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BACHELOR THESIS

The Variational Structure  
of Physical Principles:  
the cases of Classical, Relativistic and  
Statistical Mechanics

La Struttura Variazionale  
dei Principi Fisici:  
i casi della Meccanica Classica,  
Relativistica e Statistica

*Supervisors:*

Prof. Giampaolo CO'

Prof. Adriano BARRA

*Student:*

Miriam AQUARO

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# Acronyms

- **C-W** Curie-Weiss
- **H-J** Hamilton-Jacobi
- **IRS** Inertial reference system
- **ODE** Ordinary differential equation
- **PDE** Partial differential equation
- **TL** Thermodynamic limit. The limit for the particle number  $N$  and the volume  $V$  going to infinity while the density of the system  $\rho = N/V$  remains constant.

# Abstract

In this thesis work, three disciplines of physics i.e. classical, relativistic and statistical mechanics, are structured through a common base: the principle of least action (or Hamilton's principle). The main goal of this thesis is to demonstrate that even statistical mechanics, despite its probabilistic structure, can be constructed starting from the calculus of variations. If in classical mechanics we minimize the action (in order to obtain the physical path), in thermodynamics we minimize the free energy  $F$ . In our treatment, we shall use another thermodynamic quantity i.e. the pressure  $A = \beta f$ , where  $f$  is the free energy per site  $f = \frac{F}{N}$ . In order to develop the connection between the various mechanics we introduce the Curie-Weiss model in which  $N$  spins interact through pairwise couplings with each other (and it is also the simplest model to show a phase transition). The Curie-Weiss model (C-W) can be solved exactly through mean-field theory or by using Guerra's interpolation method. The interpolation method consists in obtaining the C-W pressure in the thermodynamic limit (TL) by introducing a generalized pressure  $A(\beta, t)$  with  $t$  a real parameter. The pressure  $A(\beta, t)$  evaluated at  $t = 0$  is that of a model with  $N$  independent spins, whereas,  $A(\beta, t = 1)$  is the original C-W pressure. Using the fundamental theorem of calculus we obtain  $A(\beta, t = 1)$ . The analogy between classical and statistical mechanics starts with the resolution of the model through a mechanical analogy. The pressure, now parametrized in terms of the real parameters  $x, t$ , in the TL, satisfies the Hamilton-Jacobi (HJ) equation for the free particle of unit mass and is therefore treated as an action. The momentum, the spatial derivative of the action, becomes the magnetization and the pressure  $A(t, x)$  is obtained as the integral of the Lagrangian over time. Applying the principle of least action to the expression of the pressure  $A(x, t)$  we obtain the self-consistency relation of the magnetization (the equation satisfied by the order parameter at equilibrium). The analogy has another important aspect, Noether symmetries of classical mechanics correspond, in the statistical counterpart, to the self-averaging properties of the model. Away from the critical point, the magnetization, in the TL, is self-averaging, i.e. it has no fluctuations. The C-W model can be generalized to show a relativistic structure. Now, analogously to the classical case, the relativistic pressure satisfies the relativistic H-J equation for a relativistic free particle with unitary mass at rest. We go on showing the coherence of such generalization: all relativistic equations, including the self-consistency equation and the self-averaging relations can be Taylor expanded for small values of  $m$  to obtain again the classical C-W model relations. We also describe the properties of the phase transition of the C-W model, with particular attention to the divergence of the amplified fluctuations of  $m$  (amplified by a factor of  $\sqrt{N}$ ) at the critical point and of the connection between the phenomenon of spontaneous symmetry breaking and the bifurcations typically seen in mathematical physics.

# Riassunto

In questo lavoro di tesi tre discipline della fisica, i.e. la meccanica classica, relativistica e statistica vengono strutturate mediante una base comune: il principio di minima azione (o principio di Hamilton). L'obiettivo più arduo e innovativo del lavoro è dimostrare che anche la meccanica statistica, la cui base probabilistica la allontana dal determinismo della meccanica analitica, può essere costruita a partire dal calcolo variazionale. Se nella meccanica classica, ciò che minimizziamo per trovare il cammino fisico è l'azione, per la termodinamica risulta essere l'energia libera  $F$ . Nella nostra trattazione useremo al posto dell'energia libera un'altra quantità termodinamica che è la pressione  $A = \beta f$ , dove  $f$  è l'energia libera per sito  $f = \frac{F}{N}$ . Per raggiungere lo scopo introduciamo il modello di Curie-Weiss in cui  $N$  spin interagiscono con interazione a due corpi fra di loro ed è inoltre il modello più semplice a mostrare una transizione di fase. Il modello di Curie-Weiss (C-W) può essere risolto con soluzione esatta in campo medio o con il metodo dell'interpolazione di Guerra. Il metodo dell'interpolazione consiste nel trovare la pressione nel limite termodinamico (TL) del modello di C-W introducendo una  $A(\beta, t)$  con  $t$  parametro reale, che per  $t = 0$  corrisponde ad una pressione di un modello ad  $N$  spin indipendenti e per  $t = 1$  alla pressione del modello di C-W. Utilizzando il teorema fondamentale del calcolo integrale riusciamo a ricavare  $A(\beta, t = 1)$  mediante la sola conoscenza dei risultati del modello a spin indipendenti. L'analogia tra meccanica classica e statistica comincia con la risoluzione del modello tramite un' analogia meccanica in cui, la pressione, parametrizzata ora in  $x, t$  parametri reali, nel limite termodinamico (TL), soddisfa l'equazione di Hamilton-Jacobi (H-J) per la particella libera di massa unitaria e dunque viene promossa ad azione. Il momento, derivata spaziale dell'azione, diventa la magnetizzazione e la pressione  $A(t, x)$  viene ricavata come integrale della lagrangiana rispetto al tempo. Applicando il principio di minima azione all'espressione della pressione ottenuta  $A(x, t)$  ricaviamo esattamente la relazione di auto-consistenza della magnetizzazione (espressione utilizzata in letteratura per l'equazione che definisce il parametro d'ordine all'equilibrio). L'analogia presenta un ulteriore aspetto, le simmetrie di Noether della meccanica classica corrispondono, nella controparte statistica, alle proprietà di auto-media della magnetizzazione. Lontano dal punto critico, la magnetizzazione, nel TL gode infatti della proprietà di *self-averaging* ovvero non presenta fluttuazioni. Il modello di C-W può essere esteso ad una versione relativistica. Adesso, analogamente al caso classico, la pressione relativistica soddisfa l'equazione relativistica di H-J, invariante sotto trasformazioni di Lorentz, per una particella libera relativistica con massa a riposo unitaria. Si procede in modo analogo al caso precedente e si dimostra anche la coerenza del modello: tutte le relazioni relativistiche, tra cui auto-consistenza e proprietà di auto-media possono essere sviluppate per piccoli valori della magnetizzazione per riottenere quelle del C-W classico. Nel lavoro si descrivono anche le proprietà della transizione di fase del C-W, con particolare attenzione alla divergenza delle fluttuazioni amplificate (di  $\sqrt{N}$ ) al punto critico e delle correlazioni tra il fenomeno di rottura spontanea di simmetria e le biforcazioni tipiche della fisica matematica.

# Chapter 1

## Introduction

This thesis is dedicated to the mathematical similarity between the formulations of the variational principles in various branches of the mechanics: classical, relativistic and statistical ones. To be more specific, ultimate aim of this thesis is to show the existence of a mathematical bridge connecting different physical variational principles that, at a first glance, may appear to have very little to share. In particular the main duality we want to show is how the least action principle, hegemonic in mechanics, accounts perfectly also for thermodynamics. In classical and relativistic analytical mechanics this variational principle rules the equation of a massive system and its use, in this framework, is crystal-clear.

In the microscopic description of thermodynamics, i.e. in the equilibrium statistical mechanics, we choose a rather different route to deal with the system. According to the principles of thermodynamics we require, simultaneously, both the minimization system energy and the entropy maximization. These two different principles tend to drift the system toward opposite limit (maximum order versus maximum disorder) but we can, pragmatically, satisfy both of them at once by minimizing the free energy. By using the Curie-Weiss (C-W) model (i.e. the simplest model capturing a phase transition, with  $N$  spin sites corresponding to  $N$  magnetic moments that interact with each other through pairwise interactions), we show that its free energy naturally obeys an Hamilton-Jacobi (H-J) partial differential equation (PDE) typical of Lagrangian mechanics. Then, by identifying its free energy with the action, in this mechanical analogy, we see that the least action principle for this action effectively reproduces the correct self-consistency equation for the model order parameter (in our case the magnetization) usually obtained by an entirely statistical mechanical driven path.

The analogy between analytical and statistical mechanics is actually by far deeper. In this thesis, we study its consequences and we prove that symmetries in the analytical mechanical framework (i.e. Noether symmetries) have a natural dual representation in terms of self-averaging properties of the model in the statistical mechanical counterpart. Further more, by deriving the H-J equation in the space-coordinate we obtain a Riemann-Hopf equation for the magnetization. Within this duality, Riemann-Hopf PDE is the archetype of Hopf bifurcation and symmetry breaking is naturally represented as a classical bifurcation (and the phase transition itself is nothing but a shock in the system's evolution).

Finally, we extend the analogy to its relativistic limit and we investigate the consequences in statistical mechanics. We reverse the perspective and use generalizations in analytical mechanics to study their consequences in statistical mechanics. In particular, in the relativistic extension, the free energy no longer obeys the classical H-J equation, rather its relativistic Klein-Gordon-like extension. The analogy keeps holding in full depth and the extension from classical to relativistic scenario implies, by a statistical mechanical perspective, models

whose interactions are no longer just pairwise as in the C-W model. Pairwise interactions are the minimal requirement, beyond the one body terms that deal with the external fields, to have collective phenomena as phase transitions. These models are far from exhaustive and, much more general interactions among several spins are likewise possible (as it is indeed the case, e.g. for instance in the case of structural glasses and all those systems lacking critical behaviour in general). Taking the low momentum limit of the relativistic Hamiltonian we obtain again the classical Hamiltonian with pairwise interactions, in this sense the relativistic model is more exhaustive as not only it contains the simple classical case but also considers more complicate spins interactions. To accomplish this journey across the various mechanics, a short introduction both to analytical mechanics (in its classical as well as in its relativistic formulation) and statistical mechanics is mandatory and it is provided in the first part of the thesis (the first three Sections, one for each kind of mechanics we will need). These preliminary sections introduce the key quantities, concepts and results that we need to develop the mechanical analogy, the real bulk of the thesis, discussed, in details, in chapter 5. Finally an appendix clarifies a rather technical, but important, point on the mathematical existence of all the functions that we consider.

# Chapter 2

## Classical Mechanics in a nutshell

In this section we introduce all the main quantities to be used when working with mechanical systems. In particular, we discuss the role of the principle of least action in terms of the Lagrangian, the Hamiltonian and, ultimately, how to frame it within the H-J perspective.

### 2.1 Action Principle, Lagrangian Formulation

Every mechanical system is characterized by a definite function

$$\mathcal{L}(q_1, q_2, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n) \quad (2.1)$$

called *Lagrangian*, where the set of generalized coordinates  $q_1, q_2, \dots, q_n$  and their time derivatives  $\dot{q}_1, \dot{q}_2, \dots, \dot{q}_n$  completely describes the system. In the simplest case  $\mathcal{L} = T - V$ , where  $T$  is the kinetic energy and  $V$  the potential energy of the system.

In order to introduce the principle of least action (or Hamilton's Principle) we define another important quantity in analytical mechanics, i.e. the action via the next

**Definition 1.** *The action is the integral of the Lagrangian over time*

$$S = \int_{t_1}^{t_2} \mathcal{L}(q_1, q_2, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n) dt. \quad (2.2)$$

The physical path followed by the system satisfies the principle of least action introduced in the next

**Theorem 1.** *The motion of the system from time  $t_1$  to time  $t_2$  is such that the action  $S$ , defined in Definition 1, has a stationary value along the actual path of the motion.*

The proof of this theorem is given in chapter 2 of Ref. [Gol02].

