS^2/k_B T}. \tag{4.4}$$

This time represents the average time it takes the system to jump from one minimum of Fig. 4.1 to the other.

### 4.2 Finite size and superparamagnetic limit

For the 1d Ising model, through the inequalities in Eq. (3.31), we commented that for small enough system sizes ferromagnetism – possibly present at $T = 0$ – is stable against thermal fluctuations. Indeed, Eqs. (3.69) allow drawing similar conclusions for system with continuous symmetry: both for $d=1$ and $d=2$ ferromagnetism is not destroyed at finite temperature if the system is small enough. Under this condition, the averages of transverse spin components do not necessarily diverge and the inequality $\langle (S^\alpha)^2 \rangle \ll \langle (S^z)^2 \rangle$ may be fulfilled.

Bistability is a crucial property for most of the applications of nanosized magnets (nanomagnetism). Thus an important question to be addressed is: “what do we understand for bistability when dealing with a real nanomagnet?” Rephrasing what we have just stated about small enough systems, we can answer that when a magnetic lattice does not extend indefinitely, correlations – either of short- or long-range nature – may always develop; the system as a whole then behaves like a giant classical spin. In the presence of uniaxial anisotropy, similar arguments as for a single classical spin (macrospin), described by Eq. (4.2), then apply. In particular, the most relevant quantity is the average escape rate from the minima of the total anisotropy energy, located at $\theta = 0, \pi$ (see Fig. 4.1). One possible way to pass from one of the two configurations to the other one is a rigid (coherent) rotation of all the spins$^1$.

The relaxation time for such a mechanism is nothing but a generalization of Eq. (4.4):

$$\tau \sim e^{DS^2/k_B T}. \tag{4.5}$$

$^1$For mesoscopic systems, processes which involve non-uniform magnetization reversal may be more convenient.
with \( v = N_x N_y N_z \). Often the magnetic anisotropy is defined per unit volume \( K_v = D/a^3 \) so that the usual volume \( V = a^3 N_x N_y N_z \) can be used in Eq. (4.5). Due to the exponential dependence on the system size, the characteristic time given in Eq. (4.5) can become very large even for nanomagnets. Referring again to Fig. 4.1, assume to magnetize the system by means of an external field, thus lowering the energy of one of the two minima corresponding to opposite magnetization. This essentially allows preparing the system in a chosen state. Then remove the external field. Now, due to the exponential divergence of Eq. (4.5), the system may behave as if it had undergone a magnetic phase transition, i.e. it may show a remanent magnetization. **But** such a situation corresponds to

- a metastable state
- which is not an equilibrium state (one cannot associate to it a free energy \( G \) in the same meaning as, e.g., in chapter 3).
- If one could wait long enough, \( t \gg \tau \), an average zero magnetization would be obtained (in the absence of an external field).
- A similar scenario is recovered irrespectively of the dimensionality of the lattice as far as \( \xi > N_\nu \) for all \( \nu = x,y,z \).

**Superparamagnetic limit**

For magnetic memory manufacturing, the quest to increase the density of data storage calls for reducing the linear dimensions of nanomagnets. Even if reducing the linear dimensions of a magnetic unit prevents the occurrence of a magnetic phase transition, one can just require that bistability holds for “long enough”. The required time over which one can reasonably assume that a nanomagnet remains in the desired metastable state depends on the practical application it is supposed to be used for. **But**, according to Eq. (4.5) and more general approaches, the relaxation time decreases when reducing the linear size of a nanomagnet. As a consequence, when the total volume becomes too small bistability is lost. This intrinsic constraint to the linear dimensions of a bistable magnetic unit is called superparamagnetic limit.

**4.3 Domain walls in the classical Heisenberg model**

In chapter 2 we gave a justification for the use of the Heisenberg exchange interaction which is isotropic. If we add to the classical Heisenberg Hamilto-
nian (Eq. (3.3)) an anisotropy term like the one in Eq. (4.1) we get
\[
\mathcal{H} = -\frac{1}{2} J \sum_{|\mathbf{n}-\mathbf{n}'|=1} \hat{S}(\mathbf{n}) \cdot \hat{S}(\mathbf{n}') + g\mu_B \sum_{\mathbf{n}} \mathbf{B} \cdot \hat{S}(\mathbf{n}) - D \sum_{\mathbf{n}} (\hat{S}^z(\mathbf{n}))^2. \tag{4.6}
\]

When \( D \) becomes large with respect to \(|J|\), the model described by Hamiltonian (4.6) can be replaced with the two following models
\[
\frac{D}{|J|} \rightarrow +\infty \quad \text{Ising model} \tag{4.7}
\]
\[
\frac{D}{|J|} \rightarrow -\infty \quad \text{XY / planar model}.
\]

### Domain walls: discrete lattice

In the following, we consider the Hamiltonian (4.6) taking:

- \( D > 0 \), uniaxial anisotropy
- \( J > 0 \), ferromagnetic exchange interaction (parallel alignment of nearest-neighboring spins is favored).

The study of the model described by the Hamiltonian (4.6) can be significantly simplified by substituting the quantum spin operators \( \hat{S}(\mathbf{n}) \) with classical vectors \( \mathbf{S}(\mathbf{n}) \). This simplification is justified by thinking that a sort of “collective” spin can be associated with a group of spins coupled ferromagnetically \((J > 0)\). Such groups can emerge in a magnetic system due to either long-range order or short-range correlations. In the latter case, the correlation length needs to be large enough. In both situations the collective spin can be so large that its quantum-mechanical character becomes negligible\(^2\).

In the appropriate temperature regimes, the results are then the same if the classical approximation is assumed at the level of single effective spins.

For many theoretical and applicative aspects of magnetism, **domain walls**, i.e. the boundaries between regions with opposite magnetization, play a crucial role. In particular, their structure and the energy associated with the creation of a domain wall in a uniformly magnetized configuration are

\(^2\)Remarkably, in this sense the classical-spin approximation is more justified for low temperatures than for high ones. In the paramagnetic limit \((k_B T/J >> 1)\) one has to recover a behavior described by the Brillouin function, in which the quantum nature of each spin is relevant \((S^2 \rightarrow S(S + 1))\).
relevant (see sketch in Fig. 3.2 for the Ising case). These features can be evaluated letting the spin direction vary only along one spatial direction. This *effectively* reduces the problem to a mono-dimensional one:

$$\mathcal{H}_H = -\sum_{i=1}^{N_x} \left[ J \vec{S}_i \cdot \vec{S}_{i+1} + D (S^z_i)^2 \right], \quad (4.8)$$

where $\vec{S}_i$ are classical spins and the constants $J$ and $D$ have to be thought of per unit length or per unit surface if the dimensionality of the original lattice was $d=2$ or $d=3$, respectively.

With the Hamiltonian (4.8), the domain wall can be larger than one lattice spacing. In fact, spreading the wall over more than one lattice spacing reduces the global exchange-energy cost. On the other hand, the anisotropy term would favor configurations with as less spins misaligned to the easy axis, $z$, as possible. The domain-wall profile results from the *competition* between these two energies (two opposite limits are reported in the insets of Fig. 4.4).

The lowest-energy deviations from the uniform state can be parameterized

Figure 4.4: One-wall energy in $J$ units *vs* $D/J$: minimum energy solution of the non-linear equation (4.11) computed numerically (solid line); continuum limit solution (dashed line). Inset: spin profile *vs* lattice distance: sharp wall (low-right) and broad wall for $D/J = 10^{-2}$ (up-left).
through the angle that each spin forms with the $z$ axis, $\theta$, as

$$\mathcal{E}_H = \sum_{i=1}^{N_x} \left[ J - J \cos (\theta_{i+1} - \theta_i) + D \sin^2 \theta_i \right].$$

(4.9)

The energy cost for creating a domain-wall in a uniformly magnetized configuration is given by the spin profile which fulfills the boundary conditions

$$\begin{cases}
\theta_1 = \pi \\
\theta_{N_x} = 0
\end{cases}$$

(4.10)

and minimizes the energy (4.9) with respect to $\theta_i$:

$$\frac{\partial \mathcal{E}_H}{\partial \theta_i} = \sin (\theta_i - \theta_{i-1}) - \sin (\theta_{i+1} - \theta_i) + \frac{D}{J} \sin (2\theta_i) = 0.$$  

(4.11)

Eq. (4.11) can be solved numerically and the solution provides the spin profile with respect to which the energy (4.9) is stationary. The true lowest-energy profile can be obtained comparing different solutions, among which the sharp-wall profile (see lower-right inset of Fig. 4.4):

$$\begin{cases}
\theta_i = \pi & \text{for } 1 \leq i < \frac{N_x}{2} \\
\theta_i = 0 & \text{for } \frac{N_x}{2} \leq i \leq N_x
\end{cases}$$

(4.12)

which is also a solution of (4.11). In Fig. 4.4 the resulting energy (solid line) is compared with that obtained from a continuum limit calculation (dashed line) – that we are going to present in the next paragraph – as a function of the ratio $D/J$.

### 4.4 Continuum formalism

Referring to the classical version of Hamiltonian (3.3), we rewrite in a different way the exchange-interaction term:

$$\mathcal{H}_{exch} = -\frac{1}{2} J \sum_{|n-n'|=1} \vec{S}(n) \cdot \vec{S}(n') = -J \sum_{n} \sum_{\mu} \vec{S}(n) \cdot \vec{S}(n + e_\mu)$$

(4.13)

where $\mu = x, y, z$ (spatial directions) and $e_\mu$ is the unit vector along $\mu$. Notice that

$$\left| \vec{S}(n) - \vec{S}(n + e_\mu) \right|^2 = \left| \vec{S}(n) \right|^2 + \left| \vec{S}(n + e_\mu) \right|^2 - 2 \vec{S}(n) \cdot \vec{S}(n + e_\mu).$$

(4.14)
With the hypothesis that the direction along which each classical spin \( \vec{S}(n) \) is pointing varies smoothly from one lattice site to the other (index \( n \)), one can describe \( \vec{S}(n) \) as a vector field which is a smooth function of a continuum spatial variable \( r = an, a \) being the lattice spacing. This approximation is justified

- In the classical isotropic Heisenberg chain \((D = 0)\) at low temperatures. In fact, the lowest lying excitations – which actually destroy ferromagnetism for \( d \leq 2 \) – are spin-waves with very long wavelength (in the following we will show that for small wave vectors \(|q| \rightarrow 0\) the spectrum of fluctuations is gapless).

- When the walls separating domains with opposite spin directions are broad enough. Further on, we will render this statement quantitative. In the presence of ferromagnetic \((J > 0)\) exchange interaction and uniaxial anisotropy \((D > 0)\), such a requirement is fulfilled for \( J \gg D \).

Thus one has,

\[
\vec{S}(n + e_\mu) - \vec{S}(n) \approx \vec{S}(r + ae_\mu) - \vec{S}(r) \approx a \partial_\mu \vec{S}(r) \quad (4.15)
\]

where in the first passage we have taken the continuum limit and in the second one we have performed a Taylor expansion. Combining Eq. (4.14) with Eq. (4.15), the exchange interaction between the spin located in \( r \) and half of its nearest neighbors is obtained

\[
\begin{align*}
- J \sum_\mu \vec{S}(n) \cdot \vec{S}(n + e_\mu) \\
\approx \frac{1}{2} Ja^2 \sum_\mu \left| \partial_\mu \vec{S}(r) \right|^2 - J \sum_\mu \left| \vec{S}(r) \right|^2 \\
= \frac{1}{2} Ja^2 \sum_{\mu,\nu} (\partial_\mu S^\nu(r) \cdot \partial_\mu S^\nu(r)) - J \bar{\varepsilon} \sum_\nu (S^\nu(r) \cdot S^\nu(r))
\end{align*}
\]

(4.16)

with \( \bar{\varepsilon} \) number of nearest neighbors and \( \nu = x, y, z \) label of the spin components. Normally, the first term is written as

\[
\left| \nabla \vec{S}(r) \right|^2 = \sum_{\mu,\nu} (\partial_\mu S^\nu(r) \cdot \partial_\mu S^\nu(r)) = \\
= (\partial_x S^x(r))^2 + (\partial_y S^y(r))^2 + (\partial_z S^z(r))^2 \\
+ (\partial_x S^y(r))^2 + (\partial_y S^x(r))^2 + (\partial_z S^y(r))^2 \\
+ (\partial_x S^z(r))^2 + (\partial_y S^z(r))^2 + (\partial_z S^z(r))^2.
\]

(4.17)
Taking the usual continuum limit for the sum
\[ \sum \ldots \simeq \frac{1}{a^d} \int \ldots d^d x, \] (4.18)
the classical and continuum version of Hamiltonian Eq. (4.6) is finally obtained
\begin{align*}
\mathcal{H} &= \frac{1}{2} J a^{2-d} \int \left| \nabla \vec{S}(\mathbf{r}) \right|^2 d^d x - J \frac{z}{2} \frac{1}{a^d} \int \left| \vec{S}(\mathbf{r}) \right|^2 d^d x \\
&\quad - D \frac{1}{a^d} \int |S^z(\mathbf{r})|^2 d^d x + \mu_B g \frac{1}{a^d} \int \vec{B} \cdot \vec{S}(\mathbf{r}) d^d x.
\end{align*}
(4.19)

Within the continuum model the field \( \vec{S}(\mathbf{r}) \) can be simplified as a two-component vector field or as a scalar field (see the two limits (4.7)). However, some additional constraints or effective energy terms are normally introduced in place of the stringent constraint on the spin modulus \( \left| \vec{S}(\mathbf{r}) \right|^2 = S^2 \). Of course, the latter condition is automatically fulfilled if each spin is parameterized with polar coordinates
\begin{align*}
S^x(\mathbf{r}) &= S \sin(\theta(\mathbf{r})) \cos(\varphi(\mathbf{r})) \\
S^y(\mathbf{r}) &= S \sin(\theta(\mathbf{r})) \sin(\varphi(\mathbf{r})) \\
S^z(\mathbf{r}) &= S \cos(\theta(\mathbf{r})).
\end{align*}
(4.20)

Broad domain walls: continuum limit

To the aim of computing the domain-wall energy in the continuum limit, we let the polar angles (4.20) be a function of one spatial variable only, say \( x \). For \( B = 0 \), the Hamiltonian (4.19) can then be written as
\begin{align*}
\mathcal{H} &= \frac{1}{2} J N_y N_z a S^2 \int \left[ \left( \frac{d\theta}{dx} \right)^2 + \sin^2(\theta(x)) \left( \frac{d\varphi}{dx} \right)^2 \right] dx \\
&\quad - D N_y N_z S^2 \frac{1}{a} \int \cos^2(\theta(x)) dx + \text{const}
\end{align*}
(4.21)

where we have implicitly assumed the integration domain to be a parallelepiped \( N_x N_y N_z a^3 \). The functional Eq. (4.21) can be minimized with respect to the functions \( \theta(x) \) and \( \varphi(x) \). The corresponding Euler-Lagrange equation is
\begin{equation}
\begin{cases}
J a \sin^2(\theta(x)) \frac{d^2 \theta}{dx^2} + 2 J a \sin(\theta(x)) \cos(\theta(x)) \left( \frac{d\theta}{dx} \right) \left( \frac{d\varphi}{dx} \right) = 0 \\
J a \frac{d^2 \varphi}{dx^2} - J a \sin(\theta(x)) \cos(\theta(x)) \left( \frac{d\varphi}{dx} \right)^2 - 2 \frac{D}{a} \sin(\theta(x)) \cos(\theta(x)) = 0.
\end{cases}
\end{equation}
(4.22)
The solution to Eq. (4.22) – which imposes minimization of the energy – with boundary conditions

\[
\begin{align*}
\lim_{x \to -\infty} \theta(x) &= \pi \\
\lim_{x \to +\infty} \theta(x) &= 0
\end{align*}
\]

is given by

\[
\begin{align*}
\cos(\theta(x)) &= \tanh\left(\frac{x}{\delta}\right) \\
\phi(x) &= \text{const.}
\end{align*}
\]

with \(\delta = a\sqrt{J/(2D)}\). Such a solution was proposed by Landau and Lifshitz in 1935.

