

UNIVERSITÀ DEGLI STUDI DI TRENTO

DIPARTIMENTO DI FISICA

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# XY model

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# Introduction

## 1.1 Lattice models for phase transitions

A very successful and general range of models in statistical mechanics are the ones where the components of a system are allocated on an array of lattice sites, where every component interacts only with the closest ones to it (*nearest-neighbour interaction*). This kind of models turns out to describe well a very broad range of phase transitions including ferromagnetism transitions, gas-liquid and gas-solid transitions, superconductive transitions and so on.<sup>1</sup>

The case in consideration here will be the one for *ferromagnetic* transitions.

Being defined on a lattice means basically a discretization of space, a caveat that fits very well if the system in consideration is a metal whose atoms are situated in a crystal structure. The crystalline nature of metals enables to introduce another simplification in this kind of models: considering the atoms as harmonic oscillators swinging around the equilibrium point we can neglect the kinetic energy of these atoms and consider only the interactions between them. It has to be said that this kind of facilitation turns out to be good enough also for the other kinds of transitions listed above.

## 1.2 Hamiltonian of ferromagnetic lattice systems

Being interested in the magnetic interactions of atoms we consider them as magnetic dipoles having a magnetic moment  $\mu$ . Every magnetic dipole in the  $N$  lattice sites will have a magnitude  $\mu = g\mu_B\sqrt{J(J+1)}$ , with  $g$  being the Landé factor,  $\mu_B$  the Bohr magneton and  $J$  being the total angular momentum quantum number. The orientations of the magnetic momenta are given by the multiplicity of  $J$ :  $(2J+1)$ . These magnetic dipoles will interact with each other and will interact with an eventual external field  $\mathbf{B}$ .

The net magnetization of the system  $\overline{M}$  will depend on both the tempera-

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<sup>1</sup>The foregoing discussion is heavily based on Pathria (1972) section 12.3

ture  $T$  and the field  $B$  ( $\bar{M} \equiv \bar{M}(T, B)$ ). Studying the *spontaneous magnetization*  $\bar{M}(0, B)$  of a *critical temperature*  $T_c$  can be defined as the threshold temperature for  $\bar{M}(0, B) \neq 0$ : above  $T_c$  the thermal agitation will be too big to allow a spontaneous magnetization to form, then at  $T_c$  the system will perform a *ferromagnetic transition*.

Detailed studies beyond the scope of this tractation have shown that ferromagnetic properties arise when  $J = \frac{1}{2}$  and so it can be assumed that this kind of phenomena are due to electrons spin. Then we can rewrite the magnetic moment as  $\mu = 2\mu_B \sqrt{s(s+1)}$ , where  $g = 2$  is the Landé factor for electrons and  $s$  is the spin of the electron.

From quantum mechanics considerations (see Bransden, Joachain, and Plivier 2003) it can be shown that the interaction energy between two electrons can be expressed as  $K_{ij} \pm J_{ij}$  with  $i$  and  $j$  being the two indices indicating two neighboring electrons. The plus and minus sign are determined based on  $S$  the total spin of the two electrons: the plus corresponding to the case  $S = 0$  and the minus to one with  $S = 1$ , where only  $J_{ij}$  is due to the spin configuration.

Then the energy difference between the "parallel" spin configuration and the "antiparallel" spin configuration is

$$\Delta E = E_{\uparrow\uparrow} - E_{\uparrow\downarrow} = -2J_{ij}$$

Defining the scalar product operator of the spin of the two electrons as

$$\mathbf{s}_j \cdot \mathbf{s}_i = \frac{1}{2}S(S+1) - s(s+1)$$

is easy to show that the interaction energy between the spins can be written as

$$E_{ij} = \text{const.} - 2J_{ij}(\mathbf{s}_i \cdot \mathbf{s}_j)$$

The exact value of the constant is irrelevant since any constant can be added to the potential energy. Still from quantum mechanical considerations can be seen  $J_{ij}$  fall very rapidly with the distance, supporting our initial caveat of regarding only the nearest-neighbors interactions.

## 1.3 $n$ -vector model

### 1.3.1 Ising Model

### 1.3.2 Heisenberg Model

# XY model

## 2.1 Definition

## 2.2 2D case

## 2.3 3D case

# Montecarlo simulation

## 3.1 Monte Carlo Theory

## 3.2 Implementation

## 3.3 Results

# Conclusion

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