#### 2.1.1 Calculus of variations: Euler-Lagrange Equations

As a consequence of Theorem 1, we require the action to be stationary for the physical path with respect to any neighboring paths. For simplicity we consider a one dimensional system. We denote the set of all the possible paths as  $q(t, \alpha)$  with  $\alpha$  a real parameter and  $q(t, 0)$  the



physical path. We consider small variations with respect to the physical path:

$$q(t, \alpha) = q(t, 0) + \alpha \epsilon(t), \quad \epsilon(t_1) = \epsilon(t_2) = 0. \quad (2.3)$$

The stationary condition becomes:

$$\left. \frac{dS}{d\alpha} \right|_{\alpha=0} = 0, \quad (2.4)$$

hence:

$$\frac{dS}{d\alpha} = \int_{t_1}^{t_2} \left( \frac{\partial \mathcal{L}}{\partial q} \frac{\partial q}{\partial \alpha} + \frac{\partial \mathcal{L}}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial \alpha} \right) dt, \quad (2.5)$$

and integrating by parts the second term in eq. (2.5) the integral becomes:

$$\frac{dS}{d\alpha} = \int_{t_1}^{t_2} \left( \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} \right) \frac{\partial q}{\partial \alpha} dt + \left. \frac{\partial \mathcal{L}}{\partial \dot{q}} \epsilon(t) \right|_{t_1}^{t_2}. \quad (2.6)$$

The third term in the above equation vanishes and  $S$  can have a stationary value if and only if:

$$\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} = 0. \quad (2.7)$$

This implies the following

**Proposition 1.** *A system with  $n$  degrees of freedom possesses  $n$  equations of motion of the form:*

$$\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = 0, \quad (2.8)$$

which describe its time evolution.

### 2.1.2 Noether's Theorem

Because of the remarkable role played, in this thesis, by symmetries, we consider the next theorem:

**Theorem 2.** *Consider a single parameter family of maps*

$$q_i(t) \rightarrow Q_i(s, t) \quad s \in \mathbb{R}, \quad (2.9)$$

such that

$$Q_i(0, t) = q_i(t). \quad (2.10)$$

This transformation is said to be a continuous symmetry of the Lagrangian  $\mathcal{L}$  if

$$\frac{\partial}{\partial s} \mathcal{L}(Q_i(s, t), \dot{Q}_i(s, t), t) = 0. \quad (2.11)$$

For each such symmetry there is a conserved quantity. [Ton15]

*Proof.*

$$\begin{aligned} \left. \frac{\partial \mathcal{L}}{\partial s} \right|_{s=0} &= \left. \frac{\partial \mathcal{L}}{\partial Q_i} \frac{\partial Q_i}{\partial s} \right|_{s=0} + \left. \frac{\partial \mathcal{L}}{\partial \dot{Q}_i} \frac{\partial \dot{Q}_i}{\partial s} \right|_{s=0} = \\ &= \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) \frac{\partial Q_i}{\partial s} \Big|_{s=0} + \left. \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \frac{\partial \dot{Q}_i}{\partial s} \right|_{s=0} = \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \frac{\partial Q_i}{\partial s} \Big|_{s=0} \right) = 0, \end{aligned} \quad (2.12)$$

where we have used Euler-Lagrange equation.  $\square$

### Example: the motion of a *free particle*

The motion of a free particle has space-time symmetries: indeed if we write the Lagrangian (for simplicity the direction of motion is taken along the  $x$  axis) as

$$\mathcal{L} = \frac{1}{2} m \dot{x}^2, \quad (2.13)$$

we can observe that if  $x' \rightarrow x + s\epsilon$  the Lagrangian remains unchanged. According to Noether's theorem there is a conserved quantity (momentum conservation):

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} s = \frac{\partial \mathcal{L}}{\partial x} s = 0 \rightarrow \frac{\partial \mathcal{L}}{\partial \dot{x}} = m\dot{x} = \text{const.} \quad (2.14)$$

In this case, the Lagrangian does not depend on  $x$  and we say that  $x$  is a cyclic coordinate. Now we derive the conservation of energy. This arises when the Lagrangian is independent of time, that is  $\partial \mathcal{L} / \partial t = 0$ :

$$E = \frac{\partial \mathcal{L}}{\partial \dot{x}} \dot{x} - \mathcal{L}, \quad (2.15)$$

therefore

$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{x}} \dot{x} \right) - \frac{d\mathcal{L}}{dt} = \\ &= \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} \dot{x} + \frac{\partial \mathcal{L}}{\partial \dot{x}} \ddot{x} - \left( \frac{\partial \mathcal{L}}{\partial \dot{x}} \ddot{x} + \frac{\partial \mathcal{L}}{\partial x} \dot{x} + \frac{\partial \mathcal{L}}{\partial t} \right) = -\frac{\partial \mathcal{L}}{\partial t} = 0, \end{aligned} \quad (2.16)$$

where we have used again Euler-Lagrange equation. In this example we have chosen a one-dimensional Galilean trajectory since it is a key ingredient to be used in Chapter 5.

## 2.2 Hamiltonian Formulation

Another approach to study mechanical systems is the so called Hamiltonian formulation of classical mechanics. The idea behind this theoretical scheme is based on the description of a  $n$ -dimensional system in a  $2n$  dimensional space (called phase space) instead of a  $n$  dimensional one. We have to solve  $2n$  first-order independent differential equations to describe the motion of the system. The set of independent variables  $\{q_i, \dot{q}_i\}$  is replaced by  $\{q_i, p_i\}$  where we have eliminated  $\dot{q}_i$  in favour of the momentum  $p_i$  defined as

$$\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = p_i. \quad (2.17)$$

We have to find a function of  $\{q_i, p_i\}$  that contains the same information as the Lagrangian. The procedure for switching variables in this manner is the Legendre transformation introduced implicitly in the next

**Definition 2.** *The Hamiltonian or Hamilton's function of a system is a function of the coordinates and momenta, generated by the following Legendre transformation:*

$$\mathcal{H}(q_i, p_i, t) = \dot{q}_i p_i - \mathcal{L}(q_i, \dot{q}_i, t). \quad (2.18)$$

This definition gives rise automatically to the next

**Theorem 3.** *The evolution of a system characterized by the Hamiltonian  $\mathcal{H}$  is described by the following  $2n$  equations of motion:*

$$\begin{aligned} \dot{q}_i &= + \frac{\partial \mathcal{H}}{\partial p_i}, \\ \dot{p}_i &= - \frac{\partial \mathcal{H}}{\partial q_i}, \end{aligned} \quad (2.19)$$

called canonical equations.

For the proof see chapter 8 of Ref. [Gol02]. The time derivative of the Hamiltonian is:

$$\dot{\mathcal{H}} = \frac{\partial \mathcal{H}}{\partial t} = - \frac{\partial \mathcal{L}}{\partial t}. \quad (2.20)$$

As we have already seen (see eq.s (2.15), (2.16)), if the Hamiltonian does not depend explicitly on time we have energy conservation law. However, we could also use other independent quantities to describe the evolution of the system in its phase space. To this purpose a particularly useful set of transformations are those called canonical transformations.

**Definition 3.** *A transformation from the old variables  $(q_i, p_i)$  to the new variables  $(Q_i, P_i)$  is said to be canonical if the new equations of motion for  $P(q_i, p_i), Q(q_i, p_i)$  are of the form*

$$\begin{aligned} \dot{Q}_i &= + \frac{\partial \mathcal{H}'}{\partial P_i}, \\ \dot{P}_i &= - \frac{\partial \mathcal{H}'}{\partial Q_i}, \end{aligned} \quad (2.21)$$

where  $\mathcal{H}'$  is the Hamiltonian expressed with the new variables.

We can associate a generating function to every canonical transformation. In order to find the expression of the different generating functions we introduce the following

**Theorem 4.** *If  $Q(q_i, p_i)$  and  $P(q_i, p_i)$  are canonical, they must satisfy Hamilton's principle:*

$$\delta \int_{t_1}^{t_2} (P_i \dot{Q}_i - \mathcal{H}'(Q_i, P_i)) dt = 0. \quad (2.22)$$

At the same time the old variables satisfies the same principle:

$$\delta \int_{t_1}^{t_2} (p_i \dot{q}_i - \mathcal{H}(q_i, p_i)) dt = 0. \quad (2.23)$$

Thus it holds that:

$$\dot{q}_i p_i - \mathcal{H}(q_i, p_i) = P_i \dot{Q}_i - \mathcal{H}'(Q_i, P_i) + \frac{dF}{dt}. \quad (2.24)$$

Here we show how it is possible to obtain the expression of a generating function, with independent variables the old and new coordinates, known as a type 1 generating function :  $F_1(Q_i, q_i, t)$ . First we write explicitly the time derivative of  $F_1$  in eq. (2.24):

$$\dot{q}_i p_i - \mathcal{H}(q_i, p_i) = P_i \dot{Q}_i - \mathcal{H}'(Q_i, P_i) + \frac{\partial F_1}{\partial t} + \frac{\partial F_1}{\partial q_i} \dot{q}_i + \frac{\partial F_1}{\partial Q_i} \dot{Q}_i. \quad (2.25)$$

Since  $q_i$  and  $Q_i$  are separately independent in eq. (2.25) the equivalence holds only if:

$$\begin{aligned} p_i &= \frac{\partial F_1}{\partial q_i}, \\ P_i &= -\frac{\partial F_1}{\partial Q_i}. \end{aligned} \quad (2.26)$$

There are only three other types of generating functions obtained through Legendre transformation switching the set of independent variables. In Table 2.1 we show all the possible generating functions and their derivatives.

Generating functions	Generating functions derivatives
$F = F_1(q_i, Q_i, t)$	$p_i = \frac{\partial F_1}{\partial q_i}, \quad P_i = -\frac{\partial F_1}{\partial Q_i}$
$F = F_2(q_i, P_i, t) - \sum_i Q_i P_i$	$p_i = \frac{\partial F_2}{\partial q_i}, \quad Q_i = \frac{\partial F_2}{\partial P_i}$
$F = F_3(p_i, Q_i, t) + \sum_i q_i p_i$	$q_i = -\frac{\partial F_3}{\partial p_i}, \quad Q_i = -\frac{\partial F_3}{\partial Q_i}$
$F = F_4(p_i, P_i, t) + \sum_i q_i p_i - \sum_i Q_i P_i$	$p_i = \frac{\partial F_4}{\partial q_i}, \quad Q_i = \frac{\partial F_4}{\partial P_i}$

Table 2.1: Generating Functions

Finally, it holds that

**Proposition 2.** *The new Hamiltonian  $\mathcal{H}'$  is related to the old one  $\mathcal{H}$  through the relation*

$$\mathcal{H}' = \mathcal{H} + \frac{\partial F}{\partial t}. \quad (2.27)$$

### 2.2.1 Hamilton-Jacobi Theory

A deeply related but somehow alternative approach to address the evolution of these mechanical systems is obtained by using a canonical transformation from  $q_i(t), p_i(t)$  to a new set of constant quantities which may be exactly the same coordinate and momenta but evaluated at the starting point, i.e.  $q_i(t_0), p_i(t_0)$ . This technique, known as Hamilton-Jacobi theory, is obtained by solving the H-J equation as stated in the next

**Theorem 5.** *The H-J equation, for a system described by the Hamiltonian  $H$ , is*

$$\mathcal{H}\left(q_1, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}\right) + \frac{\partial S}{\partial t} = 0, \quad (2.28)$$

where  $S$  is the action defined in Definition 1.

Note that by solving this PDE we are obtaining a solution to the original mechanical problem too.

*Proof.* In order to obtain the Hamilton-Jacobi equation we impose the transformed Hamiltonian  $\mathcal{H}'$  to be identically zero. The equations of motion are then:

$$\begin{aligned} \frac{\partial \mathcal{H}'(Q_i, P_i)}{\partial P_i} &= \dot{Q}_i = 0, \\ \frac{\partial \mathcal{H}'(Q_i, P_i)}{\partial Q_i} &= -\dot{P}_i = 0. \end{aligned} \quad (2.29)$$

Thus eq. (2.27) becomes

$$\mathcal{H}(q_i, p_i) + \frac{\partial F}{\partial t} = 0. \quad (2.30)$$

We choose  $F_2(q_i, P_i, t)$ , which is a type 2 generating function so we have:

$$p_i = \frac{\partial F_2}{\partial q_i}. \quad (2.31)$$

Finally, we obtain the PDE for  $F_2$  by substituting eq. (2.31) in (2.30):

$$\mathcal{H}\left(q_i, \frac{\partial F_2}{\partial q_i}\right) + \frac{\partial F_2}{\partial t} = 0. \quad (2.32)$$

The function  $F_2$  is called Hamilton's principal function and it is a function of  $n$  constant momenta. The physical meaning of  $F_2$  is obtained by an examination of its total time derivative:

$$\frac{dF_2}{dt} = \frac{\partial F_2}{\partial q_i} \dot{q}_i + \frac{\partial F_2}{\partial P_i} \dot{P}_i + \frac{\partial F_2}{\partial t} = p_i \dot{q}_i - \mathcal{H} = \mathcal{L}. \quad (2.33)$$

The Hamilton's principal function differs from the indefinite time integral of the Lagrangian only by a constant. For this reason we can always identify  $F_2$  with the action  $S$  as they differ, at least, by a constant.