The energy density associated with the spin profile (4.24) is \(E_w = 2\sqrt{2}S^2\sqrt{DJ}\) (per unit length for \(d=2\) and per unit surface for \(d=3\)). In Fig. 4.4 the domain-wall energy obtained numerically for the discrete-lattice calculation (solid line) is compared with that obtained in the continuum limit (dashed line) as a function of the ratio \(D/J\). The agreement is already good for ratios \(D/J < 0.3\). In the opposite limit, the discrete lattice calculation recovers the domain-wall energy of the Ising model \(E_w = 2JS^2\) (sharp domain wall defined by Eqs. (4.12)).

In those relevant limits one has

\[
\begin{align*}
J \ll D &\Rightarrow \delta = a \\
J \gg D &\Rightarrow \delta = a\sqrt{\frac{J}{2D}} > 1
\end{align*}
\]

and \(E_w = 2S^2J\) and \(E_w = 2\sqrt{2}S^2\sqrt{DJ}\).

For \(J \ll D\), the wall-energy cost equals the Ising case and follows from having \(\delta = a\). Concerning \(J \gg D\), \(E_w\) is one-soliton energy\(^3\). As one can appreciate in Fig. 4.4, the two regimes are very well recovered and the transition region, where none of the two limits (4.25) is expected to hold, is surprisingly narrow. The crossover between the sharp-wall (\(\delta = a\)) and the broad-wall (\(\delta > a\)) regime\(^4\) occurs at \(D/J = 2/3\).

In summary, the conditions (4.25) provide a criterion for the simplification of the classical Heisenberg model in terms of

\[
\begin{align*}
\text{Ising model} &\quad D/J \geq 2/3 \\
\text{continuum limit} &\quad D/J \leq 0.3
\end{align*}
\]

\(^3\)Sometimes the domain-wall width is defined with some numerical factors of difference with respect to \(\delta: \pi\sqrt{J/(2D)}\) or \(\sqrt{2J}/D\) for instance.

\(^4\)The crossover ratio \(D/J = 2/3\) can be obtained analytically by analyzing the stability of the sharp-wall profile, Eqs. (4.12), against small deviations between successive angles \(\theta_i\) (B. Barbara, *Journal de Physique* 34, p. 139 (1973)).
Typically, metallic nanowires of technological relevance fall in the broad-wall regime. In fact, materials like Co, Ni, Fe or Permalloy are characterized by $D \simeq 1 - 10$ K ($\sim 0.1 - 1$ meV) and $J \simeq 100 - 500$ K ($\sim 10 - 50$ meV) corresponding to a domain-wall width of the order $10 - 100$ nm.
4.5 Dipolar interaction

Let us focus on a material that fulfills all the ground-state requirements to give rise to ferromagnetism, as defined in the first two chapters and summarized at the beginning of chapter 3. Assume that ferromagnetism has also “survived” at finite temperatures, meaning that there is a phase with spontaneous magnetization, which requires

- the dimensionality of the magnetic lattice to be \( d \geq 2 \) for systems with uniaxial anisotropy (Ising-like)
- the dimensionality of the magnetic lattice to be \( d = 3 \) for systems with continuous symmetry (Heisenberg or XY).

In the first class of materials ferromagnetism is destroyed by thermally excited domain walls for \( T > T_C \) (with \( T_C = 0 \) for \( d = 1 \)). In systems with continuous symmetry ferromagnetism is destroyed by thermally excited spin waves (or linear excitations in general) for \( T > T_C \) (with \( T_C = 0 \) for \( d = 1, 2 \)). Now the question is: is there any other mechanism that can destroy or frustrate the “surviving” ferromagnetism? The answer is positive; namely, the dipole-dipole magnetostatic interaction neglected in the previous chapters generally acts in this sense. Some exceptions to this general trend are represented by special sample geometries – briefly discussed towards the end of this chapter – for which dipolar interaction stabilizes ferromagnetism.

Magnetostatic dipole-dipole interaction

The pairwise dipolar interaction arises directly from Maxwell equations and reads

\[
\mathcal{H}_{dd} = \frac{\mu_0}{4\pi} \left[ \frac{\vec{\mu}_1 \cdot \vec{\mu}_2}{r_{12}^3} - 3 \left( \frac{\vec{\mu}_1 \cdot \vec{r}_{12}}{r_{12}^5} \right) \left( \frac{\vec{\mu}_2 \cdot \vec{r}_{12}}{r_{12}^5} \right) \right].
\]

For our purposes, pointlike dipoles are the magnetic moments of each magnetic atom in the classical approximation \( \vec{\mu}_i = -g\mu_B \vec{S}_i \) (\( i = 1, 2 \))\(^5\) and \( \vec{r}_{12} = \vec{r}_1 - \vec{r}_2 \). Since thermal effects may be considered at different levels of approximation, we prefer to distinguish the ground-state magnetic moment \( \vec{\mu}_i = -g\mu_B \vec{S}_i \) from its thermal average \( \vec{m}_i = \langle \vec{\mu}_i \rangle_{th} \) introduced in the previous chapter. The typical strength of the dipole-dipole energy is generally small compared to the exchange energy. However, its characteristics impose to handle the dipolar interaction with extreme caution.

\(^5\)For other applications \( \vec{\mu}_i \) could be, e.g., the electron or the nucleus magnetic moments.
1. Consider just two pointlike magnetic moments that interact via the dipole-dipole interaction (4.27): The sign and the intensity of the dipolar interaction strongly depend on the relative orientation of the two interacting magnetic moments and on their relative spatial position \( r_{12} \).

2. In contrast to the exchange interaction, the dipolar interaction couples spins located indefinitely far from each other and the decay of its strength with the distance is relatively slow: \( 1/r^3 \) (long-ranged).

**Equally spaced dipoles**

![Figure 4.5: Different sample configurations of two dipoles \( \vec{\mu}_i \) \((i = 1, 2)\), placed at a fixed distance \( r_{12} \). The different values of the interaction energy, \( E \), are given in units \( E_{dd} = \frac{\mu_0}{4\pi} \frac{\mu^2}{r_{12}^3} \).]

To fix the ideas about point 1), let us consider two dipoles at a fixed distance so that the relevant energy scale is given by \( E_{dd} = \frac{\mu_0}{4\pi} \frac{\mu^2}{r_{12}^3} \). Referring to the configurations in Fig. 4.5, it is clear that when for some reasons (other energies or geometrical constraints)

- two interacting magnetic moments are forced to lie perpendicularly to the direction of \( \vec{r}_{12} \), then the antiparallel alignment is favored by the dipolar interaction (cases a) and b) in Fig. 4.5);

- two interacting magnetic moments are forced to lie along the direction of \( \vec{r}_{12} \), then the dipolar interaction favors their parallel alignment (cases c) and d) in Fig. 4.5).

In an absolute sense, the configuration c) has the lowest energy of those reported in Fig. 4.5.
Parallel dipoles

In order to evaluate the dependence of the energy \((4.27)\) on the relative orientation in space of the two point-like dipoles, \(\vec{\mu}_1\) and \(\vec{\mu}_2\), it can be useful to set the origin of the spatial coordinates in \(\vec{\mu}_1\), with the \(z\) axis parallel to the direction of \(\vec{\mu}_1\) itself. Then choose \(\vec{\mu}_1 \parallel \vec{\mu}_2\). The resulting energy only depends on the polar angle \(\theta\) defined as the angle that the vector \(\vec{r}_{12}\) forms with the \(z\) axis of our reference frame or, equivalently, with any of the two parallel magnetic moments, \(\vec{\mu}_1\) and \(\vec{\mu}_2\). Within this geometry, the interaction energy \((4.27)\) reduces to

\[
\mathcal{H}_{dd} = \frac{\mu_0 \mu_1 \mu_2}{4\pi r_{12}^3} (1 - 3\cos^2 \theta). \tag{4.28}
\]

Eq. \((4.28)\) is very interesting because it shows that the dipole-dipole interaction is

- \textbf{ferromagnetic} for \(\theta \in [0, \theta_M]\) and \(\theta \in [\pi - \theta_M, \pi]\)
- \textbf{antiferromagnetic} for \(\theta \in [\theta_M, \pi - \theta_M]\)

Figure 4.6: Plot of the interaction energy \((4.28)\) as a function of the polar angle \(\theta\) (rad). The energy values, \(E\), are given in units \(E_{dd} = \mu_0 \mu_1 \mu_2 / 4\pi r_{12}^3\). Regions with \(E < 0\) correspond to \textbf{ferromagnetic} coupling, while regions with \(E > 0\) correspond to \textbf{antiferromagnetic} coupling.
where $\theta_M$ is the *magic angle* such that $\cos^2(\theta_M) = 1/3$ (see Fig. 4.6). Exactly at the magic angle the dipolar interaction vanishes, meaning that in this geometrical configuration the two magnetic moments don’t “feel” each other, for what concerns the dipolar interaction.

![Diagram](image)

**Figure 4.7**: Dipolar-frustrated configurations. a) The vectors $\vec{r}_{12}$, $\vec{r}_{23}$ and $\vec{r}_{13}$ lie all on the same plane and all the magnetic moments are constrained to be aligned along the indicated direction: up (green) or down (violet). b) and c) All the four dipoles are assumed to lie onto the same plane; the red “F” indicates the *frustrated* bonds and black “S” *satisfied* bonds.

Fig. 4.7 evidences how the dipolar interaction easily introduces *frustration* as far as more than two magnetic moments are considered. The configuration a) in Fig. 4.7 represents three magnetic moments magnetized out of plane lying at the vertices of an equilateral triangle. The spins at the bottom of the sketch (up-green and down-violet) minimize their interaction energy by aligning antiparallelly to each other, as in the case of Fig. 4.5 b. Then, according to Fig. 4.6, the two bonds $r_{13}$ or $r_{23}$ correspond to ferromagnetic coupling because for these specific cases $\theta = \pi/6 < \theta_M$. Thus both states up or down of the third spin – the one located at the upper vertex – will produce the frustration of one of the two bonds $r_{13}$ or $r_{23}$.

Fig. 4.7 b) and c) refer to a situation in which the four magnetic moments lie onto the same plane. Due to the fact that the configuration c) of Fig. 4.5 is to the global minimum of the two-dipole interaction, the vertical bonds are first fulfilled (ferromagnetic). The horizontal bonds (antiferromagnetic) and the diagonal bonds (ferromagnetic) cannot be satisfied at the same time, so that some frustration is introduced anyway: frustrated bonds are highlighted with red. A detailed calculation shows that, eventually, the configuration in Fig. 4.7 c has a lower energy for a square lattice.

The triangle (a) and the square (b) of Fig. 4.7, can be thought of as unit cells of a 2d triangular and square lattice respectively: one can easily imagine that, when passing to the thermodynamic limit, many different configurations will
have the same, or nearly the same, energy. This fact typically gives rise to very complex behaviors, such as glassiness, metastability, order induced by disorder, spin-ice behavior, etc.

4.6 Dipolar interaction in extended systems

In extended systems, the dipolar interaction (4.27) is always present and it involves all the magnetic moments. The resulting contribution to the total energy is

\[
\mathcal{H}_{\text{dip}} = \frac{1}{2} \frac{\mu_0}{4\pi} \sum_{\mathbf{n} \neq \mathbf{n}'} \left[ \frac{\mathbf{\mu}_\mathbf{n} \cdot \mathbf{\mu}_\mathbf{n}'}{r_{\mathbf{n}\mathbf{n}'}^3} - 3 \left( \frac{\mathbf{\mu}_\mathbf{n} \cdot \mathbf{r}_{\mathbf{n}\mathbf{n}'}}{r_{\mathbf{n}\mathbf{n}'}^5} \right) \left( \frac{\mathbf{\mu}_\mathbf{n}' \cdot \mathbf{r}_{\mathbf{n}\mathbf{n}'}}{r_{\mathbf{n}\mathbf{n}'}^5} \right) \right]
\]

(4.29)

where the sum is extended over all the different couples (note the factor 1/2!) labeled by \( \mathbf{n} \) and \( \mathbf{n}' \), and \( r_{\mathbf{n}\mathbf{n}'} = a(\mathbf{n} - \mathbf{n}') \) (of course the modulus is \( r_{\mathbf{n}\mathbf{n}'} = a |\mathbf{n} - \mathbf{n}'| \)). Evaluating the term (4.29) is usually complicated analytically and computationally expensive in numerical calculations (due to the long-range character of the dipolar interaction). Thus, in practice, one tries to neglect the dipolar contribution or simplify it taking advantage from the fact that the dipole-dipole interaction normally has a much smaller strength than the exchange interaction. With the help of Table 3.1 one can easily get convinced of this. The strength of the nearest-neighbor dipolar interaction is \( \frac{\mu_0 (g\mu_B S)^2}{4\pi a^3} = M_0^2 a^3 \) (if the saturation magnetization \( M_0 \) is expressed in the Gauss system, \( M_0^2 \) has the units erg/cm\(^3\)). Putting the proper numbers one finds that this energy is of the order of few Kelvins or smaller. However, there are cases in which the dipolar interaction may affect crucially the macroscopic behavior of a magnetic system. In the following we will give some examples.

