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XY model

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Contents

Introduction

1.1 Lattice models for phase transitions

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

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 fit very well if the system unde stydu is a metal whose atoms are almost locked in a crystalline structure. The crystalline nature of metals enables to introduce another semplification 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 considering only the magnetic interactions between them. It has to be said that this kind of facilitation turns out to be adequate also for other kinds of transitions and for very different materials from metals.

1.2 Hamiltonian of ferromagnetic lattice systems

Being interested in the magnetic interactions of atoms we consider them as a magnetic dipoles having a magnetic moment μ. Every magnetic dipole in the N lattice sites will have a magnitude $\mu = g\mu_B\sqrt{J(J+1)}$, with g being the Landè factor, μ_B the Bohr magneton and J being the total angolar momentum quantum number. The total number of possible orientations of the magnetic momenta in space is given by the multiplicity of J: $(2J+1)$. This magnetic dipoles will interact witch 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 temperature T

[1] The foregoing discussion is heavily based on Pathria (1972) section 12.3

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

Detailed studies beyond the scope of this treatment 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 electons spin. Then the magnetic moment can be rewritten as $\mu = 2\mu_B\sqrt{s(s+1)}$, where $g = 2$ is the Landè 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 the two electron: the plus corresponding to the case $S = 0$ and the minus to one with $S = 1$, where only J_{ij} depends on 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 electron 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 irrilevant since any constant can be added to the potential energy. Still from quantum meachanical considerations can be seen that J_{ij} falls very rapidly when the distance beetwen thw two spins increases, supporting our initial caveat of regarding only the neirest-neighbors interactions.

1.3 *n*-vector model

In statistical mechanics the formalization of the ideas presented in the previous sections for ferromagnetic lattice models is the so called n-vector model. A n-vector model is a system of interacting spins on crystalline lattice as the ones described above. This formalization was developed by Stanley (see Stanley 1968) and he was able to show that most of the critical proprerties of this kind of systems

depends only on the dimension of the lattice and on the dimensionality of the spins in the system.

To put it in a mathematical formal way we have a n-vector model when we can describe a system composed of n-dimensional spins as unit-length vectors, located on the sites of d dimensional lattice.

The evolution of the system is described by the following Hamiltonian

$$H = -J \sum_{n.n.} \mathbf{s}_i \cdot \mathbf{s}_j \tag{1.1}$$

where the meaning of the symbols follows directly from the one used in the previous sections and the subscript $n.n.$ means the summation goes over only on the nearest-neighbor spins.

Equation 1.1 shows that *ferromagnetic* phenomena are possible when $J > 0$ since the configuration $\uparrow\uparrow$ is energetically favorable in respect to the $\uparrow\downarrow$ configuration, then otherwise if $J < 0$ *antiferromagnetic* phenomena could arise.

Obviously in the presence of an external field the Hamiltonian will be modified in the following way

$$H = -J \sum_{n.n.} \mathbf{s}_i \cdot \mathbf{s}_j - h \sum_{i} \mathbf{s}_i \tag{1.2}$$

where now J is the J in equation 1.1 divide by $k_B T$ and $h = \mu B / k_B T$, where B is the magnitude of the external magnetic field. As a consequence magnetization properties will depend also on the field.

1.3.1 Ising Model

The Ising model was the first of the ferromagnetic lattice models invented, much before Stanley's formalization, in 1920 by professor Wilhelm Lenz who gave it as problem to his student Ernst Ising. [2]

The Ising model is basically the n-vector model for $n = 1$: the spins are considered as a one dimesional vector that can take only two values: up and down. This is simplest physically important case ($n = 0$ being of importance merely from a mathematical point of view) and was solved analytically in the $d = 1$ case by Ising in 1924. He showed no transitions can occur in such a model, but it was the ground zero for the development of much more complicated models for higher dimensions.

In the following years also the case for $d = 2$ was solved and transitions were shown to be possible. Analytical solutions for higher dimension are still to be found, if there are some, and are definitely outside of the scope of this treatment.

[2] check `https://en.wikipedia.org/wiki/Ising_model`

1.3.2 Heisenberg Model

The Heisenberg model is the n-vector model for $n = 3$ and require a quantum mechanical treatment and is obviously the closest one to a description of reality. Being more complex as a model means it is a tremendously more difficult problem to tackle and it requires a mathematical and quantum mechanics formalizations called Potts models [3] that integrates also the n-vector models.

The Heisenberg model has multiple apllications in quantum mechanics and it is one of the most studied model of magnetism. [4]

[3] check `https://en.wikipedia.org/wiki/Potts_model`

[4] For a detailed view of Heisenberg model see Nolting and Ramakanth (2009)

XY model

2.1 Definition

The $n = 2$ n-vector model is the one of interest in this treatment and it is the so called *XY model*. The name is due to the fact that the spin is a two dimensional vector lying on the xy plane. Introduced in the 1950s, this model was actually used to describe quantum lattice gas and superfluid transitions, then in the late 1960s it was adopted to model ferromagnets.

As in any n-vector model properties of the system are detrmined also by the dimensionality of the lattice considered to describe the system. In the 1 dimensional case there exists an exact solution in the absence of an external field. Being exactly solvable means an exact form for the partition function can be found and thermodinamical properties can be derived theoretically. When periodic boundaries conditions are applied, using the statistical mechanics *transfer-matrix method*, first introduced by Kramers and Winnier in the study of the Ising model in 1941[1], the partition function can be written in a very simple form as

$$Z = 2\pi I_0(\beta J) \tag{2.1}$$

where $I_0(x)$ is the first modified Bessel function and $\beta = 1/k_B T$. From equation 2.1 the specific heat, and other thermodinamical quantities, can be exactly derived and is plotted in figure 2.1 below. [2]

The most physically interesting cases are the 2 dimensional and the 3 dimensional one and they will be discussed in detais in the following sections.

2.2 2D case

2.3 3D case

[1] see Kramers and Wannier 1941

[2] source `https://upload.wikimedia.org/wikipedia/commons/6/68/1D_XY_Specific_Heat.svg`

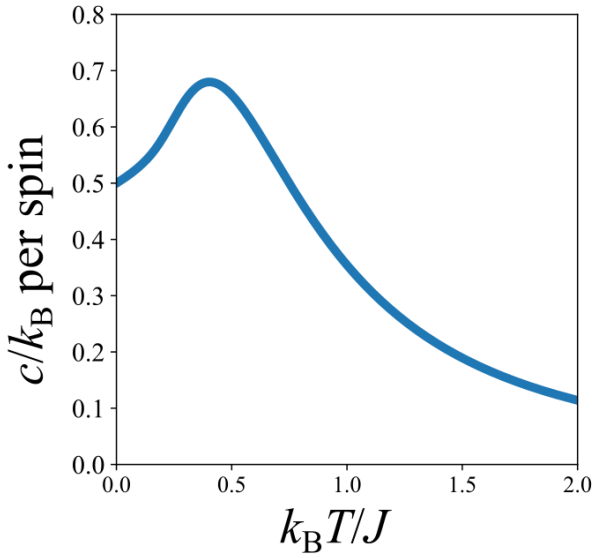

Figure 2.1: Exact specific heat of 1D XY model

Montecarlo simulation

3.1 Monte Carlo Theory

3.2 Implementation

3.3 Results

Conclusion

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