The PDE

$$\mathcal{H}\left(q_1, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}\right) + \frac{\partial S}{\partial t} = 0 \quad (2.34)$$

is the so-called H-J equation. A possible solution to the H-J equation can be written as

$$S = S(q_1, \dots, q_n, \alpha_1, \dots, \alpha_{n+1}) \quad (2.35)$$

which, remarkably, depends on  $n + 1$  independent constant of integration. One of them is solely added to  $S$  as the action does not appear directly in eq. (2.34) but only its partial derivatives. We are free to choose the other  $n$  independent constants to be the new momenta:

$$\alpha_i = P_i \quad (2.36)$$

These new momenta are connected with the initial values of  $q_i$  and  $p_i$  through the following relations:

$$\frac{\partial S(q_i, \alpha_i, t)}{\partial q_i} = p_i, \quad (2.37)$$

$$\frac{\partial S(q_i, \alpha_i, t)}{\partial \alpha_i} = \beta_i = Q_i \quad (2.38)$$

We can solve for  $q_i$  in eq. (2.38) and find:

$$q_i = q_i(\alpha, \beta, t), \quad (2.39)$$

then substituting  $q_i(\alpha, \beta, t)$  in eq. (2.37) we have:

$$p_i = p_i(\alpha, \beta, t) \quad (2.40)$$

The two eq.s (2.39) and (2.40) constitute the desired complete set of Hamilton's equations of motion in terms of the new constant momenta and coordinates. Moreover, the Hamilton's principal function turns out to be the generator of a canonical transformation to constant coordinates and momenta.  $\square$

In the next chapters we shall make use of the Lagrangian, Hamiltonian and H-J equation for the free particle. For this reason we rewrite their expressions:

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}m\dot{x}^2, \\ H &= \frac{p^2}{2m}, \end{aligned} \quad (2.41)$$

$$\frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 + \frac{\partial S}{\partial t} = 0. \quad (2.42)$$

# Chapter 3

## Relativistic Mechanics in a nutshell

### 3.1 Einstein Principle of Relativity

The Principle of Relativity asserts that all the laws of Nature are identical in all inertial reference systems (IRS). From the Principle of Relativity it follows that the speed of light is the same in all IRS.

An event is characterized by four coordinates  $x, y, z, t$  and the interval between two events is defined as follows:

**Definition 4.** *The length of the interval between two events is:*

$$s(1, 2) = \sqrt{c^2(t_2 - t_1)^2 - (x_2 - x_1)^2 - (y_2 - y_1)^2 - (z_2 - z_1)^2}. \quad (3.1)$$

The interval between two events is a number and its value is the same in all IRS. This invariance is a consequence of the constancy of light velocity. The interval between two events can be interpreted as the distance between two points in the Minkowski space (a combination of three-dimensional Euclidean space and time into a four-dimensional manifold). Because of the invariance of the interval  $s(1, 2)$  the allowed transformations are trivial parallel displacement of the origin, and rotations in  $SO(3, 1)$ . These rotations contains hyperbolic functions in place of trigonometric functions because the geometry of the Minkowski space is no longer Euclidean, and they constitute the so called Lorentz transformations.

We write the formula of transformation from an inertial reference frame  $A$  to another one  $A'$  moving relative to  $A$  with constant velocity  $v$  along the  $x$  axis as:

$$x = \frac{x' + vt'}{\sqrt{1 - \frac{v^2}{c^2}}}, \quad y = y', \quad z = z', \quad t = \frac{t' + \frac{v}{c^2}x'}{\sqrt{1 - \frac{v^2}{c^2}}}. \quad (3.2)$$

#### 3.1.1 Relativistic Mechanics

We have to define the notation used in this section. The space-time coordinates  $(ct, x, y, z) = (ct, \mathbf{x})$  are denoted by the contravariant four-vector:

$$x^\alpha := (x^0, x^1, x^2, x^3) := (ct, x, y, z). \quad (3.3)$$

The covariant four-vector  $x_\alpha$  is obtained by changing the sign of the space components:

$$x_\alpha := (x_0, x_1, x_2, x_3) := (ct, -x, -y, -z) = g_{\alpha\beta}x^\beta \quad (3.4)$$

where  $g_{\alpha\beta}$  is the metric tensor:

$$g_{\alpha\beta} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \quad (3.5)$$

**Remark 1.** In eq. (3.4) we have used the usual Einstein convention, which implies a sum on the repeated indexes.

We define the relativistic action for the motion of a free massive particle via the next

**Definition 5.** The relativistic action for a free particle is written as

$$S = -mc \int_{S_1}^{S_2} ds \quad (3.6)$$

where  $m$  indicates the rest mass of the particle.

The action must be a scalar since physical laws remain the same in every IRS i.e. the action is invariant under Lorentz transformations:

$$ds = \sqrt{dx^\alpha g_{\alpha\beta} dx^\beta} = \sqrt{dx_i dx^i}. \quad (3.7)$$

Expanding the sum in the definition of  $S$  (Definition 5) and factorizing  $cdt$  we obtain:

$$S = -mc^2 \int_{S_1}^{S_2} \sqrt{\left(1 - \frac{1}{c^2 dt^2} (dx^2 + dy^2 + dz^2)\right)} dt = -mc^2 \int_{t_1}^{t_2} \sqrt{1 - \frac{\mathbf{v}^2}{c^2}} dt. \quad (3.8)$$

Defining Lorentz's factor as  $\gamma := \frac{1}{\sqrt{1 - \frac{\mathbf{v}^2}{c^2}}}$  eq. (3.8) becomes:

$$S = -mc^2 \int_{t_1}^{t_2} \frac{1}{\gamma} dt. \quad (3.9)$$

Remembering that the action is the integral of the Lagrangian over time (see eq. (1)) we identify the integrand of eq. (3.8) with the relativistic Lagrangian:

$$\mathcal{L} = -mc^2 \sqrt{1 - \frac{\mathbf{v}^2}{c^2}}. \quad (3.10)$$

We can then calculate the relativistic Hamiltonian by using Definition 2:

$$\mathcal{H} = \mathbf{p} \cdot \mathbf{v} - \mathcal{L} = \frac{mc^2}{\sqrt{1 - \frac{\mathbf{v}^2}{c^2}}} = c \sqrt{m^2 c^2 + \mathbf{p}^2} \quad (3.11)$$

where  $\mathbf{p} = \frac{\partial \mathcal{L}}{\partial \mathbf{v}}$ . Expanding the Hamiltonian for small  $\beta := v/c$  we obtain the classical limit



(as expected):

$$\mathcal{H} \approx mc^2 + \frac{1}{2}m\mathbf{v}^2, \quad (3.12)$$

or equivalently

$$\mathcal{H} \approx mc^2 + \frac{\mathbf{p}^2}{2m}, \quad (3.13)$$

where in both cases the former term  $mc^2$  is the rest energy and the latter term is the classical kinetic energy.

We apply the least action principle to find the physical path followed by the free particle.

$$\delta S = -mc \int_{S_1}^{S_2} \delta(ds) = 0. \quad (3.14)$$

We observe that:

$$\delta(ds^2) = 2ds\delta(ds) = -2g_{\alpha\beta}\delta(dx^\alpha)dx^\beta, \quad (3.15)$$

so we can write  $\delta(ds)$  as

$$\delta(ds) = -g_{\alpha\beta} \frac{\delta x^\beta}{ds} \frac{dx^\alpha}{ds} ds. \quad (3.16)$$

Thus we have

$$\delta S = mc \left( \int_{S_1}^{S_2} ds \frac{d}{ds} \left( g_{\alpha\beta} \delta x^\alpha \frac{dx^\beta}{ds} \right) - \int_{S_1}^{S_2} ds \delta x^\alpha g_{\alpha\beta} \frac{d^2 x^\beta}{ds^2} \right). \quad (3.17)$$

The first term in the r.h.s. of the above equation vanishes since it is evaluated at the boundaries; we thus find the equation of motion:

$$mc \frac{d^2 x^\beta}{ds^2} = 0. \quad (3.18)$$

Defining the four velocity as  $cdx^\beta/ds := u^\beta$  and observing that  $ds = cdt/\gamma$ , by comparing definition (5) and eq. (3.9), we have:

$$c \frac{d^2 x^\beta}{ds^2} = \frac{du^\beta}{ds} = \frac{\gamma}{c} \frac{du^\beta}{dt} = 0, \quad (3.19)$$

thus the result is a constant velocity for the free particle in a four-dimensional form.

# Chapter 4

## Statistical Mechanics in a nutshell

In this section we shall provide a formulation of the statistical mechanics in a simple and quite-direct way. As explained in the introduction, these first sections are conceived as a syllabus of the main observables and equations to follow the derivation of the results presented in chapter 5. In particular, while analytical mechanics (in its classical or relativistic formulation) mathematically relies upon an extensive use of PDE, statistical mechanics relies upon an extensive use of probability theory.

Let us consider a system whose energy values are discrete e.g.  $E_1, \dots, E_N$  and we assign a probability to each of them. We identify the state  $|n\rangle$  characterized by the energy value  $E_n$ , by using the formalism adopted in quantum mechanics for the sake of simplicity.

### 4.1 The free energy and related definitions

**Definition 6.** *Thermodynamics systems at fixed temperature  $T$  follow the Boltzmann distribution. The probability that the system is in a state  $|n\rangle$  with energy  $E_n$  is:*

$$p(n) = \frac{\exp(-\beta E_n)}{\sum_m \exp(-\beta E_m)} = \frac{\exp(-\beta E_n)}{Z}, \quad \beta = \frac{1}{k_B T}, \quad (4.1)$$

Where  $k_B$  is the Boltzmann constant.

The probability  $p(n)$  lies at the core of statistical mechanics, and defines the Canonical Ensemble. The denominator of (4.1) is the partition function  $Z$  and contains all the information we need to describe the thermodynamic behaviour of the system. We can write the free energy, the main observable in the canonical formulation of statistical mechanics, in term of  $Z$  via the next

**Definition 7.** *The Free Energy associated to a physical system in thermodynamic equilibrium at temperature  $T$ , with partition function  $Z$  is:*

$$F = -\frac{1}{\beta} \log Z = U - \frac{\mathcal{S}}{k_B \beta} \quad (4.2)$$

Where  $U$  is the mean value of the energy of the system over all the configurations and  $\mathcal{S}$  is its related entropy.

From now on, we will work with natural units where  $k_B = 1$ . In general, just like for the

energy, all physical observables can be calculated through ensemble averages according to the next

**Definition 8.** *The mean value of an observable  $O$  is defined as follows:*

$$\langle O \rangle = \frac{\sum_n O_n \exp(-\beta E_n)}{Z}, \quad (4.3)$$

where  $O_n$  is the value of the observable  $O$  when the system is in the state  $|n\rangle$ .

## 4.2 The Curie-Weiss model: a first glance

We consider a lattice in  $d$  spatial dimensions, containing  $N$  sites. Each lattice site is characterized by a discrete variable which can assume only two possible values:

$$\sigma_i = \pm 1. \quad (4.4)$$

We can conceive this variable as that associated to two spin states corresponding to spin up and down configurations. Physically this discrete variable could represent the magnetic dipole moments of atomic spins. We can associate an energy to any particular configuration (out of the  $2^N$  possible ones) of spins  $\boldsymbol{\sigma}$  via the next

**Definition 9.** *Introduced a real positive defined spin-spin coupling  $J > 0$ , the Hamiltonian for the CW model of  $N$  spin sites in presence of a magnetic field  $B$  reads as*

$$H(\boldsymbol{\sigma}) = -B \sum_i^N \sigma_i - \frac{J}{N} \sum_{1 \leq i < j \leq N} \sigma_i \sigma_j, \quad (4.5)$$

where  $\sigma_i = \pm 1$  is called *Ising spin*.

The first term in the above definition accounts for the presence of an external magnetic field  $B$  while the last term introduces an interaction between all pairs of spins in the lattice. We have chosen  $J > 0$  so the pairs of spins prefer to be aligned and such system is called *ferromagnet*. On the contrary, in case of a negative coupling  $J < 0$ , in which the pairs of spins prefer to be antialigned, the system is called *anti-ferromagnet*. We can rewrite the Hamiltonian in definition (9) in the following way:

$$H(\boldsymbol{\sigma}) = -B \sum_i^N \sigma_i - \frac{J}{2N} \sum_{ij}^{NN} \sigma_i \sigma_j + \frac{J}{2}, \quad (4.6)$$

where the constant term  $\frac{J}{2}$  can be ignored in the TL. This is a central point since at equilibrium, thus in the statistical mechanical framework we are addressing, thermodynamic observables must be extensive and linear function of  $N$ . It is possible to check that, in the above equation, the first two terms at the r.h.s. are  $O(N)$  while the last one is  $O(1)$ .