**Continuum limit**

The continuum version of the dipolar energy given in Eq. (4.29) can be obtained by setting \( \mathbf{\mu}_\mathbf{n} = -g\mu_B \mathbf{S}_\mathbf{n} \) followed by the usual substitution

\[
\sum \cdots \approx \frac{1}{a^d} \int \cdots d^d r,
\]

(4.30)
which yields

\[
\mathcal{H}_{\text{dip}} = \frac{\mu_0 (g\mu_B S)^2}{8\pi a^3} \frac{1}{a^{2d-3}} \int d^d r \int d^d r' \frac{\vec{S}(\vec{r}) \cdot \vec{S}(\vec{r}')}{|\vec{r} - \vec{r}'|^{3}} d^d r' - \\
-3 \frac{\mu_0 (g\mu_B S)^2}{8\pi a^3} \frac{1}{a^{2d-3}} \int d^d r \int \left\{ \frac{\vec{S}(\vec{r}) \cdot (\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|^5} \right\} d^d r' + \\
+ \frac{\mu_0 (g\mu_B S)^2}{6 a^3} \frac{1}{a^{2d-3}} \int d^d r \int \vec{S}(\vec{r}) \cdot \vec{S}(\vec{r}') \delta(\vec{r} - \vec{r}') d^d r' \tag{4.31}
\]

The unit lengths \(a\) have been grouped in such a way that the characteristic energy scale of the dipolar interaction \(\Omega = \frac{\mu_0 (g\mu_B S)^2}{4\pi a^3}\) is separated from the geometrical terms. The term \(\delta(\vec{r} - \vec{r}')\) arises from a detailed magnetostatic calculation. It essentially accounts for the fact that the pointlike-dipole approximation has to include this term to compensate the divergence at short distances, \(\vec{r} \simeq \vec{r}'\). Thus the total magnetostatic energy is not ill-defined.

**Bulk magnets**

An estimate of the dipolar interaction energy of one magnetic moment with all the others is given by the following integral

\[
\int_{N^d} \frac{d^d r}{r^3} \tag{4.32}
\]

that is convergent for \(d<3\) but diverges logarithmically for \(d=3\). Actually, the anisotropy of the dipole-dipole interaction reduces the divergence. In three dimensions, the magnetostatic energy is said to be conditionally convergent: for uniformly magnetized bodies its value is finite but depends on the shape of the sample (see paragraph 4.6). A robust, but often overlooked, theorem of statistical physics demonstrates that a phase with uniform magnetization cannot be the ground state in the thermodynamic limit. Therefore – to some extent – we have to restart from zero-temperature configurations and evaluate under which exceptional conditions dipolar interaction does not prevent the occurrence of ferromagnetism.

Let us express Eq. (4.29) as

\[
\mathcal{H}_{\text{dip}} = -\frac{1}{2} \sum_n \vec{\mu}_n \cdot \vec{B}^\text{ext}_n \tag{4.33}
\]
with $\vec{B}_{\text{ext}}$ magnetic induction created at the position of the magnetic moment $\vec{\mu}_n$ by all the other magnetic dipoles in the sample. This field can also be expressed through the continuous magnetization density (or simply magnetization), $\vec{M}(r)$, introduced in elementary courses as a coarse-grained quantity. In fact, $\vec{M}(r)$ already represents an average over an elementary volume whose magnetic moment is $\vec{\mu} = \vec{M}(r)d^3r$. Replacing the magnetic moment $\vec{\mu}_n$ with a uniformly magnetized sphere, its own contribution to the field $\vec{B}$ at its location can be estimated: $\vec{B}_{\text{sph}}(r) = \frac{2}{3}\mu_0\vec{M}(r)/\mu_0$. Therefore, the magnetic induction created inside this infinitesimal spherical cavity (Lorentz cavity) by all sources outside it is equal to the total magnetic induction minus the self contribution, that is

$$B_{\text{ext}}^n = \vec{B} - \frac{2}{3}\mu_0\vec{M} = \mu_0\left(\vec{H} + \frac{1}{3}\vec{M}\right),$$

where the definition $\vec{B} = \mu_0\left(\vec{H} + \vec{M}\right)$ has been used in the last passage. In the standard formalism of macroscopic electromagnetism, the magnetostatic energy given in Eq (4.33) then reads

$$\mathcal{H}_{\text{dip}} = -\frac{\mu_0}{2} \int_{V_M} \left(\vec{H}(r) + \frac{1}{3}\vec{M}(r)\right) \cdot \vec{M}(r)d^3r. \quad (4.35)$$

The integral is restricted to the volume $V_M$ of the magnetized body, i.e. where $M \neq 0$. However, noting that the region in which $M = 0$ will not contribute to the integral, $V_M$ can be extended to the whole space. This allows rewriting\(^7\) the energy (4.36) as

$$\mathcal{H}_{\text{dip}} = \frac{\mu_0}{2} \int H^2(r)d^3r - \frac{\mu_0}{6} \int M^2(r)d^3r. \quad (4.36)$$

The first term on the right-hand side is called the demagnetizing energy and is positive definite. A “rule of thumb” to minimize this energy can be provided recalling that, for a given magnetization density $\vec{M}(r)$, the stray field (or demagnetizing field) $\vec{H}$ is minus the gradient of is the scalar magnetic

---

\(^6\)More precisely, it is $\vec{m} = \langle \vec{\mu} \rangle_{\text{th}} = \vec{M}(r)d^3r$, but for the present purposes it is convenient to keep considering the dipolar interaction at $T = 0$, for which $\vec{m} = \vec{\mu}$.

\(^7\)One uses the fact that $-\int \vec{B} \cdot \vec{M}d^3r = \int H^2d^3r - \frac{\mu_0}{4}\int \vec{B} \cdot \vec{H}d^3r/\mu_0 = \int H^2d^3r$; the integral of $\vec{B} \cdot \vec{H}$ over the whole space vanishes because $\vec{B} \cdot \vec{H} = -\vec{B} \cdot \nabla \phi_m = -\nabla \cdot (\phi_m \vec{B}) + \phi_m \nabla \cdot \vec{B} = -\nabla \cdot (\phi_m \vec{B})$; the last term becomes an integral on a surface placed infinitely far from the sources of the fields $\vec{B}$ and $\vec{H}$. The scalar magnetic potential $\phi_m$ will be introduced in the following.
potential (see, e.g., “Classical Electrodynamics,” J. D. Jackson)

\[ \phi_m(r) = \frac{1}{4\pi} \int_V \frac{\rho_m(r')}{|r-r'|} d^3r' + \frac{1}{4\pi} \int_{\Sigma_V} \frac{\sigma_m(r')}{|r-r'|} d\Sigma' \], \hspace{1cm} (4.37)

where

\[ \rho_m = -\nabla \cdot \vec{M} \quad \text{and} \quad \sigma_m = \vec{M} \cdot \hat{n} \hspace{1cm} (4.38) \]

are the volume and surface charge density, respectively (\(\hat{n}\) normal to the surface \(\Sigma_V\)). Within this formalism, \(\vec{H}\) is formally equivalent to the electric field generated by an effective Coulomb charge distribution \(\rho_m(r)\). Therefore the demagnetizing energy is minimized by configurations for which there are as less magnetic charges as possible. Even if derived in a coarse-grained context, the validity of this “rule of thumb” is quite general and provides the correct hints also in the discrete-lattice formalism. For instance, it correctly prescribes that Bloch domain walls have a lower energy than Néel domain walls in bulk magnets (see below).

The second term in Eq. (4.36) gives an extensive lower bound to the dipolar energy that is independent of sample shape: this fact will be used as a supporting argument for the Griffiths’ theorem.

### Bloch and Néel domain walls

In section 4.4 of the present chapter we investigated how domain walls with a finite width \(\delta\) emerge from the competition between the anisotropy and the exchange energy. The “compromise” which minimizes the domain-wall energy is represented by the solution (4.24) that we recall here for convenience:

\[
\begin{align*}
\cos(\theta(x)) &= \tanh \left( \frac{x}{\delta} \right) \\
\varphi(x) &= \text{const.}
\end{align*}
\hspace{1cm} (4.39)
\]

All the solutions with constant \(\varphi(x)\) give the same energy if inserted in the Hamiltonian (4.21). Now we ask ourselves whether the introduction of the dipolar energy term (5.59) may favor one specific value of \(\varphi(x)\). The two extreme cases are named

\[
\begin{align*}
\varphi(x) &= \frac{\pi}{2} \quad \forall x \hspace{1cm} \text{Bloch domain wall} \\
\varphi(x) &= 0 \quad \forall x \hspace{1cm} \text{Néel domain wall}.
\end{align*}
\hspace{1cm} (4.40)
\]

More specifically the magnetization for these two cases will be

\[
\begin{align*}
\vec{M} &= M_0 (0, \sin(\theta(x)), \cos(\theta(x))) \hspace{1cm} \text{Bloch domain wall} \\
\vec{M} &= M_0 (\sin(\theta(x)), 0, \cos(\theta(x))) \hspace{1cm} \text{Néel domain wall}.
\end{align*}
\hspace{1cm} (4.41)
\]
Figure 4.8: From Introduction to the Theory of Ferromagnetism by A. Aharoni. Energy per unit wall area, $\gamma$, (solid curves) as a function of the thickness for a permalloy film magnetized in plane. Dashed curves display the domain-wall width ($q \propto \delta$ in our notation).

with $\theta(x)$ given by Eq. (4.39). In the bulk case (3d), it is evident that the Bloch wall always has a lower energy since

$$\vec{\nabla} \cdot \vec{M} = \partial_x M_x + \partial_y M_y + \partial_z M_z \begin{cases} = 0 & \text{Bloch domain wall} \\ \neq 0 & \text{Néel domain wall} \end{cases}$$

so that only the Néel domain wall produces some magnetic charges $\rho_m = -\vec{\nabla} \cdot \vec{M}$. This rule-of-thumb prediction is confirmed by detailed calculations and experiment. The situation is analogue for thin films (2d) with the easy axis pointing out of plane. For thin films magnetized in the $xz$ plane (with easy axis parallel to $z$), the surface charges $\sigma_m$ produced by a Bloch wall ($M_y$ needs to point out of plane) can be so large that the Néel wall becomes energetically more convenient. In this case, surface charges (Bloch wall) are replaced by volume charges $\rho_m$. The solid curves in Fig. 4.8 display the domain-wall energy corresponding to a Bloch and a Néel wall, computed
with the phenomenological parameters of permalloy (alloy of \(\approx 20\%\) Fe and \(\approx 80\%\) Ni), as a function of the film thickness. Indeed, for this specific material with this specific geometry, up to thicknesses of the order of 60 nm the Néel wall has a lower energy.

**Uniformly magnetized samples**

Given a (generally non-uniform) magnetization profile \(\vec{M}(r)\), the demagnetizing field \(\vec{H}(r)\) is related to it by a 3-by-3 tensor \(N_D(r)\)

\[
\vec{H}(r) = -N_D(r)\vec{M}(r)
\]

(4.43)
called *demagnetizing tensor*. This tensor is generally difficult to calculate and depends on the shape of the sample. For the special case of uniform magnetization inside a sample of ellipsoidal shape, \(\vec{H}(r)\) is also uniform and \(N_D\) becomes a diagonal matrix:

\[
N_D = \begin{pmatrix}
N_{xx} & 0 & 0 \\
0 & N_{yy} & 0 \\
0 & 0 & N_{zz}
\end{pmatrix}
\]

(4.44)

whose elements are different for different ellipsoids but their sum (trace) is always equal to one: \(N_{xx} + N_{yy} + N_{zz} = 1\). The demagnetizing energy for a uniformly magnetized ellipsoid reduces to

\[
\mathcal{H}_D = \frac{1}{2} \mu_0 V \left( N_{xx}M_x^2 + N_{yy}M_y^2 + N_{zz}M_z^2 \right)
\]

(4.45)

Within this approximation, the dipolar interaction produces a term which—at least at a coarse grained level—is formally equivalent to the anisotropy introduced at the beginning of this chapter. This is the origin of the so-called *shape anisotropy*.

For a uniformly magnetized sphere one finds in textbooks \(N_{xx} = N_{yy} = N_{zz} = 1/3\), consistently with the complete equivalence of the principal axes and the unitary trace of the demagnetizing tensor. By elongating or compressing a sphere along one direction (\(z\) in Fig. 4.9), prolate or oblate ellipsoids are obtained. Also for these cases simple formulas exist. Taking \(z\) as the axis of elongation (compression) of a prolate (oblate) ellipsoid, the demagnetizing coefficients along the other two equivalent directions are given by \(N_{xx} = \frac{1}{2} - N_{zz}\). An indefinitely elongated ellipsoid approaches a needle or a nanowire, for which \(N_{zz} = 0\) and \(N_{xx} = N_{yy} = 1/2\). Therefore, the shape anisotropy favors the direction along the wire axis. An indefinitely flat oblate ellipsoid approaches a disk or a thin film. For this geometry the
0 ≤ N_{zz} ≤ \frac{1}{3} \Rightarrow \text{prolate ellipsoid}

N_{zz} = 0 \Rightarrow \text{cylinder}

\frac{1}{3} ≤ N_{zz} ≤ 1 \Rightarrow \text{oblate ellipsoid}

N_{zz} = 1 \Rightarrow \text{disk}

Figure 4.9: Sketch of prolate and oblate ellipsoids with the relative ranges of \( N_{zz} \), and the corresponding limits of an elongated needle (cylinder) and a flat disk, respectively. For both ellipsoids the demagnetizing coefficients along the two equivalent directions are related to \( N_{zz} \) as \( N_{xx} = N_{yy} = (1 - N_{zz})/2 \).

direction perpendicular to the plane is a hard axis, for what concerns the shape anisotropy. In other words, in thin films the shape anisotropy provides an easy plane contribution to the anisotropy. However, it is worth reminding that here we are just considering configurations with uniform magnetization. More general configurations will be treated in the following, in which case the dipolar contribution to the total energy cannot simply be expressed as a shape anisotropy.