The partition function for the C-W model is

$$Z = \sum_{\{\boldsymbol{\sigma}\}} \exp \left[ \beta B \sum_i^N \sigma_i + \beta \frac{J}{2N} \sum_{ij}^{NN} \sigma_i \sigma_j \right], \quad (4.7)$$

here the sum over  $\{\boldsymbol{\sigma}\}$  means over all configurations of spins, we no longer have a sum over

energy levels since each configuration  $\{\sigma\}$  parameterizes a particular energy level indirectly. As usual in statistical mechanics we can characterize the macroscopic behaviour of a physical system through order parameters. For the present model this is introduced by the next

**Definition 10.** *The magnetization associated to a particular configuration  $\{\sigma\}$  is*

$$m(\sigma) = \frac{1}{N} \sum_i^N \sigma_i, \quad (4.8)$$

whose average value can be obtained through

**Observation 1.**

$$\langle m \rangle = \frac{1}{N} \left\langle \sum_{i=1}^N \sigma_i \right\rangle = \frac{1}{N\beta} \frac{\partial \log Z}{\partial B} = -\frac{1}{N} \frac{\partial F}{\partial B}. \quad (4.9)$$

We plan to find an explicit expression of the free energy, in terms of the order parameter, the magnetization, and then we impose at the same time a minimization of the energy and a maximization of the entropy. This typically leads to a self-consistency equation for the order parameter whose inspection allows us to obtain the phase diagram of the system under consideration. In this context the self-consistency equation is used to indicate the equation satisfied by the magnetization at equilibrium [Bar08].

Among the various methods to achieve this goal we present in this section two of them. A first one is more related to a theoretical physics methodology and a second one, addressed in Section (4.3), to a mathematical physics approach.

The first approach needs a new formulation of the partition function. For this purpose we substitute the sum in eq. (4.7) with a sum over the magnetization together with a sum over the configurations at  $m$  fixed:

$$Z = \sum_m \sum_{\{\sigma\}|_m} \exp(-\beta H[\sigma]) = \sum_m \exp(-\beta F(\beta, m)), \quad (4.10)$$

where, in the second term, we have written  $Z$  in terms of the free energy using relation (4.2) and  $m$  is the magnetization (4.8) which lies in the range  $-1 \leq m \leq 1$ . The magnetization acquires only discrete values, quantized in units of  $2/N$ . In the TL we can transform eq. (4.10) of  $Z$  in an integral:

$$Z = \frac{N}{2} \int_{-1}^1 dm \exp(-\beta F(\beta, m)). \quad (4.11)$$

Eq. (4.2) defines the free energy only at equilibrium (where our interest lies), where the magnetization takes a specific value, that given in eq.(4.9). Because of that, we can consider the  $F$  function in eq. (4.11) as an effective free energy depending also on the magnetization  $m$  of the specific configuration of the system. It is customary to define the free energy per unit spin.

**Definition 11.** *The free energy per unit site is defined as follows*

$$f(\beta, m) = \frac{F(\beta, m)}{N}, \quad (4.12)$$

In the above definition, we have normalized the extensive free energy by dividing it by  $N$ , in order to obtain the intensive free energy, or the free energy per site. While extensive quantities fluctuate in the TL, intensive quantities do not. We shall prove in Appendix A that, in the TL, these quantities exist. Intensive quantities have distributions that, in the TL, typically collapse on a Dirac delta. For this reason handling with these quantities is usually more convenient for practical purposes. We introduce another intensive thermodynamic quantity, the pressure  $A$ , as it will be used in Section 4.3:

**Definition 12.** *The pressure is related to the free energy per unit site through*

$$A = -\beta f. \quad (4.13)$$

Note that the above observable has been called *pressure* (or *mathematical pressure*) in a series of papers by Francesco Guerra, Lon Rosen and Barry Simon [Gue75, Gue76, Gue73], but it is not related to the pressure as usually defined by physicists. It is a useful redefinition of the free energy.

By using Definition (11) we can write

$$Z = \int dm \exp(-\beta N f(\beta, m)), \quad (4.14)$$

where the coefficient  $N/2$  is omitted since it is unimportant for the physics. To simplify the writing, in the following expressions we shall omit the  $\beta$  dependence in the Free Energy. In the TL the integral in (4.14) is well approximated by the value of  $m$  which minimizes  $f(m)$ . This approximation is known as the *saddle point* or *steepest descent* [Gou99]. Thus

$$Z \approx \exp(-\beta N f(m_{min})) \implies F(\text{thermo}) \approx F(m_{min}) \quad (4.15)$$

and it is easy to see that the equilibrium value of the magnetization turns out to be  $m_{min}$ .

### 4.2.1 The mean field approximation

A successful approach to study spin systems is the mean-field approximation, which consists in assuming that each spin interacts with the rest of the network of its peers in a homogeneous average way, regardless to the Euclidean distance within the lattice. The single spin in the network feels not only the force stemming from the applied magnetic field, but also the magnetic field generated by all the other spins. In our case since we are studying the C-W model that already is a mean field model such approximation is actually the exact solution. Rewriting (4.6) as:

$$H(\sigma) = - \sum_i^N \sigma_i (B + \frac{J}{2N} \sum_j^N \sigma_j) = \sum_i^N h_i^{\text{eff}}(\sigma) \sigma_i, \quad (4.16)$$

eq. (4.16) defines the single particle effective Hamiltonian  $h_i^{\text{eff}}$ . The structure of the Hamiltonian is the sum of each spin multiplied by its correspondent effective field  $h_i^{\text{eff}}$  which also depends on the spins. Whereas the effect of the external magnetic field  $B$  is time-independent, the coupling term  $\propto J$  contained in  $h_i^{\text{eff}}$  yet will fluctuate in time due to thermal noise (even at equilibrium). The mean field approximation consists in ignoring these details and substituting the fluctuating values of the neighboring variables by their statistical average. To

this purpose we take the mean value of  $h_i^{\text{eff}}$ :

$$\langle h_i^{\text{eff}}(\boldsymbol{\sigma}) \rangle = -(B + \frac{J}{2N} \sum_j^N \langle \sigma_j \rangle) = -(B + \frac{J}{2} \langle m \rangle), \quad (4.17)$$

where  $\langle m \rangle$  is defined in eq. (4.9). We can rewrite the Hamiltonian in eq. (4.6) as:

$$H(\boldsymbol{\sigma}) = - \sum_i^N \sigma_i (B + \frac{J}{2} \langle m \rangle) \implies \frac{H}{N} = -B \langle m \rangle - \frac{1}{2} J \langle m \rangle^2, \quad (4.18)$$

At this point the sum over the configuration  $\{\boldsymbol{\sigma}\}|_m$  in eq. (4.10) is easy to compute since the number of configurations corresponding to a fixed value for the magnetization is

$$\Omega = \frac{N!}{N_{\uparrow}!(N - N_{\uparrow})!}, \quad (4.19)$$

with

$$m = \frac{N_{\uparrow} - N_{\downarrow}}{N}. \quad (4.20)$$

By using Stirling's formula [Sem18] we obtain

$$\log \Omega \approx N \log N - N_{\uparrow} \log N_{\uparrow} - (N - N_{\uparrow}) \log(N - N_{\uparrow}), \quad (4.21)$$

$$\frac{\log \Omega}{N} \approx \log 2 - \frac{1}{2}(1 + m) \log(1 + m) - \frac{1}{2}(1 - m) \log(1 - m). \quad (4.22)$$

**Observation 2.** *Multiplying by the Boltzmann constant the logarithm of the number of configurations in eq. (4.19) we obtain the so called Boltzmann entropy  $\mathcal{S}$ . Rewriting eq. (4.22) as*

$$\frac{\log \Omega}{N} = -\frac{N_{\uparrow}}{N} \log \left( \frac{N_{\uparrow}}{N} \right) - \frac{N_{\downarrow}}{N} \log \left( \frac{N_{\downarrow}}{N} \right). \quad (4.23)$$

*We can conceive  $-\frac{N_{\uparrow}}{N}$  as the probability for the single spin system to be up (and we have an analogous expression for the down state). Thus eq. (4.23) turns up to be Shannon definition of entropy, namely  $-\sum_i p_i \log p_i$  where  $p_i$  is the probability of the single event to happen. This definition is introduced in the close framework of information theory [Jay57]).*

In mean field approximation, the partition function  $Z$ , eq. (4.10), becomes:

$$Z = \sum_m \exp(-\beta N f(m)) \approx \sum_m \Omega(m) \exp(-\beta H(m)). \quad (4.24)$$

By substituting the expression (4.18) for the Hamiltonian, and using eq. (4.22) we obtain the following expression for the effective free energy:

$$f(m) \approx -Bm - \frac{1}{2} J m^2 - \frac{1}{\beta} \left[ \log 2 - \frac{1}{2}(1 + m) \log(1 + m) - \frac{1}{2}(1 - m) \log(1 - m) \right]. \quad (4.25)$$

**Observation 3.** We have already demonstrated in eq. (4.15) that in the TL the magnetization reaches its equilibrium value i.e. that defined in eq. (4.9). Thus we write, for the sake of simplicity,  $\langle m \rangle$  instead of  $m$  in the next equations. If we call  $P(m)$  the probability distribution of the magnetization, it results that  $\lim_{N \rightarrow \infty} P(m)$  is a Dirac delta.

Now we impose the stationarity condition as discussed in section 4.2:

$$\frac{\partial f}{\partial \langle m \rangle} = 0 \implies \beta(B + J\langle m \rangle) = \frac{1}{2} \log \left( \frac{1 + \langle m \rangle}{1 - \langle m \rangle} \right). \quad (4.26)$$

Thus magnetization at equilibrium obeys the so called self-consistency condition

$$\langle m \rangle = \tanh(\beta B + \beta J \langle m \rangle). \quad (4.27)$$

We can consider  $B_{\text{eff}} = B + J\langle m \rangle$  the effective magnetic field experienced by each spin containing the extra contribution from the other spins. Figure 4.1 shows the behaviour of  $m$  at equilibrium as a function of  $B$  for different value of the temperature. The magnetization is dimensionless whereas  $T$  and  $B$  are in units of  $k_B$ . Note that, for  $T > 1$  the magnetization is a continuous function of the magnetic field, while this is no longer true for temperatures under  $T = 1$ . In subsection 4.3.1 we shall prove that, at  $T = 1$ , the system undergoes a phase transition.

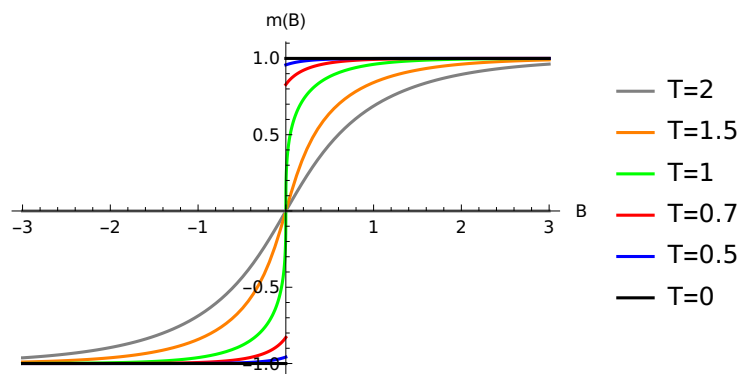


Figure 4.1: Behaviour of  $m$  at equilibrium as a function of  $B$  for different value of the temperature.

### 4.3 The C-W model: a deeper look

In this section we introduce a powerful scheme to solve mean field models: the Guerra's interpolation approach [Bar08].

From now on we set  $B \equiv 0$  and we rewrite the Hamiltonian  $\mathcal{H}(\boldsymbol{\sigma})$  of the mean field ferromagnetic model (C-W) in term of the magnetization as

$$H_N(m) = -\frac{JN}{2}m^2, \quad (4.28)$$

where again, noting that  $|m| \leq 1$ , we remark the linear dependence in  $N$  of eq. (4.28). The partition function of the system is thus

$$Z_N(\beta) = \sum_{\boldsymbol{\sigma}} \exp(-\beta \mathcal{H}_N(\boldsymbol{\sigma})) = \sum_{\boldsymbol{\sigma}} \exp\left(\frac{\beta J N m^2}{2}\right). \quad (4.29)$$

At the core of Guerra's scheme lies the introduction of a more general partition function  $Z_N(\beta, t)$  depending on a real parameter  $t \in [0, 1]$  and a tunable parameter  $\psi \in \mathbb{R}$  to be chosen later.

$$Z_N(\beta, t) = \sum_{\sigma} \exp\left(t \frac{\beta J N m^2}{2} + (1-t) N m \psi\right). \quad (4.30)$$

The situation at  $t = 0$  corresponds to a trivial one-body problem, in which the  $N$  spins are independent from each other. The resulting partition function is:  $Z_N(\beta, 0) = Z_1(\beta, 0)^N$ , where

$$Z_1(\beta, 0) = \sum_{\sigma=\pm 1} \exp(\sigma \psi) = 2 \cosh \psi \quad (4.31)$$

is the single spin partition function. Thus  $Z_N(\beta, 0)$  becomes:

$$Z_N(\beta, 0) = Z_1(\beta, 0)^N = (2 \cosh \psi)^N. \quad (4.32)$$

The situation at  $t = 1$  corresponds to the C-W model.