**Griffiths’ theorem**

Equation (4.45) shows that the demagnetizing energy of a uniformly magnetized ellipsoid – but the result can be generalized to other shapes – is proportional to the sample volume (extensive). The second, negative term
on the right-hand side of Eq. (4.36) also brings an extensive contribution to the total magnetostatic energy. We can, thus, conclude that the dipolar energy per spin is finite (at odds with the first rough estimate based on the divergence of the integral (4.32) for $d=3$). As anticipated, its value depends on the shape of the sample, right through the demagnetizing energy.

Before coming back to our original question, we need to quote an important theorem. In 1968 Griffiths\(^8\) proved that the free energy per spin (thus also the energy per spin at $T = 0$) of a magnetic system is shape-independent in the thermodynamic limit. The existence of a shape independent lower bound in the energy (4.36) is a basic ingredient of the proof. Besides this, Griffiths showed that the free energy per spin decreases with increasing sample size. These two results imply that the free energy converges to a shape-independent value in the limit of large system size. A weak but significant requirement for the proof is that all three linear dimensions of the sample increase to infinity, which leaves the possibility to have exceptions in low dimensional systems (see next section). On the other hand, we have just seen that the energy of a 3d ferromagnet is shape-dependent. One can argue that this is also the case when the magnetization is not uniform but not globally compensated either (i.e., there is a net magnetization along some direction).

In conclusion, Griffiths’ theorem implies that the equilibrium state of a bulk magnet cannot be ferromagnetic: rather the total magnetization of a large enough sample, or portions of it, exactly compensates to zero.

At this point the reader may speculate whether the exchange interaction, neglected so far in this discussion, possibly manages to stabilize a ferromagnetic ground state in 3d. As a simple counterexample one can think of splitting a bulk magnet into two equal domains with opposite magnetization so to obtain a globally vanishing magnetization. The cost to create the domain wall scales like its own surface but the reduction of the dipolar energy is proportional to the volume. Thus, at sufficiently large spatial scales, the dipolar interaction always dominates, imposing some non-uniform, generally complicated, magnetization distribution (domain structure, curling, etc.) as ground state. In this sense, three-dimensional ferromagnetism can only be a mesoscopic phenomenon or a metastable phase.

In the next sections we will suggest a route to quantify the length scale over which ferromagnetism can actually be realized.

4.7 Dipolar interaction in low-dimensional systems

Griffiths’ theorem does not apply to thin films because they extend indefinitely only along two spatial directions. For this reason a phase with uniform magnetization in 2d systems would not violate this theorem. Among the configurations with uniform $\vec{M}$, we have seen that the shape anisotropy favors a phase with in-plane magnetization. This is indeed the ground state of a Heisenberg Hamiltonian with dipolar interaction and without other anisotropy terms (e.g., magnetocrystalline anisotropy produced by spin-orbit coupling). Below we will see that such a phase remains stable up to some finite temperature.

**Dipolar interaction in 2d Heisenberg systems**

In the spirit of previous sections, we will just provide some arguments to convince the reader that the Heisenberg model with dipolar interaction actually admits spontaneous magnetization. A rigorous demonstration is beyond the scope of the course. The in-plane phase favored by shape anisotropy still has a residual degeneracy, for planar rotations of the magnetization, which makes this model akin to the two-dimensional XY model with dipolar interaction.

In section 3.6 the divergence of the integral
\[
\langle (S^\alpha)^2 \rangle \approx \frac{k_B T}{(2\pi)^d} \int d^d q \frac{\Gamma(q)}{\Gamma(q)}
\]
for $d=2$, $B = 0$ and in the absence of uniaxial anisotropy was used to prove that ferromagnetism is not stable at finite temperature in systems with continuous symmetry. To the leading order in small $q$, the dipolar interaction modifies the spectrum of fluctuations as $\Gamma(q) \simeq Jq^2 + \gamma \Omega q$ (with $\Omega$ strength of dipole-dipole interaction and $\gamma$ some numerical factor). As a consequence, transverse fluctuations do not diverge anymore as the linear dimensions of the film are increased; more precisely
\[
\langle (S^\alpha)^2 \rangle \simeq \frac{k_B T}{J} \int_{q_{\text{min}}}^{q_{\text{max}}} dq \frac{d}{q + \gamma \Omega / J} \simeq \frac{k_B T}{J} \ln \left( \frac{q_{\text{max}} + \gamma \Omega / J}{q_{\text{min}} + \gamma \Omega / J} \right) < \infty.
\]
Remember that the dependence on the system size is contained in $q_{\text{min}} = \pi/N_\alpha$ that vanishes in the limit of $N_\alpha \to \infty$. In conclusion, the dipolar interaction stabilizes ferromagnetism up to some finite temperature for the 2d isotropic Heisenberg model.

Adding an in-plane uniaxial anisotropy to this model will certainly not
destabilize magnetic order. However, by removing the original planar de-
generacy, this additional anisotropy may drive the system towards the Ising
universality class. This is indeed observed in Fe films of few atomic layers
deposited on W(110) substrate. These films are model realizations of the
2d Ising model as they obey the predicted scaling behavior for $T \sim T_C$ over
eighteen orders of magnitude (see Fig 4.10). As pointed out in *Nature* 378 p.
597, neither the dipolar interaction nor other effects neglected in the ideal
model seem to affect the 2d-Ising critical behavior observed in Fe/W(110).

2d systems magnetized out-of-plane

A completely different situation occurs in films with out of plane magne-
tocrystalline anisotropy, strong enough to overcome the shape anisotropy. In
these systems the dipolar interaction is frustrated and tends to “destroy”
ferromagnetism (see Fig. 4.5 b). An example is represented by atomically
thin Fe on Cu(001). Here the competition between the ferromagnetic exchange
interaction – originating ferromagnetism for $T < T_C$ – and dipolar
interaction – frustrating ferromagnetism on a larger scale – produces a sort
of phase separation between regions of positive and negative magnetization
perpendicular to the film plane (see the scheme in Fig. 4.11). In other words,
ferromagnetism is limited to some spatial regions in which all the magnetic
moments point along the same direction. Such regions are called magnetic
CHAPTER 4. MAGNETIC DOMAINS AND DOMAIN WALLS

Figure 4.11: The competition between exchange interaction and the dipolar interaction originates a modulated phase in magnetic films magnetized out of plane.

domains. The whole scenario holds below the Curie temperature, thus magnetic domains need not be confused with the spatial regions defined by the correlation length $\xi$. In Fig. 4.12 some images of different magnetic-domain patterns observed in Fe/Cu(001) films are shown.

Dipolar interaction in 1d systems

The ground state of a one-dimensional array of dipoles interacting only via dipole-dipole interaction is one of the two ferromagnetic configurations sketched in Fig. 4.13 with all the magnetic moments aligned along the chain axis. One may wonder whether the long-range character of dipolar interaction could stabilize ferromagnetism at finite temperature in 1d systems. Some more insight can be gained applying the Landau argument – reproposed in the previous chapter (Fig. 3.2) to exclude long-range magnetic order at finite

\footnote{Remember that c) corresponds to the global minimum among the configurations considered in Fig. 4.5.}
temperature in the Ising chain – to the following Hamiltonian

\[ H = -\Omega_\alpha \sum_{i\neq j}^{N} \frac{\sigma_i \sigma_j}{|i-j|^\alpha} \]  

(4.48)

in which the exchange interaction is not limited to nearest neighbors and \( \sigma_i = \pm 1 \) are Ising variables (we assume \( \Omega_\alpha > 0 \)). For an infinite chain, it can be shown\(^{10}\) that creating a domain wall (as sketched in Fig. 4.13) decreases the Gibbs free energy for any finite temperature when \( \alpha > 2 \). Indeed, the dipolar interaction falls in this range (\( \alpha = 3 \)) and is therefore not long-ranged enough to stabilize ferromagnetism in one dimension. For completeness, we mention that the model with Hamiltonian (4.48) is compatible with ferromagnetism at finite \( T \) for \( 0 < \alpha < 2 \). The case \( \alpha = 2 \) is a bit pathological and displays a Kosterlitz-Thouless phase transition\(^{11}\).

Even if it cannot stabilize long-range magnetic order, the dipolar interaction

---


affects – to some extent – the elementary excitations that destroy ferromagnetism in 1d systems, namely spin-waves in isotropic spin chains or domain wall in spin chains with uniaxial anisotropy. By this, dipolar interaction may in turn affect short-range order and modify, e.g., the dependence of the correlation length $\xi(T)$ on temperature. In any case, its role is generally less severe in 1d than in higher dimensions.

### 4.8 Ferromagnetism and magnetic domains

The scenario described schematically in Fig. 4.11 is just a particular case in which the competition between exchange and dipolar energy gives rise to a configuration with zero global magnetization. Qualitatively, this is very similar to what prescribed by Griffiths’ theorem for bulk magnets (films are not contemplated by the theorem). Such a configuration is the compromise that produces the least demagnetizing energy (i.e. as less magnetic charges as possible) with the minimum frustration of the exchange interaction. What results from the competition between these two energies is generally different depending

- on the easy-axis direction (determined by the sum of magnetocrystalline anisotropy, shape anisotropy, etc.)
- on the geometry of the sample

so that each case needs to be evaluated on its own. As a simple example, let us consider – again – a 2d system magnetized out of plane and evaluate the energy variation associated with the creation of a domain wall from a uniformly magnetized state (see Fig 4.14). Both the exchange energy and uniaxial anisotropy contribute to the domain-wall energy $\mathcal{E}_w$, thoroughly discussed in the previous sections and whose values are summarized schematically in Eq. (4.25). When deriving those results we assumed that the spin profile was a function of one spatial variable only. Now we consider a film of finite thickness $t$ and a domain wall developing indefinitely along the $y$ direction, so that the total increase of the exchange and anisotropy energy is $N_y N_z \mathcal{E}_w$, with $N_z = t/a$. For a film magnetized out of plane and with thickness $t$ of few monolayers the dipolar energy (5.59) can be approximated as

$$\mathcal{H}_{\text{dip}} = \frac{1}{2} \Omega \frac{t^2}{a^3} \int \int \frac{S_z(r) S_z(r')}{|r - r'|^3} \, d^2 r \, d^2 r' \, .$$

(4.49)

Splitting the $xy$ plane into two half-planes and reversing the magnetization (along $z$) of one of the two half-planes produces
Figure 4.14: Sketch of the two configurations corresponding to the energy difference evaluated in Eq. (4.50). Arrows represent magnetic moments pointing \textit{out of plane}.

A decrease of the dipolar energy by a factor

$$
\Delta \mathcal{E}_{\text{dip}} = 2N_y \Omega \frac{t^2}{a^2} \int_0^{N_x a/2} dx \int_{-N_x a/2}^{0} dx' \int_{-\infty}^{+\infty} \frac{1}{[(x - x')^2 + y^2]^{3/2}} dy; \quad (4.50)
$$

the integral over \(dx\) is performed starting from a length scale equal to the domain-wall width \(\delta\) in order to avoid an unphysical divergence. In other words, spins located inside the domain wall have been ideally “removed” from the calculation of the dipolar energy. Note that \(\Delta \mathcal{E}_{\text{dip}}\) in Eq. (4.50) represents the variation of the interaction energy between the two half-planes; the magnetostatic self-energy of the two half-planes remains the same. The integral in Eq. (4.50) can be performed analytically and gives

$$
\Delta \mathcal{E}_{\text{dip}} = 4N_y \Omega \frac{t^2}{a^2} \ln \left( \frac{N_x a + 2\delta}{4\delta} \right). \quad (4.51)
$$

The condition \(\Delta \mathcal{E}_{\text{dip}} = N_y N_z \mathcal{E}_w\) gives the minimum linear dimension \(N_x\) that a slab should have in order that splitting the uniform state into domains becomes favorable. In the realistic limit of \(N_x a \gg \delta\), one finds that for \(N_x\) larger than the threshold value

$$
N_x \simeq \frac{4\delta}{a} \exp \left( \frac{\mathcal{E}_w a}{4\Omega t} \right) \quad (4.52)
$$

it is convenient for the system to split into domains of opposite \textit{out-of-plane} magnetization. From this rough calculation one expects the typical size of domains to be \(L_{eq} \simeq \bar{N}_x a / 2\). The exponential dependence on the ratio \(\mathcal{E}_w / \Omega\) is typical of \(d=2\). For the 3d case, a further integration would be involved in the evaluation of \(\Delta \mathcal{E}_{\text{dip}}\) which, eventually, would result in a much weaker dependence of the domain size \(L_{eq}\) on the ratio \(\mathcal{E}_w / \Omega\).
Chapter 4. Magnetic Domains and Domain Walls

Striped pattern

Figure 4.15: Schematic view of the striped ground state of a ferromagnetic film magnetized out of plane in the presence of the dipolar interaction and $B = 0$. Stripes of different colors represent regions of opposite out-of-plane magnetization. The typical stripe width is $L_{eq}$.

In spite of the crude approximations that have been performed to obtain Eq. (4.52), the predicted scaling with $E_w/\Omega$ and with the film thickness $t$ match with the optimal stripe width for an ideal stripe pattern at $T = 0$ (see Fig. 4.15). This pattern corresponds to the ground state of a film magnetized out of plane in the presence of dipolar interaction and zero external field. Detailed calculations\textsuperscript{12} yield for $\Omega \ll D \ll J$

$$L_{eq} = \frac{10}{3\pi} \delta \exp \left( \frac{E_w a}{4\Omega t} \right)$$

(4.53)

and for $\Omega \ll J \ll D$ (Ising domain wall)

$$L_{eq} = L_0 \exp \left( \frac{Ja}{2\Omega t} \right)$$

(4.54)

with $L_0 = 0.871a$. Remembering that in the second case $E_w = 2J$ and $\delta = a$, both Eqs. (4.53) and (4.54) confirm the scaling predicted by Eq. (4.52) on the basis of heuristic arguments.
Ferromagnetism or domain phases?