The physical interpretation of this approach is the following: since in the TL the average of the magnetization does not fluctuate, we search for a  $\psi$ , a *fictitious interaction*, that correctly reproduces the statistics generated by the spins at the lowest order. In this case the spins  $\sigma_i$  do not distinguish between the field generated by its peers, i.e. the term  $-\frac{J}{2N} \sum_{ij}^{NN} \sigma_i \sigma_j$  in the Hamiltonian, and the effective field carried by  $\psi$ . Thus we can solve an effective one-body model with all the thermodynamic characteristics of the real pairwise model.

To achieve this task, we generalize the definition of the pressure  $A_N(\beta) \rightarrow A_N(\beta, t)$  and use the fundamental theorem of calculus.

**Definition 13.** We define the generalized C-W pressure  $A_N(\beta, t)$  as

$$A_N(\beta, t) = \frac{1}{N} \log(Z_N(\beta, t)). \quad (4.33)$$

**Proposition 3.** According to the fundamental theorem of calculus the C-W, the pressure can be written as follows

$$A_N(\beta, t = 1) = A_N(\beta, t = 0) + \int_0^1 \partial_t A_N(\beta, t) dt, \quad (4.34)$$

where

$$\partial_t A_N(\beta, t) = \frac{\partial}{\partial t} \left( \frac{1}{N} \log(Z_N(\beta, t)) \right) = \frac{\beta J}{2} \langle m^2 \rangle - \psi \langle m \rangle, \quad (4.35)$$

where we have used the expression (4.30) for  $Z_N(\beta, t)$ . We can find the expression for  $A_N(\beta, t = 0)$  by considering eq. (4.32):

$$A_N(\beta, t = 0) = \frac{1}{N} \log((2 \cosh \psi)^N) = \log 2 + \log(\cosh \psi). \quad (4.36)$$

In order to obtain an expression for  $A_N(\beta, t)$  we have to integrate eq. (4.35). Because the



magnetization is self-averaging [Gen09], i.e. it has no fluctuations in the TL away from phase transition point, it is useful to write  $m$  as its average  $\bar{m}$  plus a fluctuation  $\Delta$  which is suppose to vanish in the TL:

$$m = \bar{m} + \Delta, \quad (4.37)$$

where

$$\bar{m} = \lim_{N \rightarrow \infty} \langle m \rangle. \quad (4.38)$$

By substituting relation (4.37) into eq. (4.35) and writing  $\langle \Delta \rangle$  according to its definition in eq. (4.37), we obtain:

$$\partial_t A_N(\beta, t) = -\frac{\beta J}{2} \bar{m}^2 + \frac{\beta J}{2} \langle \Delta^2 \rangle + \beta J \bar{m} \langle m \rangle - \psi \langle m \rangle, \quad (4.39)$$

this expression indicates that it is convenient to choose  $\psi = \beta J \bar{m}$  in order to eliminate the coefficient of  $\langle m \rangle$ . In the TL  $\langle \Delta^2 \rangle \rightarrow 0$ , since the magnetization is a self-averaging order parameter and its distribution becomes a Dirac delta. Finally, we obtain the following easily integrable expression:

$$\partial_t A_N(\beta, t) = -\frac{\beta J}{2} \bar{m}^2 + \frac{\beta J}{2} \langle \Delta^2 \rangle \underset{N \rightarrow \infty}{=} -\frac{\beta J}{2} \bar{m}^2. \quad (4.40)$$

In the TL  $A_N(\beta, t) \rightarrow A(\beta, t)$ , as we show in appendix A. We can introduce the following

**Proposition 4.** *The C-W pressure in the TL is*

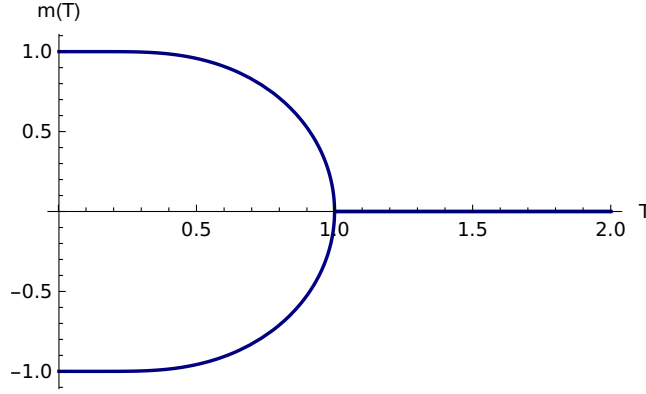
$$\begin{aligned} A(\beta, t = 1) &= A(\beta, t = 0) - \int_0^1 \frac{\beta J \bar{m}^2}{2} dt = \\ &= \log 2 + \log(\cosh(\beta J \bar{m})) - \frac{\beta J}{2} \bar{m}^2, \end{aligned} \quad (4.41)$$

where we have used eq. (4.36).

In order to obtain the self-consistency relation we impose the stationarity condition

$$\begin{aligned} \partial_{\bar{m}} A(\beta, t = 1) &= \partial_{\bar{m}} (\log 2 + \log(\cosh(\beta J \bar{m})) - \frac{\beta J}{2} \bar{m}^2) = \\ &= \beta J \tanh(\beta J \bar{m}) - \beta J \bar{m} = 0, \end{aligned} \quad (4.42)$$

and find again the self-consistency relation. In figure 4.2 we show the magnetization as a function of  $T$ , obtained by solving the self-consistency equation with  $J = 1$ . The magnetization is dimensionless and the temperature is in units of  $k_B$ . We can see that starting from the high noise limit (i.e.  $T = \infty$ ) and going back toward  $T = 0$  there is a point, called critical point, where the magnetization is no longer zero. There is a phase transition toward not-zero values. We shall prove in subsection 4.3.1 that the critical temperature is  $T = 1$  where, as we can see in figure 4.2, the magnetization turns off abruptly.


 Figure 4.2: Behaviour of  $m$  as a function of  $T$ .

### 4.3.1 Fluctuations and critical temperature

The occurrence of a phase transition is the result of two competitive effects. The first one tends to minimize the energy and introduce order in the system by aligning the spins (i.e.  $m \rightarrow \pm 1$ ), the second tends to maximize the entropy and drives the system to a random spins configuration, i.e. a null magnetization [Mus10]. When these two opposite requirements balance reciprocally the system experiences a huge stress and undergoes a critical behaviour whose features we shall present in the following.

We have already observed (4.2) that the magnetization turns off abruptly at  $T = 1$  in figure . A way to obtain the critical temperature  $T_c$  is by carrying out a Taylor expansion of eq. (4.42) and then solving for  $T$ :

$$\bar{m} = \tanh(\beta J \bar{m}) \sim \beta J \bar{m} + \frac{\beta^3 J^3}{3} (\bar{m})^3. \quad (4.43)$$

We obtain  $T_c = J$  by neglecting the last term in eq. (4.43). In our case  $T_c = 1$  since we have set  $J = 1$ .

In figure 4.2 we see that the magnetization is a continuous function of the temperature and, for this reason, the critical phenomenon is called a continuous phase transition or a second order phase transition. The name second order phase transition is due to the fact that the discontinuity affects the fluctuations of the magnetization that diverge at  $T_c$ .

To be more precise, the amplified magnetization fluctuations become infinitely strong at the critical temperature:

$$T = T_c, \quad \lim_{N \rightarrow \infty} (N(\langle m^2 \rangle - \langle m \rangle^2)) = \lim_{N \rightarrow \infty} \langle N \Delta^2 \rangle \rightarrow \infty. \quad (4.44)$$

We can prove expression (4.44) by using Guerra's interpolation scheme. Our aim is to evaluate the mean value of  $N \Delta^2$ .

We start by adding a source term  $hN(N \Delta^2)$ , with  $h$  a real parameter, inside the exponential of the partition function in eq. (4.30) such that the new partition function is

$$\mathcal{Z}_N = \sum_{\sigma} \exp(t \frac{\beta J N m^2}{2} + (1-t) N m \beta \bar{m} J + h N (N \Delta^2)), \quad (4.45)$$

where we have substituted  $\psi = \beta J \bar{m}$  for the fictitious interaction. Using Definition (4.33) we write the new pressure  $\mathcal{A}_N$ :

$$\mathcal{A}_N = \frac{1}{N} \log \mathcal{Z}_N. \quad (4.46)$$

According to the fundamental theorem of calculus we write  $\langle N\Delta^2 \rangle_{t=1}$  as

$$\langle N\Delta^2 \rangle_{t=1} = \langle N\Delta^2 \rangle_{t=0} + \int_0^1 [\partial_t \langle N\Delta^2 \rangle_t] dt, \quad (4.47)$$

with

$$\langle N\Delta^2 \rangle = \partial_h \mathcal{A}_N|_{h=0}. \quad (4.48)$$

Using eq. (4.45) we find that

$$\begin{aligned} \partial_t \langle N\Delta^2 \rangle &= \frac{N\beta J}{2} \langle m^2 N\Delta^2 \rangle - N\beta J \bar{m} \langle m N\Delta^2 \rangle + \\ &+ -\frac{N\beta J}{2} \langle N\Delta^2 \rangle \langle m^2 \rangle + N\beta J \bar{m} \langle m \rangle \langle N\Delta^2 \rangle. \end{aligned} \quad (4.49)$$

Again we write  $m = \bar{m} + \Delta$  as we did in eq. (4.37), thus

$$\langle m^2 \rangle = -\bar{m}^2 + 2\langle m \rangle \bar{m} + \langle \Delta^2 \rangle, \quad (4.50)$$

where we have used  $\langle \Delta \rangle = \langle m \rangle - \bar{m}$ . Finally, by substituting eq. (4.50) into eq. (4.49) we obtain:

$$\partial_t \langle N\Delta^2 \rangle = \frac{N\beta J}{2} (N\langle \Delta^4 \rangle - N\langle \Delta^2 \rangle^2). \quad (4.51)$$

We want to investigate how fluctuations behave close to  $T_c$ . It is easier to approach  $T_c$  from the ergodic region (i.e. for  $T > T_c$ ) since all the distributions of the various observables, e.g. magnetization, free energy, entropy and energy are Gaussian as it can be shown by using a simple Central Limit Theorem argument [Bar08]).

$\Delta$  is also Gaussian in the ergodic region so satisfies the relation:

$$\langle \Delta^4 \rangle = \langle \Delta^2 \rangle \langle \partial_\Delta \Delta^3 \rangle = 3\langle \Delta^2 \rangle^2. \quad (4.52)$$

The latter expression is proved in appendix B. Eq. (4.51) becomes the following ODE

$$\partial_t \langle N\Delta^2 \rangle = \beta J \langle N\Delta^2 \rangle^2. \quad (4.53)$$

We define  $y = \langle N\Delta^2 \rangle$  and solve the ODE in eq. (4.53) by separation of variables:

$$\int_{y(0)}^{y(1)} \frac{1}{y^2} dy = \beta J \int_0^1 dt, \quad (4.54)$$

where  $y(0) = \langle N\Delta^2 \rangle_{t=0}$  and  $y(1) = \langle N\Delta^2 \rangle_{t=1}$ . By integrating both sides of eq. (4.54) we obtain:

$$\langle N\Delta^2 \rangle_{t=1} = \frac{\langle N\Delta^2 \rangle_{t=0}}{1 - \beta J \langle N\Delta^2 \rangle_{t=0}}. \quad (4.55)$$

In order to calculate  $\langle N\Delta^2 \rangle_{t=0}$ , i.e. the mean value of the amplified fluctuations in the independent spins case ( $t = 0$ ), we add a source term in the exponential of  $Z_N(\beta, t = 0)$  (eq. (4.30)). The latter becomes:

$$\mathcal{Z}_N(\beta, 0) = \sum_{\sigma} \exp(\beta J \bar{m} \sum_i \sigma_i + h m N). \quad (4.56)$$

and the corresponding pressure is

$$\mathcal{A}_N(\beta, 0) = \frac{1}{N} \log \mathcal{Z}_N(\beta, 0). \quad (4.57)$$

In the TL

$$A(\beta, 0) = \log 2 + \log(\cosh(\beta J \bar{m} + h)). \quad (4.58)$$

The source term allow us to write  $\langle N\Delta^2 \rangle_{t=0}$  as:

$$\langle N\Delta^2 \rangle_{t=0} = \partial_h^2 A|_{h=0} = \partial_h^2 (\log 2 + \log(\cosh(\beta J \bar{m} + h)))|_{h=0} = 1 - \tanh^2(\beta \bar{m} J), \quad (4.59)$$

where the first equality can be proved directly by substituting the pressure with eq. (4.57). However  $\bar{m} = 0$  in the ergodic region (as we can see in figure 4.2 for  $T > T_c$ ), so

$$\begin{aligned} \langle N\Delta^2 \rangle_{t=0} &= 1, \\ \langle N\Delta^2 \rangle_{t=1} &= \frac{1}{1 - \beta J}. \end{aligned} \quad (4.60)$$

It results that  $N(\langle m^2 \rangle - \langle m \rangle^2)$  is a mero-morphic function with a pole at the critical temperature  $T = J$ . There is only a single pole and away from the critical point the magnetization is self-averaging (in the high temperature region it is null). The fluctuations exploding at the critical point are those amplified by a factor  $N$ , i.e. the diverging term is  $N(\langle m^2 \rangle - \langle m \rangle^2)$ . The correct amplification for each single magnetization is  $\sqrt{N}$  perfectly in agreement with the Central Limit Theorem [Bar18].

Another important aspect of this continuous phase transition is the *spontaneous symmetry breaking*. Figure 4.3 shows the intensive free energy per unit site as a function of the magnetization for different values of the temperature. The function plotted in figure 4.3 is obtained by substituting in Definition 12 the expression for the C-W pressure, eq. (4.41), and solving for the extensive free energy per unit site:

$$f(m, \beta) = -\frac{1}{\beta} A(m, \beta) = -\frac{1}{\beta} \left( \log 2 + \log(\cosh(\beta J m)) - \frac{\beta J}{2} m^2 \right). \quad (4.61)$$

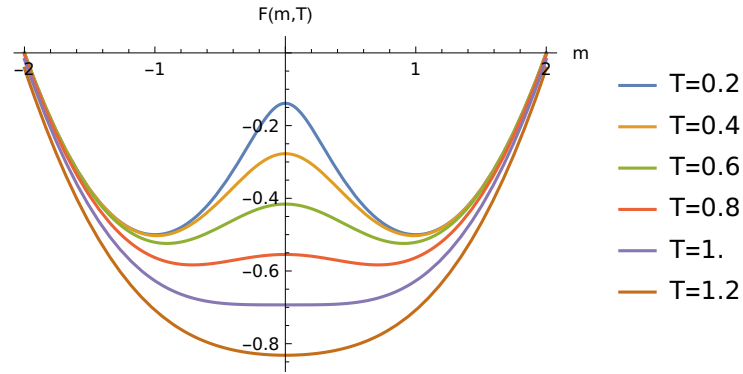


Figure 4.3: Free Energy as a function of  $m$  for different temperatures.

Figure 4.3 shows that, above the critical temperature, the free energy has a parabolic shape around  $m = 0$ . At the critical temperature  $T = 1$  the parabolic shape leaves toward a quartic shape. For lower temperatures, the free energy is bimodal, symmetric around zero. The free energy is invariant under the change  $m \rightarrow -m$ , this is because the Hamiltonian of the C-W model in eq. (4.28) also enjoys this symmetry. Below  $T_c$  the free energy selects one of the two ground states, corresponding to a minimum of the free energy. Whichever choice breaks the symmetry and when a symmetry of a system is not respected by the ground state we say that the symmetry is spontaneously broken.

# Chapter 5

## The Duality

In the previous chapters we have introduced all the concepts, observables and main theorems that we need to show the mechanical analogy. In other words the mathematical duality that lies at the core of the variational principles in analytical and statistical mechanics.

### 5.1 The classical mechanical analogy for the C-W model

In this section we shall show how it is possible to describe the thermodynamic behaviour of the C-W model by using an analogy with the analytical mechanics without relying on the statistical mechanics techniques. Through this mechanical analogy [Bar14], whose study is the main goal of this thesis, the duality will start to emerge and will be confirmed and extended later on, when we shall apply it to incorporate also the relativistic mechanics. We

define a generalized Guerra's action:

**Definition 14.** *By introducing two real parameter  $t, x$  (that can be thought of as fictitious time and fictitious space coordinates) we define the generalized Guerra's action as*

$$A_N(t, x) = \frac{1}{N} \log \sum_{\sigma} \exp \left( -\frac{t}{2N} \sum_{i,j}^{NN} \sigma_j \sigma_i + x \sum_i^N \sigma_i \right), \quad (5.1)$$

for  $t = -\beta J$  and  $x = \beta B$  we recover the statistical expression of the pressure of the C-W model.

**Observation 4.** *The following relations can be proved by using Definition (14):*

$$\begin{aligned} \frac{\partial}{\partial t} A_N(t, x) &= -\frac{1}{2} \langle m^2 \rangle, \\ \frac{\partial}{\partial x} A_N(t, x) &= \langle m \rangle. \end{aligned} \quad (5.2)$$

**Definition 15.** *We define the potential  $V_N(t, x)$*

$$V_N(t, x) = \frac{1}{2} (\langle m^2 \rangle - \langle m \rangle^2). \quad (5.3)$$

In the TL,  $V_N(t, x)$  vanishes since the magnetization is self-averaging.

**Proposition 5.** *Remembering the relations in (5.2) and the definition (5.3), by construction, Guerra's action satisfies the following Hamilton-Jacobi equation:*

$$\frac{\partial}{\partial t} A_N(t, x) + \frac{1}{2} \left( \frac{\partial}{\partial x} A_N(t, x) \right)^2 + V_N(t, x) = 0 \quad (5.4)$$

Eq. (5.4) has the same form of a H-J PDE, eq. (2.34). For this reason it is immediate to define the  $p_N$  and Lagrangian  $\mathcal{L}_N$  as:

$$\begin{aligned} p_N &= \frac{\partial}{\partial x} A_N(t, x) = \langle m \rangle, \\ \mathcal{L}_N &= \frac{p_N^2}{2} = \frac{1}{2} \langle m \rangle^2. \end{aligned} \quad (5.5)$$

In the TL

$$\begin{aligned} \lim_{N \rightarrow \infty} A_N &= A, & \lim_{N \rightarrow \infty} V_N(x, t) &= \lim_{N \rightarrow \infty} \frac{1}{2} (\langle m^2 \rangle - \langle m \rangle^2) = 0, \\ \lim_{N \rightarrow \infty} p_N &= p, & \lim_{N \rightarrow \infty} \mathcal{L}_N &= \mathcal{L} = \frac{1}{2} \langle m \rangle^2. \end{aligned} \quad (5.6)$$

The PDE satified by  $A(x, t)$  becomes:

$$\frac{\partial}{\partial t} A(t, x) + \frac{1}{2} \left( \frac{\partial}{\partial x} A(t, x) \right)^2 = 0, \quad (5.7)$$

which is exactly the expression of the H-J PDE of a free particle with unitary mass, eq. (5.7) with  $m = 1$  for the action  $S$ .

**Theorem 6.** *Since eq. (5.7) is the H-J equation for a free particle of unitary mass, this expression induces to identify  $A$  as the action  $S$  and we can use the standard expression for the action integral:*

$$A(t, x) = A(0, x_0) + \int_0^t \mathcal{L} dt. \quad (5.8)$$

The initial condition  $A(0, x_0)$  can be obtained directly by setting  $t = 0$  inside definition (14) resulting in:

$$A(0, x_0) = \log 2 + \log(\cosh(x_0)). \quad (5.9)$$

To calculate the integral of the Lagrangian we consider the fact that in the TL  $\mathcal{L}$  is a constant along the path given by  $x(t) = x_0 + vt = x_0 + \langle m \rangle t$ , which is the uniform straight motion for the free particle. Finally we reach the expression of Guerra Action, (14), in the TL:

$$A(t, x) = \log 2 + \log \cosh(x(t) - \langle m \rangle t) + \frac{1}{2} \langle m \rangle^2 t \quad (5.10)$$

We evaluate eq. (5.10) for  $t = -\beta J$  and  $x = 0$  to recover the definition of the statistical pressure, eq. (4.33), in the thermodynamic limit. We obtain

$$A(\beta) = \log 2 + \log \cosh(\beta J \langle m \rangle) - \frac{1}{2} \beta J \langle m \rangle^2, \quad (5.11)$$

which is exactly the same expression of the pressure obtained with statistical mechanics approach (see eq. (4.41)).

### 5.1.1 Self-averaging properties and symmetries

The duality, we have shown above in section 5.1, is not simply a remarkable. In this section we shall discuss:

- how self-averaging properties in statistical mechanics match, in their dual representation, Noether conserved currents,
- how the Hamilton principle applied to Guerra's action leads to the self-consistency equation for the magnetization,
- how the evolution of  $\langle m \rangle$  in the (t,x) space obeys the Riemann-Hopf PDE, specifically the archetype PDE for a Hopf bifurcation. We shall show that spontaneous symmetry breaking in Theoretical Physics has a dual interpretation in terms of a shock in Mathematical Physics.

**Proposition 6.** *The space-time symmetries of the free particle motion (as discussed in section 2.1.2), i.e. momentum and energy conservation, imply the following self-averaging properties of the magnetization and its momenta:*

$$\lim_{N \rightarrow \infty} (\langle m^n \rangle - \langle m \rangle^n) = 0.$$

*Proof.* The space symmetry of the motion implies  $x$  to be a cyclic coordinate, as shown in (2.14). For momentum conservation, in the TL, we can write:

$$\frac{\partial \mathcal{L}_N}{\partial x} = \frac{1}{2} \frac{\partial \langle m \rangle^2}{\partial x} = \partial_x \langle m \rangle = N \langle m \rangle (\langle m^2 \rangle - \langle m \rangle^2) \underset{N \rightarrow \infty}{=} 0, \quad (5.12)$$

where

$$\langle m \rangle = \frac{\partial}{\partial x} A_N(t, x) = \frac{1}{N} \frac{\partial}{\partial x} \log \sum_{\sigma} \exp \left( -\frac{t}{2N} \sum_{i,j} \sigma_j \sigma_i + x \sum_i \sigma_i \right). \quad (5.13)$$

The *velocity* in  $N$ , by which self-averaging is guaranteed, is exactly that obtained from the study of the fluctuations in the statistical mechanical counterpart (see subsection 4.3.1).

We have already demonstrated in eq. (2.16), that energy conservation implies  $\partial \mathcal{L} / \partial t = 0$ , thus for time symmetry the conservation law becomes:

$$\frac{\partial \mathcal{L}_N}{\partial t} = \frac{1}{2} \frac{\partial \langle m \rangle^2}{\partial t} = \partial_t \langle m \rangle = -\frac{N}{2} \langle m \rangle (\langle m^3 \rangle - \langle m \rangle \langle m^2 \rangle) \underset{N \rightarrow \infty}{=} 0, \quad (5.14)$$

where we have used eq. (5.13). In the TL we have:

$$\begin{aligned} \lim_{N \rightarrow \infty} (\langle m^2 \rangle - \langle m \rangle^2) &= 0, \\ \lim_{N \rightarrow \infty} (\langle m^3 \rangle - \langle m \rangle^3) &= 0. \end{aligned} \quad (5.15)$$



Acting on  $\partial_x \langle m \rangle$  and  $\partial_t \langle m \rangle$  with higher order derivatives  $\partial_t^n$  we obtain:

$$\lim_{N \rightarrow \infty} (\langle m^n \rangle - \langle m \rangle^n) = 0. \quad (5.16)$$

So in this mathematical framework, Noether symmetries translate directly into self-averaging relations.  $\square$

**Proposition 7.** *The self-consistency relation  $\langle m \rangle = \tanh(\beta J \langle m \rangle)$  is the result of the Hamilton's principle applied to the Guerra's action, eq. (14).*

*Proof.* We perform an infinitesimal variation  $\langle m \rangle \rightarrow \langle m \rangle + \delta \langle m \rangle$  and then minimize the pressure with respect to  $\langle m \rangle$

$$\delta A(\beta) = \frac{\partial A(\beta)}{\partial \langle m \rangle} \delta \langle m \rangle = 0 = (\beta J \tanh(\langle m \rangle \beta J) - \beta J \langle m \rangle) \delta \langle m \rangle = 0, \quad (5.17)$$

thus:

$$\tanh(\beta J \langle m \rangle) = \langle m \rangle. \quad (5.18)$$

$\square$

Finally, by direct derivation of the H-J equation for the Guerra's action, i.e. eq. (5.7), with respect to  $x$  we obtain the following

**Proposition 8.** *Remembering that  $\partial_x A = \langle m \rangle$  and that  $[\partial_x, \partial_t] = 0$  since we are dealing with analytic functions (everywhere but not at the critical point), the PDE for the space-time evolution of  $\langle m \rangle$  is the following Riemann-Hopf type*

$$\frac{\partial \langle m \rangle}{\partial t} + \langle m \rangle \frac{\partial \langle m \rangle}{\partial x} = 0, \quad (5.19)$$

and this equation, also known as the inviscid Burgers equation, is the prototype of a bifurcation for the magnetization exactly as produced by the spontaneous symmetry breaking described in figure 4.2.