Similarly to what done at the end of the previous chapter, we would like to conclude the present one with another “truth table” that summarizes for which models a phase with uniform magnetization (ferromagnetic) can occur at finite temperature, in the presence or absence of dipolar interaction. Only magnetic lattices with dimensionalities \( d = 2 \) and \( d = 3 \) are considered, because in lower dimension genuine ferromagnetism can never occur (note that in Table 3.2 superparamagnetism was also considered). In the presence of dipolar interaction, films magnetized in plane (\( \parallel \)) or out of plane (\( \perp \)) behave differently, as pointed out previously. In the second type of films and in bulk magnets the uniformly magnetized phase realized in the (hypothetic) absence of dipolar interaction is generally replaced by a phase with magnetic domains and fully compensated magnetization (\( \mathcal{M} = 0 \) on macroscopic scale), when dipole-dipole interaction is considered. However, for bulk magnets Griffiths’ theorem contemplates more general configurations with vanishing global magnetization than domains, for instances with curling of \( \vec{M} \). That is the reason why for the 3d case we did not specify “domains”, which are generally realized in bulk magnets when some magnetocrystalline anisotropy is present. Remarkably, for the 2d Heisenberg model no ferromagnetism is expected at finite temperature in the absence of dipolar interaction, while, if taken into account, this interaction stabilizes a magnetically ordered planar phase. The 2d Heisenberg model is not compatible with an out-of-plane magnetized phase, which implicitly requires a uniaxial anisotropy perpendicular to the film.

\footnote{Case \( \Omega \ll D \ll J \) adapted from S. A. Pighin \textit{et al.}, J. Mag. Mag. Mat. \textbf{322} p. 3889 (2010). Case \( \Omega \ll J \ll D \) (Ising) adapted from A. B. MacIsaac \textit{et al.}, Phys. Rev. B \textbf{51} p. 16033 (1995).}

<table>
<thead>
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<th>model</th>
<th>2d ( \parallel )</th>
<th>2d ( \perp )</th>
<th>3d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heisenberg/XY + dipolar</td>
<td>YES</td>
<td>-</td>
<td>NO (Griffiths)</td>
</tr>
<tr>
<td>Ising + dipolar</td>
<td>YES</td>
<td>NO (domains)</td>
<td>NO (Griffiths)</td>
</tr>
<tr>
<td>Heisenberg/XY</td>
<td>NO</td>
<td>NO</td>
<td>YES</td>
</tr>
<tr>
<td>Ising</td>
<td>YES</td>
<td>YES</td>
<td>YES</td>
</tr>
</tbody>
</table>

Table 4.1: “Truth table” of ferromagnetism, i.e. a phase with uniform magnetization at finite \( T \), with and without including the dipolar interaction. Where not indicated, models are meant without dipolar interactions (last two rows). For \( d = 2 \) the cases with magnetization pointing in plane (\( \parallel \)) or out of plane (\( \perp \)) are distinguished.
CHAPTER 4. MAGNETIC DOMAINS AND DOMAIN WALLS

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• A. Aharoni, Introduction to the Theory of Ferromagnetism
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Chapter 5

Nanoscale magnetism

What happens when a bulk magnet is flattened to nanometric thickness? In previous chapters, we have seen that some ferromagnetism – possibly present in the ground state – may survive up to some finite temperature. A finite anisotropy is required for that (in 2d), but this condition is not that stringent. In fact, as seen previously, dipolar interaction suffices to stabilize order in the 2d Heisenberg model. Ferromagnetism in (nanometric) thin films was, e.g., crucial for observing giant magnetoresistance (GMR), for which Albert Fert and Peter Grünberg\(^1\) were awarded the Nobel prize in 2007. Apart from the enormous technological impact, this recognition was motivated by the fact that GMR was as acknowledged as a novel physical phenomenon. From this we learn that shrinking one or more spatial dimension of a macroscopic object may lead to new physics. Sticking to magnetic films, at the end of chapter 4 we mentioned that films magnetized out of plane spontaneously split into domains, because of the competition between exchange and dipolar interaction. At room temperature such domains fall in the micrometer range. Therefore, if the lateral dimensions of a film are squeezed below some sample-dependent threshold ($\lesssim \mu m$) a monodomain configuration can be stabilized, independently of the fact that dipolar interaction be frustrated or not (see Fig.5.1). Actually, in chapter 3 we have seen that finite size can also prevent a system that does not sustain ferromagnetism (for instance a spin chain) from splitting into domains because of thermal fluctuations. Eventually, in a small enough system with an uniaxial-anisotropy axis the two lowest energy configurations will be populated with the same probability at equilibrium (if $B = 0$). Thus, the question is shifted to how long it takes to reverse the magnetization from one of those configurations to the other. In other words, the question about stability of ferromagnetism at thermodynamic equilibrium

becomes a question of characteristic time scale of bistability.

Besides GMR, squeezing a magnet as much as possible is clearly desirable for a large variety of applications. Since nowadays engineering magnetic samples of nanometric size is achievable by different means, we speak about nanomagnetism. Reviewing even only the most relevant applications of nanomagnetism in a chapter would not be feasible. This is partially due to the fact that this field is relatively new and still very active so that what is literature has not been clearly established yet. However, within the appropriate time scale, magnetization dynamics is basically relevant to all applications. For this reason, we devote this chapter to dynamics. In particular, we will try to pinpoint that different physical principles – and formalisms – underlie magnetization dynamics at different time scales. Some remarks on nowadays’ applications will be made when presenting different phenomena or during the lecture, integrated with some slides.

5.1 Landau-Lifshitz dynamics

The question of how to model magnetization dynamics for different time windows and spatial scales will be addressed in large part of this chapter. Following our usual bottom-up approach, we shall start defining the dynamics of a single, atomic magnetic moment. Given the proportionality $\dot{\mu} = -g\mu_B \dot{S}$, where $\dot{S}$ has to be understood as an effective spin, this issue reduces to investigating the dynamics of a single spin. To fix the ideas, let us consider
a Hamiltonian that comprises only a Zeeman contribution:

\[ \mathcal{H} = g\mu_B \vec{B} \cdot \hat{S}. \]  

(5.1)

Classically, the time evolution of angular momenta is given in terms of Poisson brackets: \( \dot{\vec{S}}^\eta = \{\vec{S}^\eta, \mathcal{H}\} \), with \( \eta = x, y, z \). The quantum-mechanical equivalent is obtained by means of Dirac’s mapping \( i\hbar \{\hat{S}^\eta, \mathcal{H}\} \rightarrow [\hat{S}^\eta, \mathcal{H}] \), which – for our specific case – yields

\[ i\hbar \dot{\hat{S}}^\eta = [\hat{S}^\eta, \mathcal{H}] = g\mu_B \sum_\delta B^\delta [\hat{S}^\eta, \hat{S}^\delta] = g\mu_B \sum_\delta B^\delta i\epsilon_{\eta\delta\sigma} \hat{S}^\sigma, \]  

(5.2)

where \( \epsilon_{\eta\delta\sigma} \) is the Levi-Civita symbol\(^2\) and spin operators are expressed in the Heisenberg representation. Clearly, the equation above can be expressed with a cross product \( \hbar \dot{\hat{S}} = -g\mu_B \hat{S} \times \vec{B} \). Its classical version (after \( \hat{S} \rightarrow \vec{S} \)) is formally equivalent and it is usually referred as Landau-Lifshitz (LL) equation:

\[ \dot{\vec{S}} = -\gamma \vec{S} \times \vec{B} \quad \text{with} \quad \gamma = \frac{g\mu_B}{\hbar}. \]  

(5.3)

Normally, \( \vec{S} \) is not thought of as an atomic spin but rather as a coarse-grained macrospin representing the normalized magnetization of some sufficiently small volume: \( \vec{S} = -\vec{M}/M_s \) (with \( M_s \) saturation magnetization)\(^3\). In the following, this macrospin approximation will be assumed to describe nanoparticles whose magnetization is supposed to rotate rigidly. This case – in which the classical treatment is indeed more justified – may be thought of as a limit in which \( J \rightarrow \infty \). In the language of the forthcoming section 5.A, having an infinite \( J \) means that individual spins are always aligned along the exchange component of the local field (exchange field). Therefore, the latter does not contribute to dynamics nor enters the LLG equation.

Equation (5.3) describes a Hamiltonian, non-dissipative dynamics of the magnetization. Since \( \vec{S} \) is orthogonal to both \( \vec{S} \) and \( \vec{B} \), the corresponding motion is a precession with angular velocity \( \omega_L = \gamma B \). To make this point clear, we define the \( z \) direction parallel to the magnetic field: \( \vec{B} = (0, 0, B) \). Thus, Eq. (5.3) is equivalent to

\[ \begin{align*}
\dot{S}^x &= -\gamma BS^y \\
\dot{S}^y &= \gamma BS^x \\
\dot{S}^z &= 0.
\end{align*} \]  

(5.4)

\(^2\)\( \epsilon_{\eta\delta\sigma} = 1 \) for cyclic permutations of \( \eta\delta\sigma = xyz \), it is -1 for for cyclic permutations of \( \eta\delta\sigma = yzx \), and zero when at least two indices are equal.

\(^3\)Often, the classical vector \( \vec{S} \) is defined as the ratio \( \vec{M}/M_s \) or \( \vec{\mu}/(g\mu_B) \) in such a way that it tends to align along the applied field instead of the opposite direction.
This system of equations has a stationary solution of the form

\[
\begin{aligned}
S^x &= A^x \cos(\omega t) \\
S^y &= A^y \sin(\omega t) \\
S^z &= \text{const.},
\end{aligned}
\]  

which inserted in Eq. (5.4) yields

\[
\begin{aligned}
\omega A^x &= \gamma B A^y \\
\omega A^y &= \gamma B A^x.
\end{aligned}
\] (5.6)

The last set of equations admits a non-trivial solution (with \(A^x \neq 0\) and \(A^y \neq 0\)) only\(^4\) for \(\omega = \gamma B\), yielding \(A^x = A^y\). Therefore, the spin \(\vec{S}\) performs a right-hand precession about the axis along which the magnetic field is applied with a characteristic frequency \(\omega_L = \gamma B\), called Larmor frequency. Some more insight can be obtained expressing the final result in polar coordinates

\[
\begin{aligned}
S^x &= \sin \theta \cos(\omega L t) \\
S^y &= \sin \theta \sin(\omega L t) \\
S^z &= \cos \theta.
\end{aligned}
\] (5.7)

First, on the xy plane the spin \(\vec{S}\) describes a circular motion with constant angular velocity \(\varphi = \omega_L t\). Second, its projection along the field – parameterized through the \(\theta\) angle – is conserved. This second feature is the fingerprint of non-dissipative dynamics.

An experimental technique whose basic physics is described by a simple generalization of Eq. (5.4) is ferromagnetic resonance\(^5\). Besides the macrospin approximation, the demagnetizing field, introduced in Eq. (4.43), has to be considered. Under specific experimental conditions, the gyromagnetic frequency, the saturation magnetization, the anisotropy energy and the demagnetizing coefficients \((N_{xx}, N_{yy}, N_{zz})\) can be determined.

### 5.2 Landau-Lifshitz-Gilbert equation

The previous example clearly shows that Landau-Lifshitz Eq. (5.3) does not allow for energy dissipation. According to Hamiltonian (5.2), the minimal energy is realized by the configuration in which \(\vec{B}\) and \(\vec{S}\) are antiparallel, namely

\(^4\)The solution with \(\omega = -\gamma B\) gives \(A^x = -A^y\) that actually corresponds to the same physical solution.

\(^5\)Read, e.g., the Charles Kittel’s book for more details.
Figure 5.2: Schematic view of vectors involved in a Larmor precession. Due to the relation \( \vec{\mu} = -g\mu_B \vec{S} \), the damping term (gray) has a plus sign in the LLG equation for the magnetic moment (upper part) and a minus sign when LLG equation describes the dynamics of the spin \( \vec{S} \) as in Eq. (5.8).