## 5.2 The relativistic mechanical analogy for the C-W model

In this section we shall discuss a generalization of the CW model [Bar18].

**Definition 16.** *We define the Hamiltonian of the relativistic C-W model as*

$$-\frac{\mathcal{H}_N(m)}{N} = \sqrt{1 + m^2}. \quad (5.20)$$

*Note that, by Taylor expanding the r.h.s. of the above definition, we obtain interactions terms beyond the pairwise couplings:*

$$\sqrt{1 + m^2} \sim 1 - \frac{m^2}{2} + \frac{m^4}{8} - \frac{m^6}{12} + \dots$$

The above equation shows that the relativistic Hamiltonian contains interaction terms between the spins more complicate than the pairwise interactions of the classical case. For this reason the relativistic model can be considered as a more exhaustive description of the statistical system rather than the classical one.

As a natural extension, we write the relativistic Guerra's action as

$$A_N(t, x) = \frac{1}{N} \log \sum_{\sigma} \exp \left[ N \left( -t\sqrt{1+m^2} + xm \right) \right]. \quad (5.21)$$

In order to find the PDE satisfied by  $A_N(t, x)$  we evaluate its space-time derivative:

$$\begin{aligned} \frac{\partial}{\partial t} A_N(t, x) &= -\langle \sqrt{1+m^2} \rangle, \\ \frac{\partial}{\partial x} A_N(t, x) &= \langle m \rangle, \\ \frac{\partial^2}{\partial t^2} A_N(t, x) &= N(\langle 1+m^2 \rangle - \langle \sqrt{1+m^2} \rangle^2), \\ \nabla^2 A_N(t, x) &= N(\langle m^2 \rangle - \langle m \rangle^2). \end{aligned} \quad (5.22)$$

**Proposition 9.** *It holds by construction that the relativistic Guerra's action obeys the following relativistic H-J PDE:*

$$\partial_t^2 A_N - \nabla^2 A_N = N(1 - (\partial_t A_N)^2 + (\nabla A_N)^2). \quad (5.23)$$

In the covariant form the last expression becomes

$$\frac{1}{N} \square A_N + (\partial_\alpha A_N)^2 = 1. \quad (5.24)$$

This expression is relativistic invariant.

This equation is analogous to the Klein-Gordon equation of the relativistic quantum mechanics.

**Definition 17.** *We define the potential  $V_N$  in order to construct the mechanical analogy:*

$$V_N(x, t) = \frac{1}{N} \square A_N = (1 + \langle m \rangle^2) - \langle \sqrt{1+m^2} \rangle^2. \quad (5.25)$$

By calculating the space-time derivatives of  $A_N$  with respect to  $x_\alpha = (t, -x)$  we obtain

$$\begin{aligned} p_N^\alpha &= -\frac{\partial A_N}{\partial x_\alpha} = (\langle \sqrt{1+m^2} \rangle, \langle m \rangle), \\ p_N^\alpha p_{N\alpha} &= \langle \sqrt{1+m^2} \rangle^2 - \langle m \rangle^2 = 1 - V_N(x, t). \end{aligned} \quad (5.26)$$

By analogy with relativistic mechanics we define:

$$\begin{aligned} \gamma_N &= \langle \sqrt{1+m^2} \rangle, \\ \mathcal{L}_N &= -\gamma_N^{-1} = -\frac{1}{\langle \sqrt{1+m^2} \rangle}, \\ v_N &= \frac{\langle m \rangle}{\langle \sqrt{1+m^2} \rangle}. \end{aligned} \quad (5.27)$$

In the TL we have

$$\begin{aligned} V_N(x, t) &\rightarrow V(x, t) = 0, \\ A_N(x, t) &\rightarrow A(x, t), \end{aligned} \quad (5.28)$$

therefore, the quantities in eq. (5.26) and eq. (5.27) become:

$$\begin{aligned} p^\alpha &= -\frac{\partial A}{\partial x_\alpha} = (\sqrt{1 + \langle m \rangle^2}, \langle m \rangle), \\ \gamma &= \sqrt{1 + \langle m \rangle^2}, \quad v = \frac{\langle m \rangle}{\sqrt{1 + \langle m \rangle^2}}. \end{aligned} \quad (5.29)$$

**Proposition 10.** *In the TL  $A(t, x)$  obeys the relativistic H-J equation for a free relativistic particle with unitary rest mass.*

$$(\partial_\alpha A(x, t))^2 = \frac{\partial A(x, t)}{\partial x^\alpha} \frac{\partial A(x, t)}{\partial x_\alpha} = p^\alpha p_\alpha = 1. \quad (5.30)$$

*Proof.* We have just to substitute the TL of the potential of eq. (5.28) in eq. (5.24).  $\square$

In analogy to the classical case, we identify the relativistic extension of Guerra's action with the relativistic action  $S$ . In order to obtain the explicit expression of  $A(t, x)$  we use the fundamental theorem of calculus and write it as in eq. (5.8):

$$A(t, x) = A(0, x_0) + \int_0^t \frac{dA}{dt'} dt', \quad (5.31)$$

where

$$\frac{dA}{dt} = -\frac{1}{\sqrt{1 + \langle m \rangle^2}} = -\gamma^{-1} = \mathcal{L}. \quad (5.32)$$

The relativistic Lagrangian  $\mathcal{L} = -\gamma^{-1}$  is a constant along the actual path  $x = x_0 + vt$  since it is the kinetic energy of the free particle. For the sake of simplicity, from now on the direction of motion is taken along the  $x$  axis such that the magnetization and the velocity become one dimensional quantities. We can easily integrate eq. (5.31) and evaluate  $A(x, t)$

$$A(t, x) = A(0, x_0) - \int_0^t \frac{dt}{\gamma} = \log 2 + \log \cosh(x - vt) - \frac{t}{\gamma}. \quad (5.33)$$

**Remark 2.** *By differentiating  $A_N(x, t)$  with respect to  $t$  we obtain:*

$$\frac{dA_N}{dt} = -\langle \sqrt{1 + m^2} \rangle + \dot{x} \langle m \rangle. \quad (5.34)$$

*In analogy to eq. (4.37) we write the magnetization as its mean value plus the fluctuation around it:  $m = \bar{m} + \Delta$  and we carry out a Taylor expansion around  $\bar{m}$ . We obtain*

$$\frac{dA_N}{dt} = -\frac{1}{\sqrt{1 + \bar{m}^2}} + \langle m \rangle \left[ \dot{x} - \frac{\bar{m}}{\sqrt{1 + \bar{m}^2}} \right] + \langle O(\Delta^2) \rangle. \quad (5.35)$$

We impose

$$-\frac{\overline{m}}{\sqrt{1+\overline{m}^2}} + \dot{x} = 0. \quad (5.36)$$

This is the expression of the velocity obtained through the mechanical analogy (see equations in (5.26)). We substitute expression (5.36) in eq. (5.34) and obtain in the TL:

$$\frac{dA}{dt} = -\frac{1}{\sqrt{1+\langle m \rangle^2}}. \quad (5.37)$$

therefore have demonstrated that

$$\frac{dA}{dt} = \mathcal{L}, \quad (5.38)$$

confirming again the identification of  $A$  with the action  $S$  defined in definition 1.

As we have done in eq. (5.10)) we substitute  $t = -J\beta$ ,  $x = 0$  and then we use the expressions for  $v$  and  $\gamma$  in terms of the magnetization, eq.s in (5.29), to write  $A(x, t)$  in terms of  $\beta$ :

$$A(\beta) = \log 2 + \log \cosh \left[ \frac{J\beta \langle m \rangle}{\sqrt{1+\langle m \rangle^2}} \right] + \frac{J\beta}{\sqrt{1+\langle m \rangle^2}}. \quad (5.39)$$

In order to obtain the self-consistency relation, as for the classical case, we further exploit the mechanical analogy via the next

**Proposition 11.** *The self-consistency relation can be obtained by applying Hamilton's principle to the relativistic extension of Guerra's action.*

*Proof.* According to variational principle we impose the stationarity condition

$$\begin{aligned} \delta A &= \frac{\partial A(\beta)}{\partial m} \delta m = \tanh \left( \frac{\beta J \langle m \rangle}{\sqrt{1+\langle m \rangle^2}} \right) \beta J \frac{\delta m}{\left( \sqrt{1+\langle m \rangle^2} \right)^3} + \\ &- \beta J \frac{\langle m \rangle}{\left( \sqrt{1+\langle m \rangle^2} \right)^3} \delta m = 0 \implies \end{aligned} \quad (5.40)$$

$$\tanh \left( \frac{\beta J \langle m \rangle}{\sqrt{1+\langle m \rangle^2}} \right) = \langle m \rangle. \quad (5.41)$$

which is the relativistic self-consistency relation.  $\square$

### 5.2.1 Self-averaging properties and symmetries

In the TL  $A(t, x)$  satisfies the relativistic H-J equation for a free relativistic particle. As a consequence, just like in the classical case, the symmetries of such motion give important information regarding the self-averaging properties of the magnetization as established by the next

**Proposition 12.** *The space-time symmetries of the relativistic free particle motion, i.e. four*

momentum conservation and energy conservation, imply the self-averaging properties of the magnetization.

*Proof.* We observe that the Lagrangian in the infinite volume limit does not depend on  $x$  (it is a cyclic coordinate) thus

$$\frac{\partial \mathcal{L}_N}{\partial x} = N\gamma_N^{-2} \left( \langle m\sqrt{1+m^2} \rangle - \langle m \rangle \langle \sqrt{1+m^2} \rangle \right) \underset{N \rightarrow \infty}{=} 0. \quad (5.42)$$

We have already demonstrated that as a consequence of the space symmetry of the motion we have 4-velocity conservation (eq. (3.19) holds). Considering that the system has unitary mass it turns out that the 4-velocity  $u^\beta$ , eq.(3.19), has the same expression of the 4-momentum. Recalling 4-momentum expression in the finite volume case (see eq. 5.26), we define

$$u_N^\beta := (\langle \sqrt{1+m^2} \rangle, \langle m \rangle). \quad (5.43)$$

We insert this expression in eq. (3.19) and obtain

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{1}{\gamma} \frac{du_N^\beta}{dt} = 0 \implies \\ \frac{d}{dt} \langle \sqrt{1+m^2} \rangle = N \left( \langle 1+m^2 \rangle - \langle \sqrt{1+m^2} \rangle^2 \right) - \\ + N\dot{x} \left( \langle m\sqrt{1+m^2} \rangle - \langle m \rangle \langle \sqrt{1+m^2} \rangle \right) \underset{N \rightarrow \infty}{=} 0 \end{aligned} \quad (5.44)$$

and

$$\begin{aligned} \frac{d\langle m \rangle}{dt} = N \left( \langle m\sqrt{1+m^2} \rangle - \langle m \rangle \langle \sqrt{1+m^2} \rangle \right) + \\ + N\dot{x} \left( \langle m^2 \rangle - \langle m \rangle^2 \right) \underset{N \rightarrow \infty}{=} 0. \end{aligned} \quad (5.45)$$

□

In the TL we obtain the following limits:

$$\begin{aligned} \lim_{N \rightarrow \infty} \left( \langle m\sqrt{1+m^2} \rangle - \langle m \rangle \langle \sqrt{1+m^2} \rangle \right) &= 0 \\ \lim_{N \rightarrow \infty} \left( \langle m^2 \rangle - \langle m \rangle^2 \right) &= 0 \\ \lim_{N \rightarrow \infty} \left( \langle 1+m^2 \rangle - \langle \sqrt{1+m^2} \rangle^2 \right) &= 0. \end{aligned} \quad (5.46)$$

**Remark 3.** *Equation*

$$\lim_{N \rightarrow \infty} \left( \langle 1+m^2 \rangle - \langle \sqrt{1+m^2} \rangle^2 \right) = 0 \quad (5.47)$$

can also be obtained by imposing energy conservation:

$$\begin{aligned}
 \lim_{N \rightarrow \infty} \frac{\partial \mathcal{L}_N}{\partial t} &= - \lim_{N \rightarrow \infty} \frac{\partial}{\partial t} \frac{1}{\langle \sqrt{1+m^2} \rangle} = \\
 &= \lim_{N \rightarrow \infty} \frac{1}{\langle \sqrt{1+m^2} \rangle^2} \left( \langle 1+m^2 \rangle - \langle \sqrt{1+m^2} \rangle^2 \right) = 0 \implies \\
 \lim_{N \rightarrow \infty} \left( \langle 1+m^2 \rangle - \langle \sqrt{1+m^2} \rangle^2 \right) &= 0.
 \end{aligned} \tag{5.48}$$

### 5.2.2 The standard C-W model as the classical limit

Relativistic mechanics is the correct kinematic description at high velocity, but Newtonian mechanics is an adequate approximation at small velocity compared to the speed of light; this is because Lorentz transformation turns into Galilean transformation in the limit  $v \ll c$ . Similarly we can show how the relativistic extension of C-W turns into the classical C-W model in the limit  $\langle m \rangle \ll 1$  as expected.