\( \vec{\mu} \parallel \vec{B} \). But if \( \theta \) is conserved throughout the dynamics the energy minimum, attained for \( \theta = \pi \), can never be reached. On the contrary, at macroscopic time scales, experience suggests that the magnetization generally tends to align along an applied field. Already Landau and Lifshitz proposed to solve this apparent inconsistency by introducing a damping term. We start from the alternative version of the damped LL equation proposed by Gilbert:

\[
\dot{\vec{S}} = -\gamma \vec{S} \times \vec{B} - \alpha \vec{S} \times \dot{\vec{S}}. \tag{5.8}
\]

The last term can be written in a different way using Eq. (5.8) itself:

\[
\vec{S} \times \dot{\vec{S}} = -\gamma \vec{S} \times (\vec{S} \times \vec{B}) - \alpha \vec{S} \times (\vec{S} \times \dot{\vec{S}}); \tag{5.9}
\]

in particular, the second double cross product on the right-hand side gives

\[
\vec{S} \times (\vec{S} \times \dot{\vec{S}}) = (\vec{S} \cdot \dot{\vec{S}}) \vec{S} - S^2 \dot{\vec{S}} = -\dot{\vec{S}}, \tag{5.10}
\]

where we have used the fact that \( S^2 = |\vec{S}|^2 = 1 \) so that \( \vec{S} \cdot \dot{\vec{S}} = 0 \). Thus, the Landau-Lifshitz-Gilbert (LLG) equation can equivalently be written as

\[
\dot{\vec{S}} = -\gamma \vec{S} \times \vec{B} + \alpha \gamma \vec{S} \times (\vec{S} \times \vec{B}) - \alpha^2 \dot{\vec{S}}, \tag{5.11}
\]
or better

\[
(1 + \alpha^2) \dot{\vec{S}} = -\gamma \vec{S} \times \vec{B} + \gamma \alpha \vec{S} \times (\vec{S} \times \vec{B}) .
\]  

(5.12)

It is instructive to see how the precession of the magnetization about an external field \( \vec{B} = (0, 0, B) \) is modified by the presence of the Gilbert damping. Let us first compute the double cross product on the right-hand side of Eq. (5.12):

\[
\vec{S} \times (\vec{S} \times \vec{B}) = (\vec{S} \cdot \vec{B}) \vec{S} - \vec{B} = (S^z B) \vec{S} - \vec{B} .
\]  

(5.13)

Assuming \( (S^z \simeq -1) \), Eqs. (5.4) are modified as follows

\[
\begin{align*}
(1 + \alpha^2) \dot{S}_x &= -\omega_L S_y - \alpha \omega_L S_x \\
(1 + \alpha^2) \dot{S}_y &= \omega_L S_x - \alpha \omega_L S_y \\
\dot{S}_z &= 0
\end{align*}
\]  

(5.14)

With the trial function \( S^\sigma = A^\sigma e^{-i\omega t} (\sigma = x, y) \), the condition to have non-trivial solutions is given by the vanishing of the determinant:

\[
\begin{vmatrix}
 i(1 + \alpha^2) \omega - \alpha \omega_L & -i \omega_L \\
 i(1 + \alpha^2) \omega - \alpha \omega_L & i(1 + \alpha^2) \omega - \alpha \omega_L
\end{vmatrix} = 0
\]  

(5.15)

which occurs when

\[
\omega = \frac{1}{1 + \alpha^2} \omega_L - i \frac{\alpha}{1 + \alpha^2} \omega_L
\]  

(5.16)

so that the sought for solution corresponds to

\[
\begin{align*}
S^x &= A^x e^{-i\omega'_L t} e^{-t/\tau_D} \\
S^y &= A^y e^{-i\omega'_L t} e^{-t/\tau_D}
\end{align*}
\]  

(5.17)

with

\[
\begin{align*}
\omega'_L &= \frac{1}{1 + \alpha^2} \omega_L \\
\frac{1}{\tau_D} &= \frac{\alpha}{1 + \alpha^2} \omega_L = \alpha \omega'_L .
\end{align*}
\]  

(5.18)

Remarkably, for typical values of \( \alpha = 0.1 \ldots 0.001 \), the characteristic damping time can be three orders of magnitude longer than the precessional period. This separation of time scales is crucial to understand why magnetization dynamics is mainly determined by (non-dissipative) precession at short times, while it is dictated by (dissipative) damping at longer time scales. The time regime at which damping effects becomes relevant strongly depends on the considered experimental system, on the applied field, etc. So, without taking this number too seriously, one may consider damping effects to be irrelevant in the sub-nanosecond regime.
As anticipated, in the realm of nanomagnetism it may happen that magnetization reverses because of thermal fluctuations. Within the macrospin approximation this is possible only in sufficiently small samples, of tens of nanometers or less. Such dynamics pertains a third regime – besides precessional and dissipative regime – and characterizes longer time scales. The main ideas behind the formalism through which thermally-driven magnetization dynamics is described will be sketched in section 5.4.

5.3 Systems of coupled spins

In this section the Landau-Lifshitz-Gilbert equation will be generalized to a system of coupled spins. We refer again to a Heisenberg type Hamiltonian but now we express it as

\[ H = g\mu_B \frac{1}{2} \sum_n \vec{B}_{\text{self}}(n) \cdot \vec{S}(n) + g\mu_B \sum_n \vec{B} \cdot \vec{S}(n) \]

with \( \vec{B}_{\text{self}}(n) = \frac{1}{g\mu_B} \frac{\delta H_0}{\delta \vec{S}(n)} \) (5.19)

where \( H_0 \) is the part of the Hamiltonian that does not contain the Zeeman term. The effective field \( \vec{B}_{\text{eff}}(n) = \vec{B}_{\text{self}}(n) + \vec{B} \) experienced by the spin located at the \( n \)-th lattice site results from four contributions: i) the effect of exchange interaction with the neighboring spins, ii) the magnetocrystalline anisotropy energy, iii) the interaction with the external field (Zeeman energy) and iv) the dipolar interaction with all the other spins in the lattice (magnetostatic energy). In fact, one can express in a more compact way the effective field as

\[ \vec{B}_{\text{eff}}(n) = \frac{1}{g\mu_B} \frac{\delta H}{\delta \vec{S}(n)} \] (5.20)

Details about functional derivatives and how to compute \( \vec{B}_{\text{eff}}(n) \) in practice can be found in Appendix 5.A. This field enters the LL equation that describes the time evolution of the \( n \)-th spin

\[ \dot{\vec{S}}(n) = -\gamma \frac{\vec{S}(n) \times \frac{\delta H}{\delta \vec{S}(n)}}{g\mu_B} \Rightarrow \hbar \dot{\vec{S}}(n) = -\vec{S}(n) \times \frac{\delta H}{\delta \vec{S}(n)} \] (5.21)

where we have used the fact that \( \gamma = g\mu_B/\hbar \). The Gilbert damping adds a contribution to the equation above analogous to the one given in Eq. (5.12). Generally, Eq. (5.21) corresponds to a system of coupled non-linear equations which can be solved analytically only in very special cases or at the price of
some drastic approximation. An example is represented by the macrospin approximation, within which we have derived the results presented in previous sections.

5.3.1 Spin waves

In this section we would like to study the properties of a special class of \textit{linear} solutions of the Landau-Lifshitz equation (without damping) that we already introduced to discuss the loss of ferromagnetic order in systems with continuous symmetry, that is spin waves. In order to avoid unnecessary complications, we develop the explicit calculation for a Heisenberg spin chain. The relative Hamiltonian is

$$H = -\frac{1}{2} \sum_{i \neq j=1}^{N} J \vec{S}_i \cdot \vec{S}_j - D \sum_{i=1}^{N} (S^z_i)^2 + g\mu_B B \sum_{i=1}^{N} S^z_i , \quad (5.22)$$

while the effective field experienced by the \( j \)-th spin is

$$\vec{B}_{\text{eff},j} = -\frac{1}{g\mu_B} \left[ J \left( \vec{S}_{j-1} + \vec{S}_{j+1} \right) + 2DS^z_j \hat{e}_z \right] + B\hat{e}_z \quad (5.23)$$

(\( \hat{e}_z \) being the unitary vector along the \( z \) axis). By inserting this expression for the local field in Eq. (5.21) we obtain the Landau-Lifshitz equation for a spin chain described by the Hamiltonian in Eq. (5.22):

$$\begin{align*}
\hbar \dot{S}^x_j &= S^y_j \left[ J \left( S^z_{j-1} + S^z_{j+1} \right) + 2DS^z_j - g\mu_B B \right] - J S^z_j \left( S^x_{j-1} + S^x_{j+1} \right) \\
\hbar \dot{S}^y_j &= -S^x_j \left[ J \left( S^z_{j-1} + S^z_{j+1} \right) + 2DS^z_j - g\mu_B B \right] + J S^z_j \left( S^x_{j-1} + S^x_{j+1} \right) \\
\hbar \dot{S}^z_j &= -JS^y_j \left( S^x_{j-1} + S^x_{j+1} \right) + JS^x_j \left( S^y_{j-1} + S^y_{j+1} \right) . \quad (5.24)
\end{align*}$$

This set of equations involves products of spin components, which renders it highly non-linear. However, Eqs. (5.24) can be linearized assuming the transverse spin components to be small compared to \( |S^y_j| \), \( |S^x_j| \) \( \ll |S^z_j| \) and \( |S^y_j| \) \( \ll |S^z_j| \). Then we can set \( S^x_j = S^z \) independent of the lattice position and obtain

$$\begin{align*}
\hbar \dot{S}^x_j &= S^y_j \left( 2JS^z + 2DS^z - g\mu_B B \right) - JS^z \left( S^y_{j-1} + S^y_{j+1} \right) \\
\hbar \dot{S}^y_j &= -S^x_j \left( 2JS^z + 2DS^z - g\mu_B B \right) + JS^z \left( S^x_{j-1} + S^x_{j+1} \right) \\
\hbar \dot{S}^z_j &= 0 . \quad (5.25)
\end{align*}$$
Since we seek for traveling-wave solutions, we set $S_j^\sigma = A^\sigma e^{i(\omega t - q_j)}$ with $\sigma = x, y$, which yields

$$
\begin{align*}
  i\hbar \omega A^x &= A^y [2JS^z (1 - \cos(q)) + 2DS^z - g\mu_B B] \\
  i\hbar \omega A^y &= -A^x [2JS^z (1 - \cos(q)) + 2DS^z - g\mu_B B].
\end{align*}
$$

The values of $\omega$ for which the set of Eqs. (5.26) has non-trivial traveling-wave solutions are obtained from the characteristic equation

$$
\begin{vmatrix}
  i\hbar \omega & -2JS^z (1 - \cos(q)) - 2DS^z + g\mu_B B \\
  2JS^z (1 - \cos(q)) + 2DS^z - g\mu_B B & i\hbar \omega
\end{vmatrix} = 0
$$

whence

$$
\hbar \omega(q) = |S^z| \left[ 2J (1 - \cos(q)) + 2D - g\mu_B \frac{B}{S^z} \right].
$$

If one specializes the value of $S^z = -1$, the expression on the right-hand side matches the expression of $\Gamma(q)$, given in Eq. (3.72), for a linear spin chain. Repeating the same treatment for a 2d and 3d lattice one would get exactly the same expression as Eq. (3.72). For $B = 0$ and $D = 0$, the limit of long wave-lengths gives

$$
\hbar \omega(q) \sim Jq^2.
$$

From textbooks we know that spin waves are also quantized and the specific quadratic relation given in Eq. (5.28) determines the behavior of the magnetization at low temperature. In particular, the relative decrease of the magnetization should follow the Bloch law

$$
\frac{\Delta M}{M_s} \propto T^{3/2}.
$$

It is worth remarking that this behavior is expected for the isotropic ferromagnetic Heisenberg model and for d=3. The $T^{3/2}$ Bloch law agrees with experiments on bulk magnetic systems which are well-described by such a model (with $D \simeq 0$). An example is reported in Fig. 5.3.

**Advanced applications of spin waves**

Nowadays, the interest in spin waves is mostly motivated by the possibility of creating logic devices and low-power circuits based on these type of excitations. This emerging field is called *magnonics*. A particularly hot topic relates the controlled interplay between spin waves and domain walls (DWs).
Figure 5.3: Experimental confirmation of the Bloch law given in Eq. (5.29) for a series of Gadolinium-based magnetic crystals. F. Holtzberg et al., Phys. Rev. 35, p. 1033 (1964).

It has been proposed theoretically\(^6\) that a spin wave artificially injected in a ferromagnetic nanowires should be able to displace a DW. This way of manipulating the position of a DW in a nanowire would be alternative to spin-transfer-torque approach (via injection of electric current) that still requires too much power to be appealing for the spintronic market.

S_z = \cos(\theta(x,t)) = \tanh(c(x-q)), with \( q(t) = \alpha \delta \omega'_L t \).

5.3.2 A simple model for domain-wall dynamics

By means of the LLG equation the dynamics of a domain wall (DW) under external drift can also be described. Within some approximations analytic results can be obtained. Note that the spin profile within a DW – by definition – is not uniform so that the macrospin approximation does not help. For this problem it is more convenient to use polar coordinates \( \vec{S} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \). The time evolution of the \( \theta \) and \( \varphi \) variables can be derived from the LLG equation in this coordinate system:

\[
\begin{aligned}
\dot{\theta} - \alpha \sin \theta \dot{\varphi} &= -\gamma (\vec{B}_{\text{eff}}) \varphi \\
\sin \theta \dot{\theta} + \alpha \dot{\theta} &= \gamma (\vec{B}_{\text{eff}}) \theta
\end{aligned}
\]  

(5.30)

where \( \vec{B}_{\text{eff}} \) is again given by the functional derivative of some Hamiltonian \( \mathcal{H} \) but now in polar coordinates. Limiting ourselves to consider exchange, anisotropy energy, and Zeeman interaction we have

\[
\mathcal{H} = \mathcal{H}_{\text{exch}} + \mathcal{H}_{\text{an}} + \mathcal{H}_{\text{Z}}
\]  

(5.31)

where individual contributions correspond to those given in section 5.A. From Hamiltonian (5.31) it follows

\[
\begin{aligned}
\dot{\theta} - \alpha \sin \theta \dot{\varphi} &= \gamma \frac{Ja}{g \mu B} \frac{1}{\sin \theta} \partial_x \left( \sin^2 \theta \partial_x \varphi \right) \\
\sin \theta \dot{\theta} + \alpha \dot{\theta} &= \gamma \left\{ \frac{Ja^2}{g \mu B} \sin \theta \cos \theta (\partial_x \varphi)^2 + \frac{2D}{g \mu B} \sin \theta \cos \theta + B \sin \theta - \frac{Ja^2}{g \mu B} \partial_x^2 \theta \right\}
\end{aligned}
\]  

(5.32)
Equation (5.32) is highly non-linear and cannot be solved analytically, in general. Nevertheless, we may try to do an educated guess for the DW profile, for instance starting from the static solution which minimizes the energy and fulfills antiperiodic boundary conditions. Such a DW profile was deduced in section 4.4 of the previous chapter but we repropose it here for convenience

\[
\begin{align*}
\cos \theta(x) &= \tanh(cx) \\
\varphi &= \text{const.}
\end{align*}
\]  

(5.33)

with \( ca = 1/\delta = \sqrt{2D/J} \). A reasonable way to modify this equation to include dynamics was proposed by Walker\textsuperscript{7}:

\[
\begin{align*}
\cos \theta(x, t) &= \tanh(c(x - q)) \\
q &= q(t) \quad \dot{c} = 0 \\
\varphi(x, t) &= \varphi(t)
\end{align*}
\]  

(5.34)

The time dependence is thus restricted to \( q \) (coordinate of the DW center) and the azimuthal angle \( \varphi(t) \), assumed to be independent of \( x \). We insert this ansatz into the equations of motion and use the following useful facts \( \partial_x \theta = -c \sin \theta \) and \( \dot{\theta} = c \dot{q} \sin \theta \). The corresponding equations of motion are

\[
\begin{align*}
c \dot{q} \sin \theta - \alpha \sin \theta \dot{\varphi} &= 0 \\
\sin \theta \dot{\varphi} + \alpha c \dot{q} \sin \theta &= \gamma \left\{ \frac{2D}{g_B} \sin \theta \cos \theta + B \sin \theta - \frac{J a^2}{g_B} c^2 \cos \theta \sin \theta \right\}
\end{align*}
\]  

(5.35)

Assuming \( ca = \sqrt{2D/J} \) also in the dynamic regime, the second equation simplifies and we get the final result

\[
\begin{align*}
c \dot{q} - \alpha \dot{\varphi} &= 0 \\
\dot{\varphi} + \alpha c \dot{q} &= \gamma B
\end{align*}
\]  

(5.36)

which is a system of two coupled equations for \( q \) (the DW center) and \( \varphi \). From the first equation it follows that \( c \dot{q} = \alpha \dot{\varphi} \), which inserted in the second one yields \( (1 + \alpha^2) \dot{\varphi} = \gamma B \). This means that the azimuthal angle precesses with an angular velocity formally equivalent to the Larmor frequency of a damped precession, namely \( \dot{\varphi} = \omega_L' \) (see Eq. (5.18)). Substituting this result back in the first equation, a simple expression for the DW velocity is obtained

\[
\dot{q} = \alpha \omega_L' \delta = \gamma B \frac{\alpha}{1 + \alpha^2} \delta
\]  

(5.37)

(with $\delta$ DW width). As expected, we get $\dot{q} \propto B$, meaning that if the field is parallel to the $z$ axis, more and more spins progressively align along the opposite direction in order to minimize the global energy (see Fig. 5.4).