**Proposition 13.** *The classical C-W model is the approximation of the relativistic C-W model in the low momentum limit  $\langle m \rangle \ll 1$ .*

*Proof.* We consider the low momentum limit  $\langle m \rangle \ll 1$  of

$$\tanh \left( \frac{\beta J \langle m \rangle}{\sqrt{1 + \langle m \rangle^2}} \right) = \langle m \rangle \tag{5.49}$$

and we obtain the self-consistency relation of the classical C-W model

$$\tanh \beta J \langle m \rangle = \langle m \rangle. \tag{5.50}$$

We consider the  $\langle m \rangle \ll 1$  approximation also for the relativistic self-averaging properties and we obtain

$$\begin{aligned}
 \lim_{N \rightarrow \infty} \left( \langle m \sqrt{1+m^2} \rangle - \langle m \rangle \langle \sqrt{1+m^2} \rangle \right) &= 0, \\
 \lim_{N \rightarrow \infty} \left( \langle m^2 \rangle - \langle m \rangle^2 \right) &= 0,
 \end{aligned} \tag{5.51}$$

therefore we find

$$\begin{aligned}
 \lim_{N \rightarrow \infty} \frac{1}{2} \left( \langle m^3 \rangle - \langle m \rangle \langle m^2 \rangle \right) &= 0, \\
 \lim_{N \rightarrow \infty} \left( \langle m^2 \rangle - \langle m \rangle^2 \right) &= 0,
 \end{aligned} \tag{5.52}$$

which allows us to obtain the self-averaging relations of eq. (5.15).  $\square$

# Chapter 6

## Conclusions

In this thesis we have shown the existence of a mathematical bridge connecting the different physical variational principles lying at the core of non-relativistic, relativistic and statistical mechanics.

In order to build this bridge, we used toy-models in both analytical and statistical mechanics. For the former case, in both non-relativistic and relativistic situations, we considered the Galilean motion of a free particle of unitary mass.

For the statistical mechanics we considered the C-W model consisting in an infinite one-dimensional spin chain, subject to an external magnetic field. We have considered the situation with a pairwise interaction between the various spin components of the chain. If the external magnetic field is switched off, the the model behaves as a paramagnet in the high-temperature region, while, in the low-temperature region it spontaneously acquires a magnetization, and behaves as a ferromagnet. In going from one region to the other one, the system shows a critical behaviour which is a second order phase transition. While the Hamiltonian keeps the spin-flip invariance, the state of the system relaxes and does not posseses this symmetry any more. This is a clear example of spontaneous symmetry breaking.

The basic point of our approach is the use of the Guerra-Rosen-Simon pressure [[Gue75](#), [Gue76](#), [Gue73](#)] which is a novel definition of the free energy. This quantity obeys to the H-J PDE in an analogous manner as the free-particle action in the classical Lagrangian mechanics. We used this pressure within the variational least-action principle and we found the same self-consistency relation obtained with the usual techniques of the canonical statistical mechanics. Thus the principle of least action applied in statistical mechanics effectively reproduces the free energy minimization and entropy maximization required by thermodynamics.

We exploited this analogy by demonstrating that the well-known self averaging proprieties of the magnetization in statistical mechanics are obtained via this mechanical duality as conserved currents typically described in terms of Noether symmetries in analytical mechanics.

Furthermore, we have shown that the spin-flip symmetry breaking found at the critical point in statistical mechanics turns out to be a Hopf-bifurcation in the mechanical analogy. When the C-W model acquires spontaneously a magnetization, the system undergoes to a classical shock in the language of non-linear PDE.

We have extended this analogy to its relativistic limit. Since the C-W model is described

in the mechanical duality by the classical kinetic term only, it is not difficult to obtain its relativistic extension. The Hamiltonian chosen for the extended C-W model is analogous to that of the relativistic mechanics, where the magnetization plays the role of the mechanical three-momentum.

In carrying out this relativistic extension we found that the theory predicts the presence of terms beyond the pairwise interaction which is usually the only term considered in the traditional statistical mechanics. These higher order terms can play a role in specific cases such as the structural glasses and all the systems whose phase transitions are no longer continuous in the order parameter.

As aspected, the analogy keeps holding in full depth. The pressure turns out to obey to a Klein-Gordon-like equation and the theory becomes intrinsically relativistic invariant. We exploited the connection between the two mechanics in the same way as before for the classical analogy and, finally, we demonstrated the choerence of the relativistic extension by taking the low momentum limit of the relativistic relations and we obtained again the classical ones.

At the end of our journey we can say that, from a pragmatocal point of view, the lesson we have learned is that we can explore the probabilistic evolution of a statistical system through the deterministic technique of the classical and relativistic mechanics and viceversa, hence putting a bit closer two worlds (functional analysis and probability theory) that are usually treated as separated fields of research. This bridge could thus be mathematically useful, and the existence of the duality itself constitutes a refined and comprehensive picture of the various mechanics.



# Appendix A

## Existence of the TL

Despite Physicists sometimes assume the existence of the asymptotic values of the entities of interest (first of all the free energy), it is instructive to show how to prove the existence of such limits. This is important for two reasons, the one more physical in spirit the other one more mathematical.

From a physical perspective, when dealing with (possibly more realistic) lattice models, we saw that solving for their free energy can be of extraordinary difficulty but proving the existence of all the involved observables is rather trivial (by an elementary *surface-to-volume* ratio). On the other hand, when studying mean-field models (where the surface-to-volume ratio is one by definition, as these models are effectively infinite dimensional models), questioning on the existence of the asymptotic values of their main observable can be far from simple.

It is this appendix we prove the existence of the limiting value of the free energy per site in the C-W model we studied. The underlying idea is to compare the free energy of a large system, made of  $N$  spin sites, with two -independent- subsystem made of  $N_1$ ,  $N_2$  sites respectively such that  $N_1 + N_2 = N$ . As elegantly shown by Ruelle [Rue99], if we can prove that the free energy is sub-extensive (or even super-extensive, the important point is that it does not oscillate) and that it is limited, then -due to the Fekete Lemma- the limit of the succession  $F_N, F_{N+1}, \dots, F_\infty$  must converge (at worst in the Cesaro sense). To achieve our final goal we have thus to divide the  $N$  spin system into two independent subsystems of  $N_1$ ,  $N_2$  spin sites such that  $N = N_1 + N_2$  and define the magnetization of the original system, i.e.  $m$ , and those of the two subsystems as

$$\begin{aligned} m_1(\boldsymbol{\sigma}) &= \frac{1}{N_1} \sum_i^{N_1} \sigma_i, \\ m_2(\boldsymbol{\sigma}) &= \frac{1}{N_2} \sum_{i=N_1+1}^N \sigma_i, \end{aligned} \tag{A.1}$$

such that the total magnetization can be written as

$$m(\boldsymbol{\sigma}) = \frac{N_1}{N} m_1(\boldsymbol{\sigma}) + \frac{N_2}{N} m_2(\boldsymbol{\sigma}). \tag{A.2}$$

Since the function  $x \rightarrow x^2$  is convex, obviously it must hold that

$$\begin{aligned} Z_N(\beta) &= \sum_{\sigma} \exp\left(\frac{1}{2}\beta N m^2(\sigma)\right) \leq \sum_{\sigma} \exp\left(\frac{1}{2}\beta(N_1 m_1^2(\sigma) + N_2 m_2^2(\sigma))\right) = \\ &= Z_{N_1}(\beta) Z_{N_2}(\beta). \end{aligned} \quad (\text{A.3})$$

**Remark 4.** *The function  $f(x) = x^2$  is convex so  $\forall t \in \mathbb{R}$ :*

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2), \quad (\text{A.4})$$

choosing  $t = N_1/N$  we obtain the previous inequality:

$$\left(\frac{N_1}{N}x_1 + \frac{N_2}{N}x_2\right)^2 \leq \frac{N_1}{N}x_1^2 + \frac{N_2}{N}x_2^2. \quad (\text{A.5})$$

Manipulating (A.3) in order to obtain the free energy per site (that is by taking the log at both sides of the expression and then using the properties of the logarithms) we obtain

$$Nf_N(\beta) = -\frac{1}{\beta} \log Z_N(\beta) \geq N_1 f_{N_1}(\beta) + N_2 f_{N_2}(\beta), \quad (\text{A.6})$$

and thus the free energy is a super-additive function. To check that it is also a bounded function it is enough to consider its infinite noise limit, where the free energy reduces trivially to  $(-\beta^{-1} \text{ times})$  the intensive infinite-noise entropy  $-\beta^{-1} \ln 2$  (as a consequence of a flat measure over a configuration space large as  $2^N$ ) that is a bounded function in  $N$ .

According to the Fekete lemma then  $\lim_{N \rightarrow \infty} f_N(\beta)$  exists and equals the sup  $f_N(\beta)$ . Another, equivalent, route to show the super-additive property of the intensive free energy arises also by interpolating between the original system of  $N$  spins, and two non-interacting systems, containing  $N_1$  and  $N_2$  spins, respectively. To this purpose, we consider the interpolating parameter  $0 \leq t \leq 1$  and the partition function:

$$Z_N(t, \beta) = \sum_{\sigma} \exp\left(\frac{1}{2}\beta(Ntm^2(\sigma) + N_1(1-t)m_1^2(\sigma) + N_2(1-t)m_2^2(\sigma))\right), \quad (\text{A.7})$$

where:

$$\begin{aligned} -\frac{1}{N\beta} \log Z_N(1, \beta) &= f_N(\beta), \\ -\frac{1}{N\beta} \log Z_N(0, \beta) &= \frac{N_1}{N} f_{N_1}(\beta) + \frac{N_2}{N} f_{N_2}(\beta), \end{aligned} \quad (\text{A.8})$$

and

$$-\frac{1}{N\beta} \log Z_N(t=1, \beta) = -\frac{1}{N\beta} \log Z_N(t=0, \beta) - \int_0^1 \frac{1}{N\beta} \frac{d}{dt} (\log Z_N(t, \beta)) dt, \quad (\text{A.9})$$

where the integrand turns out to be the positive quantity:

$$-\langle m^2(\sigma) - \frac{N_1}{N} m_1^2(\sigma) - \frac{N_2}{N} m_2^2(\sigma) \rangle_t \geq 0. \quad (\text{A.10})$$

Thus we obtain again the super-additive property for the free energy

$$f_N(\beta) \geq \frac{N_1}{N} f_{N_1}(\beta) + \frac{N_2}{N} f_{N_2}(\beta). \quad (\text{A.11})$$

# Appendix B

## A property of Gaussian observables

We have an observable  $x$  with Gaussian continuous probability distribution:

$$f(x, \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right), \quad (\text{B.1})$$

where

- $\mu$  is the expectation or mean of the distribution
- $\sigma$  is the standard variation
- $\sigma^2$  is the variance

**Proposition 14.** *For the Gaussian observable  $x$  we can write the following equality:*

$$\langle xg(x) \rangle = \langle x^2 \rangle \langle \partial_x g(x) \rangle, \quad (\text{B.2})$$

where  $\langle O \rangle = \int_{\mathbb{R}} O(x) f(x, \mu, \sigma^2) dx$  and  $g(x)$  is a continuous function of  $x$ .

*Proof.* We consider the mean value of  $x$  equals to zero for simplicity. We write:

$$\begin{aligned} \langle xg(x) \rangle &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{\mathbb{R}} xg(x) \exp\left(-\frac{x^2}{2\sigma^2}\right) dx = \\ &= -\sigma^2 \int_{\mathbb{R}} g(x) \partial_x \left( \exp\left(-\frac{x^2}{2\sigma^2}\right) \right) dx. \end{aligned} \quad (\text{B.3})$$

The second term in the latter equation can be integrating by parts to obtain:

$$\begin{aligned} &= -\sigma^2 \int_{\mathbb{R}} g(x) \partial_x \left( \exp\left(-\frac{x^2}{2\sigma^2}\right) \right) dx = \\ &= -\sigma^2 \int_{\mathbb{R}} \partial_x g(x) \exp\left(-\frac{x^2}{2\sigma^2}\right) dx = \langle \partial_x g(x) \rangle \langle x^2 \rangle, \end{aligned} \quad (\text{B.4})$$

where we have used in the last equality the fact that  $\langle x^2 \rangle = \sigma^2$ . □

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