Some features of this solution deserve specific comments:

1. In the absence of damping ($\alpha = 0$) the azimuthal angle precesses with an angular velocity equal to the Larmor frequency $\omega_L = \gamma B$ but the DW does not move, $\dot{q} = 0$, i.e., the global Zeeman energy does not decrease.

2. The effect of $\alpha$ is not that of slowing down the DW motion, on the contrary having $\alpha \neq 0$, is crucial for the DW to move.

3. The translational motion of the DW is – in this case – always accompanied by a steady precession $\dot{\varphi} = \omega'_L = c\dot{q}/\alpha$.

**Advanced applications of domain-wall dynamics**

The interest in magnetic DWs has experienced a sort of renaissance during the last decade. The improvement in spatial resolution with which magnetic textures could be resolved certainly played an important role. However, it was the perspective of employing DWs in spintronic devices – such as the racetrack memory – that gave the crucial boost. The effect of a polarized electric current can also be included in the LLG equation by adding two extra terms, originating from spin-transfer torque (STT). Within similar assumptions as above, after some algebra, one would get the following set of equations

$$
\begin{align*}
\dot{c}q - \alpha \dot{\varphi} &= \gamma D_{\text{int}} g B \sin(2\varphi) + cu \\
\dot{\varphi} + \alpha c\dot{q} &= \gamma B + \beta_{\text{STT}} cu
\end{align*}
$$

(5.38)

where $D_{\text{int}}$ is the intermediate-axis anisotropy; the contribution of spin-transfer torque (STT) is given by $u = j P g B/(2eM_s)$ which has the units of a velocity, $j$ being the electric current density. The term $cu$ on the right-hand side of the first equation comes from adiabatic STT, while the term $\beta_{\text{STT}} cu$ is due to the non-adiabatic contribution ($\beta_{\text{STT}}$ non-adiabaticity parameter).

Some typical curves displaying the DW velocity for different sets of parameters are reported in the following figure. The reader is invited to consider the following special cases (see exercise serie 4)

1. $D_{\text{int}} \neq 0$, $u = 0$ and $B \neq 0$;

---

8**Hint:** First, set $\dot{\varphi} = 0$ and search for the value of $\varphi = \varphi_0(B)$ which remains constant during the motion. Afterwards, look for the threshold field $B_W$ above which the condition $\dot{\varphi} = 0$ cannot be fulfilled anymore (Walker breakdown).
CHAPTER 5. NANOSCALE MAGNETISM

2.  $D_{\text{int}} \neq 0$, $u \neq 0$, $\beta_{\text{STT}} = 0$ and $B = 0$ (proceed similarly to first point) by setting $\dot{\varphi} = 0$ first).

3.  $D_{\text{int}} \neq 0$, $u \neq 0$, $\beta_{\text{STT}} \neq 0$ and $B = 0$.

Possible pinning of DWs is definitely important in applicative contexts. In the idealized picture of Eq. (5.37) an infinitesimally small field should be able to displace a DW. This result was derived in the continuum limit. It can be shown that when the continuum formalism is not applicable anymore, i.e., for sharp DWs, a finite field is required to move the DW itself. The energy barrier to be overcome is roughly given by the cost to lie the spin located at the DW center on the hard plane, namely $\Delta E = D$. At finite temperature (setting for simplicity $B = 0$), this fact suggests that DW diffusion occurs as a thermally-activated process for sharp DWs, with a diffusion coefficient $D_s \sim e^{-\beta D}$. The last dependence has been confirmed experimentally in slow-relaxing molecular spin chains (single-chain magnets). The behavior of the diffusion coefficient for broad DWs is still under debate and harder to investigate experimentally. Theoretical and numerical studies seem to be consistent with a direct proportionality between $D_s$ and temperature, as per standard Brownian motion of a particle in a viscous fluid.

What described above is usually referred as *intrinsic* pinning. In realistic samples additional contributions arise from defects, impurities, substrate roughness, etc., which go under the name of *extrinsic* pinning.

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9Some details may be found in Phys. Rev. B 84, 064415 (2011) and references therein.
5.4 Stochastic dynamics

A thorough theoretical description of magnetization reversal of a nanoparticle is given in the original article by W. F. Brown Jr.\textsuperscript{10}. Thermal effects are there taken into account by adding a fluctuating, random field $\vec{h}(t)$ to the LLG equation:

$$\dot{\vec{S}} = -\vec{S} \times \left[ \gamma \left( \vec{B}_{\text{eff}} + \vec{h}(t) \right) + \alpha \vec{S} \right]; \quad (5.39)$$

$\vec{S}$ is supposed to be a (classical) macrospin with Hamiltonian $\mathcal{H}$; the latter includes Zeeman, exchange, and anisotropy energy (possibly both of magneto-crystalline and dipolar origin). The effective field appearing in Eq. (5.39) is a generalization of the external field and reads

$$\vec{B}_{\text{eff}} = \frac{1}{g\mu_B} \frac{\delta \mathcal{H}}{\delta \vec{S}} \quad (5.40)$$

(more details are given in Appendix 5.A). The Gaussian noise $\vec{h}(t)$ is characterized by the following properties:

$$\langle h^\eta(t) \rangle = 0 \quad \langle h^\eta(t) h^\sigma(t + \Delta t) \rangle = b \delta_{\eta\sigma} \delta(\Delta t) \quad (5.41)$$

where $\langle \ldots \rangle$ stands for statistical average and $\eta, \sigma = x, y, z$. To be quantitative, these assumptions hold as long as time correlations in the random field $\vec{h}(t)$ occur at much shorter time scales\textsuperscript{11} than the Larmor period $1/\omega_L$. The constant $b$ appearing in Eq. (5.41) is to be determined by some correspondence principle with Boltzmann distribution at thermal equilibrium. As for Brownian motion, it turns out to be proportional to temperature.

Still nowadays, Eq. (5.39) represents the way to go if one wants to describe magnetization dynamics at finite temperature. Numerical simulations of this stochastic-LLG equation are computationally more demanding than its zero-temperature counterpart. Basically, averages have to be performed over many replicas of trajectories corresponding to different realization of noise $\vec{h}(t)$. This is the Langevin-dynamic approach. Recently, a mapping paradigm has been defined which allows treating the same problem with time-quantified MonteCarlo algorithms\textsuperscript{12}. Apart from improving numerical stability, up to now, the second approach did not yield a significant reduction in computational time. More optimistic perspectives arise from the implementation of both algorithms on graphic cards (GPU).


\textsuperscript{11}Based on the quantum-mechanical Nyquist formula, the spectrum of thermal fluctuations may be regarded as white up to a frequency of the order of $k_B T/\hbar$. At room temperature this yields correlation times of the order of $10^{-13}$ s, well below a typical precessional period (for instance, about an anisotropy field).

Figure 5.6: Left: qualitative energy landscape $\mathcal{H}(\theta) = -D \cos^2 \theta + g \mu_B B \cos \theta$. Indicatively, domains that are significantly populated in the high-energy barrier limit are defined by thermal energy $k_B T$: $\Gamma_1 \equiv [0, \theta_1]$ and $\Gamma_2 \equiv [\theta_2, \pi]$. Right: the two domains $\Gamma_1$ and $\Gamma_2$ are sketched on the unitary sphere with the corresponding current density $\vec{J}_\theta$.

5.4.1 Nanoparticles with uniaxial anisotropy

In order to get the flavor of the underlying formalism, we are going to repropose the calculation performed by W. F. Brown Jr. for a nanoparticle with uniaxial anisotropy. In this special case – with some additional simplifying hypotheses – the main features of stochastic dynamics may be captured without integrating Eq. (5.39) numerically.

Let $\vec{S}$ be the total spin of a nanoparticle, within the macrospin approximation. Referring to Fig. 5.6, a point $(\theta, \varphi)$ on the unitary sphere identifies the instantaneous direction along which $\vec{S}$ is pointing. In a statistical sense,

ensemble of nanoparticles

Figure 5.7: Sketch of an ensemble of nanoparticles with uniaxial anisotropy described in the text.
a surface density $W(\theta, \varphi, t)$ can be defined, which represents the probability that the considered nanoparticle points along the direction defined by $(\theta, \varphi)$ at time $t$. For the sake of simplicity, we will refer to a statistical ensemble of $n$ particles, so that $\int W(\theta, \varphi, t) \, d\Omega = n$ (see sketch in Fig. 5.7). As individual magnetic moments undergo variations, the distribution of representative points on the unit sphere changes, which results in a finite surface-current density $\vec{J}$. Because the number of particles is conserved, $W$ and $\vec{J}$ are related by a continuity equation:

$$\frac{\partial W}{\partial t} = -\nabla \cdot \vec{J}. \quad (5.42)$$

When magnetic moments in the ensemble evolve according to the LLG equation and the current density contains just a deterministic contribution one has $\vec{J} = W \hat{S}$, with $\hat{S}$ being given by Eq. (5.12). Such current describes a dissipative dynamics, but still does not account for finite temperature. The net effect of thermal fluctuations is that of providing an additional diffusive contribution to the current density of the form $-k'\nabla W$. We further assume that an external field is applied along the easy axis, so that the energy of each particle is a function of the polar angle only: $\mathcal{H}(\theta) = -D \cos^2 \theta + g\mu_B B \cos \theta$.

For what concerns the polar component $J_\theta$, two distinct scenarios occur that can be summarized as follows:

$$J_\theta = -h' \frac{\partial \mathcal{H}}{\partial \theta} W \quad \text{dissip.} \quad T = 0 \quad (5.43)$$

$$J_\theta = -h' \frac{\partial \mathcal{H}}{\partial \theta} W - k' \frac{\partial W}{\partial \theta} \quad \text{dissip. + th. diff.} \quad T \neq 0 \quad (5.44)$$

$h'$ is related to the parameters of LLG:

$$h' = \frac{\gamma g\mu_B}{\hbar^2} \frac{\alpha}{1 + \alpha^2} = \frac{1}{\hbar} \frac{\alpha}{1 + \alpha^2} \quad (5.45)$$

This correspondence is obtained after quite some labor. First, the stochastic-LLG needs to be expressed in polar coordinates, then mapped into a Fokker-Planck equation. After some mathematical manipulations, the latter takes the form of Eq. (5.42). The requirement that Boltzmann distribution be recovered for $\partial W/\partial t = 0$ allows establishing that $\beta k' = h'$.

Remarkably, in the absence of dissipation ($\alpha = 0$) the current density in Eq. (5.43) has no polar component, i.e., $J_\theta = 0$. Indeed, this is related to the fact that $\theta$ remains constant in a Larmor precession produced by a field applied along the $z$ axis (see Eq. (5.7)). Generally, the angle that

---

13The same theoretical treatment applies to a single particle provided that the probability density $W(\theta, \varphi, t)$ is normalized to one.
individual magnetic moments form with their local easy axes shall vary from one particle to the other. But those angles are constant of motion, therefore the dependence on $\theta$ of the probability distribution $W$ does not change either. Larmor precession of individual magnetic moments sustains a current along the azimuthal direction $J_\varphi \neq 0$, which does not facilitate the approach to equilibrium. In fact, if energies are not distributed according to Boltzmann statistics at $t = 0$, a non-dissipative dynamics will never bring $W(\theta, \varphi, t)$ towards thermodynamic equilibrium.

5.4.2 High-energy barrier

When the applied field is smaller than the anisotropy field $2D/(g\mu_B)$ the energy $\mathcal{H}(\theta)$ has one minimum $\mathcal{E}_1$ at $\theta = 0$, another one $\mathcal{E}_2$ at $\theta = \pi$, and one maximum $\mathcal{E}_M$ for $\theta_M = \arccos(2D/(g\mu_B B))$. We are going to derive an equation for the escape rate from one minimum to the other based on the Kramers method\textsuperscript{14}. In the high-energy-barrier limit, namely $\beta(\mathcal{E}_M - \mathcal{E}_i) \gg 1$ (for $i = 1, 2$), most of particle spins have orientations $\theta \simeq 0$ or $\theta \simeq \pi$. We may thus define two populations $n_1$ and $n_2$ corresponding to the number of particles with $0 \leq \theta \leq \theta_1$ and $\theta_2 \leq \theta \leq \pi$, respectively. In the following, we will see that the choice of $\theta_1$ and $\theta_2$ is not crucial. The probability density $W$ for intermediate polar angles $\theta_1 < \theta < \theta_2$ will be very small, though not vanishing in order to warrant a finite flow of representative points from the overpopulated towards the underpopulated minimum. Moreover, we assume that this flow can be described as constant total current across the parallels (circles parallel to the equator) of the unitary sphere (see Fig. 5.6) $I = 2\pi \sin \theta J_\theta$. Since all the representative points basically fall in the neighborhood of the poles, $\theta \simeq 0$ or $\theta \simeq \pi$, one has $n_1 + n_2 \simeq n$ and consequently $I = -\dot{n}_1 = \dot{n}_2$. Equation (5.44) allows relating the current $I$ to the populations $n_1$ and $n_2$. Within our assumptions one has

$$-k' \frac{\partial \mathcal{H}}{\partial \theta} W - k' \frac{\partial W}{\partial \theta} = \frac{I}{2\pi \sin \theta}$$

$$\Rightarrow \quad \beta \frac{\partial \mathcal{H}}{\partial \theta} W + \frac{\partial W}{\partial \theta} = -\frac{I}{2\pi k' \sin \theta}$$

$$\Rightarrow \quad \frac{\partial}{\partial \theta} \left(W e^{\beta \mathcal{H}(\theta)}\right) = -\frac{I}{2\pi k' \sin \theta} e^{\beta \mathcal{H}(\theta)}, \quad (5.46)$$

\textsuperscript{14}In the original work this formalism was developed to study the dynamics of chemical reactions: H. A. Kramers, Physica \textbf{7}, 284 (1940).
CHAPTER 5. NANOSCALE MAGNETISM

where in the last passage we multiplied the left- and right-hand side by $e^{\beta H(\theta)}$. Integrating from $\theta = 0$ to $\theta = \pi$ we get

$$W_2 e^{\beta \varepsilon_2} - W_1 e^{\beta \varepsilon_1} = -\frac{I}{2\pi k'} \Sigma_M$$

with $\Sigma_M = \int_0^\pi \frac{e^{\beta H(\theta)}}{\sin \theta} \, d\theta, \quad (5.47)$

where $W_1 = W(0)$ and $W_2 = W(\pi)$. The integral $\Sigma_M$ can be estimated expanding the energy about the maximum $H(\theta) \simeq \varepsilon_M - \kappa_M(\theta - \theta_M)^2/2$ ($\kappa_M = H''(\theta_M)$) and replacing $\sin \theta$ by $\sin \theta_M$; then, letting the extremes go to $\pm \infty$, one obtains

$$\Sigma_M = \sqrt{\frac{2\pi}{\beta \kappa_M}} \frac{e^{\beta \varepsilon_M}}{\sin \theta_M}. \quad (5.48)$$

Now we are going to show that the terms $W_i e^{\beta \varepsilon_i}$ (with $i = 1, 2$) appearing on the left-hand side of Eq. (5.47) are actually related to the populations $n_i$ in the two energy wells (polar circles in Fig. 5.6 right). To this aim, we will assume that equilibrium (Boltzmann distribution) has been attained in those two wells $0 \leq \theta \leq \theta_1$ and $\theta_2 \leq \theta \leq \pi$ (energy landscape in Fig. 5.6 left). Therefore,

$$n_i = 2\pi W_i \int_{\Gamma_i} e^{\beta [\varepsilon_i - H(\theta)]} \sin \theta \, d\theta, \simeq \frac{2\pi}{\beta \kappa_i} W_i \quad (5.49)$$

with $\kappa_1 = H''(0)$ and $\kappa_2 = H''(\pi)$. In Eq. (5.49) the original integration domains were $\Gamma_1 \equiv [0, \theta_1]$ and $\Gamma_2 \equiv [\theta_2, \pi]$ but have been extended to $[0, \pm \infty)$. Moreover, $\sin \theta$ has been expanded to the first order. Thanks to the relation (5.49) between $n_i$ and $W_i$, Eq. (5.47) can be written as

$$\frac{\beta}{2\pi} \left( n_2 \kappa_2 e^{\beta \varepsilon_2} - n_1 \kappa_1 e^{\beta \varepsilon_1} \right) = \frac{\beta}{2\pi h'} \sqrt{\frac{2\pi}{\beta \kappa_M}} \frac{e^{\beta \varepsilon_M}}{\sin \theta_M} \dot{n}_1 \quad (5.50)$$

where the relations $I = -\dot{n}_1$, $k' = \beta h'$, and Eq. (5.48) have been used. After some elementary manipulations, the equation above takes the form

$$\dot{n}_1 = \nu_2 n_2 - \nu_1 n_1 \quad \text{with} \quad \nu_i = \kappa_i h' \sin \theta_M \sqrt{\frac{\beta \kappa_M}{2\pi}} e^{-\beta (\varepsilon_M - \varepsilon_i)} \quad (5.51)$$

With the condition $n_1 + n_2 = n$ — closely related to the high-energy-barrier constraint $\beta (\varepsilon_M - \varepsilon_i) \gg 1$ — Eq. (5.51) enables describing how the two populations evolve in time:

$$\begin{align*}
n_1(t) &= \frac{\nu_2}{\nu} n + \left[ n_1(0) - \frac{\nu_2}{\nu} n \right] e^{-\nu t} \\
n_2(t) &= \frac{\nu_1}{\nu} n + \left[ n_2(0) - \frac{\nu_1}{\nu} n \right] e^{-\nu t}
\end{align*} \quad (5.52)$$
where \( \nu = \nu_1 + \nu_2 \). The inverse of this attempt frequency defines the characteristic time scale of approach towards equilibrium: the relaxation time \( \tau = 1/\nu \). At long-time scales, the ratio of the two populations tends to

\[
\frac{n_2}{n_1} = \frac{\nu_1}{\nu_2} = \frac{\kappa_1 e^{\beta E_1}}{\kappa_2 e^{\beta E_2}}.
\] (5.53)

Besides the exponential dependence on the energy at the two poles, a kind of entropic prefactor appears. The latter accounts for a possible different curvature of the energy landscape around the two minima. Thus, overall the Boltzmann distribution is recovered.

We conclude this section giving an explicit formula for the relaxation time in the case in which no magnetic field is applied. In this case \( \mathcal{H}(\theta) = -D \cos^2 \theta \), from which \( \mathcal{H}''(\theta) = 2D \cos(2\theta) \) that yields \( \kappa_1 = \kappa_2 = \kappa_M = 2D \).

The energy barrier is simply \( E_M - E_i = D \). Therefore, the attempt frequencies in Eq. (5.51) take the form

\[
\nu_1 = \nu_2 = \frac{2D}{\hbar} \frac{\alpha}{1 + \alpha^2} \sqrt{\frac{\beta D}{\pi}} e^{-\beta D} = \frac{1}{\tau_D} \sqrt{\frac{\beta D}{\pi}} e^{-\beta D}.
\] (5.54)

The term in front of the square root is the inverse of the damping time \( \tau_D \) characterizing a damped precession about a field equal to the anisotropy field \( 2D/(g\mu_B) \) (see Eqs. (5.17) and (5.18)). The leading temperature dependence clearly lies in the exponential, which is typical of thermally-activated processes across an energy barrier. This result for the escape rate from wells created by the anisotropy energy was anticipated at the beginning of chapter 4, precisely in Eq. (4.4). The additional square-root dependence on temperature has to do with the curvature at the maximum of the energy barrier. Finally, under these hypotheses, the relaxation time for an ensemble of nanoparticles described here reads:

\[
\tau = \frac{\tau_D}{2} \sqrt{\frac{\pi}{\beta D}} e^{\beta D}.
\] (5.55)

**Advanced applications of superparamagnets**

When considering a systems of coupled spins which are assumed to rotate rigidly, Eq. (5.55) defines the superparamagnetic limit. In fact, in this macrospin approximation the energy barrier for the relaxation time scales with the number of atoms in the nanoparticle, namely with its volume. When the latter becomes too small bistability is lost and with that the possibility to store information in the considered nanoparticle. This issue has been already discussed in section 4.2 of the previous chapter. Here we would like
to point out that a rigid rotation is obviously not the only way to reverse the magnetization. In macroscopic specimens, this process typically encompasses a non-homogeneous magnetization reversal. If one thinks of elongated samples (nanowires), nucleation of a domain wall (DW) at a free edge costs a fixed amount of energy, of the order of the DW energy, independently of the sample size. On the contrary, the barrier for a uniform rotation is always proportional to the particle volume, meaning that it will be favored only for very short wires. For completeness, we mention that in atomic nanowires with broad DWs, the nucleation cost may be reduced by the presence thermally-excited spin waves, which lowers the effective barrier with respect to $\mathcal{E}_w = 2\sqrt{2D\mathcal{J}}$.

A stochastic-dynamic treatment of non-homogeneous magnetization reversal is, of course, much more difficult than what exposed above and can hardly be tackled analytically for very special geometries$^{15}$.

Conclusions

Coherently with the line of the whole course, we tried to provide a crash overview of magnetization dynamics with the main focus on fundamental aspects that rule it at different time scales. The price was that of renouncing to describe specific selected topics of cutting-edge research. However, we learnt that between 10-100 ps dynamics is essentially precessional. Damping effects typically occur in the nanosecond range. While from less than microseconds to geological time scales magnetization dynamics behaves stochastically. Note that, for different reasons, all those three regimes are interesting for magnetic-storage applications.

Due to space limitations, we overlooked at least two other types of magnetization dynamics associated with flourishing research fields: ultrafast (demagnetization) dynamics, which takes place at femtosecond time scale$^{16}$, and quantum-tunneling of the magnetization observed in single-molecule magnets$^{17}$. The last ones are molecular compounds, comprising a limited number (typically between three and twelve) of paramagnetic ions coupled via the exchange interaction, in which tunneling mechanism competes with stochastic relaxation described in section 5.4.2. In particular, for some special values of the applied field (resonance) the magnetization can short-cut the energy barrier by quantum tunneling, which eventually speeds up relaxation towards equilibrium.

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$^{16}$The interested student is addressed to the course held by Yves Acremann.
CHAPTER 5. NANOSCALE MAGNETISM

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Appendices

5.A Micromagnetic limit

Beyond analytical approaches, a lot of algorithms are available that allow simulating magnetization dynamics through the integration of the LLG equation\(^{18}\). The latter is usually expressed in the continuum limit so that finite-element methods can be applied. For convenience, we list below the different contributions to the energy – which have been introduced in previous chapters – expressed in the continuum limit.

- **Exchange energy**

\[
H_{\text{exch}} = \frac{1}{2} J a^{2-d} \int \left| \nabla \vec{S}(r) \right|^2 d^d x + \text{const.} \quad (5.56)
\]

- **Magnetocrystalline-anisotropy energy**

\[
H_{\text{an}} = - D \frac{1}{a^d} \int |S_z(r)|^2 d^d x \quad (5.57)
\]

- **Zeeman energy**

\[
H_Z = \mu_B \frac{1}{a^d} \int \vec{B}^{\text{ext}} \cdot \vec{S}(r) d^d x \quad (5.58)
\]

where \(\vec{B}^{\text{ext}} = \mu_0 \vec{H}^{\text{ext}}\) is the external, applied field and does not include the contribution coming from \(\vec{M}\), the latter being accounted for in the following term.

- **Dipolar energy**

\[
H_{\text{dip}} = \frac{\mu_0}{8\pi} \Omega \frac{1}{a^{2d-3}} \int d^d r \int \frac{\vec{S}(r) \cdot \vec{S}(r')}{|r - r'|^3} d^d r' - \\
-3 \frac{\mu_0}{8\pi} \Omega \frac{1}{a^{2d-3}} \int d^d r \int \left\{ \frac{\left[ \vec{S}(r) \cdot (r - r') \right] \left[ \vec{S}(r') \cdot (r - r') \right]}{|r - r'|^5} \right\} d^d r' + \\
\frac{\mu_0}{6} \Omega \frac{1}{a^{2d-3}} \int d^d r \int \vec{S}(r) \cdot \vec{S}(r') \delta (r - r') d^d r'
\quad (5.59)
\]

with \(\Omega = \frac{\mu_0}{4\pi} \left( g \mu_B S \right)^2 a^d\).

\(^{18}\)For instance, the Object Oriented MicroMagnetic Framework (OOMMF) or Nmag or FastMag simulation packages.
The calculation of the effective field \((5.40)\) encompasses functional derivatives, which in the continuum limit read

\[
\frac{\delta \mathcal{H}}{\delta S^\sigma} = \frac{\partial f_H}{\partial S^\sigma} - \sum_{\eta,\sigma} \partial_\eta \frac{\partial f_H}{\partial (\partial_\eta S^\sigma)} + \ldots \tag{5.60}
\]

where \(\eta, \sigma = x, y, z\) and \(f_H\) is an energy density defined as \(\int f_H d^d x / d^d \). For instance, the anisotropy energy brings only a contribution along \(z\) equal to the anisotropy field

\[
B_{an}^z(r) = \frac{1}{g\mu_B} \frac{\partial f_{H_{an}}}{\partial S^z} = -\frac{2D}{g\mu_B} S^z(r). \tag{5.61}
\]

A bit more tricky is the contribution from the exchange Hamiltonian. Remembering that

\[
\left| \nabla \vec{S}(r) \right|^2 = \sum_{\eta,\sigma} \partial_\eta S^\sigma(r) \partial_\eta S^\sigma(r) \tag{5.62}
\]

the \(\sigma\) component of the effective exchange field reads

\[
B_{exch}^\sigma(r) = -\frac{1}{g\mu_B} \sum_{\eta} \partial_\eta \frac{\partial f_{H_{exch}}}{\partial (\partial_\eta S^\sigma)} = -\frac{J}{g\mu_B} a^2 \sum_{\eta} \partial_\eta^2 S^\sigma = -\frac{J}{g\mu_B} a^2 \Delta S^\sigma. \tag{5.63}
\]

The functional derivative of the Zeeman energy simply yields the applied, external field; while the effective dipolar field can be deduced similarly to the anisotropy field.

One should not forget that the continuum limit is justified when the spin profile varies smoothly from one site to the next. Quantitatively, this requires the domain-wall width to be larger than several lattice units. Such a condition is usually fulfilled in standard conductors (Fe, Ni, Permalloy, etc.) but not necessarily in molecular samples (spin chains, spin ice, molecular magnets, etc.).