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PHASE TRANSITIONS IN STRONGLY CORRELATED ELECTRONIC SYSTEMS

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Capitolo 1

Abstract

We studied the some type of phase transitions in Strongly Correlated Electronic Systems. In particular we rigorously established some exact properties of a multi-orbital Hubbard model, here formulated to describe a nematic phase transition. In the first step, using Bogoliubov's inequality, we rigorously showed that the multiorbital Hubbard model with narrow bands, eventually in the presence of the spin-orbit coupling, does not exhibit long-range nematic order, in the low dimensions. This result holds at any finite temperature for both repulsive and attractive on-site Coulomb interactions, with and without spin-orbit coupling. In the following step, using the reflection positivity method, we showed that this model supports a staggered nematic order if repulsive or attractive on-site inter-orbital and intra-orbital interactions and off-site repulsive inter-orbital interaction are considered. Depending on the dimensions of the lattice where the model is defined, the order may or not may exist. Indeed, in three dimensions the order may exist at finite temperature, and we get the condition for its existence finding out an upper bound for the critical temperature. On the other hand, for two dimensional lattices, the order may exist at least in the ground state, if the hopping amplitude is small enough.

Furthermore, in the final step, we studied the symmetry properties of the non-degenerate Hubbard model with spin-orbit interactions of Rashba and Dresselhaus type. These interactions break the rotational symmetry in spin space, so that the magnetic order cannot be excluded by using the Bogoliubov inequality method. Nevertheless, we rigorously show that the existence of the magnetic long-range orders may be ruled out when the Rashba and Dresselhaus coupling constants are equal in modulus, whereas the η-pairing can be always ruled out, regardless of the microscopic parameters of the model. These results are obtained by imposing locally the SU(2) gauge symmetry on the lattice, and rewriting the spin-orbit interactions in such a way that they are included in the path ordered of the gauge field on lattice.

In questo lavoro consideriamo alcuni tipi di transizioni di fase in Sistemi Elettronici Fortemente Correlati stabilendo, in particolare, alcuni risultati rigorosi riguardanti il modello di Hubbard multibanda dove possono presentarsi ordini a lungo raggio di tipo orbitale. In un primo passo, usando la diseguaglianza di Bogoliubov, mostriamo che il modello di Hubbard multibanda con interazione spin orbita non presenta ordine nematico in sistemi a bassa dimensionalita' . Questo risultato vale a temperatura finita e se consideriamo interazione Coulombiana on-site repulsiva o attrattiva con o senza interazione spin orbita. Nel passo successivo, usando il metodo degli Infrared Bounds e condizione di Reflection Positivity, mostriamo che il modello presenta uno Staggered Nematic order almeno nello stato fondamentale se consideriamo on-site Interazione Coulombiana repulsiva o attrattiva ed una interazione Coulombiana repulsiva fra elettroni appartenenti alla stessa banda e siti reticolari primi vicini. I sistemi considerati sono definiti su reticoli bidimensionali o tridimensionali sui quali diamo delle condizioni necessarie affinche' l'ordine esista.

Infine, considerando il modello di Hubbard non degenre su reticoli uni e bidimensionali, studiamo le sue propriet di simmetria se vengono aggiunte interazioni spin-orbita di tipo Rashba o Dresselhauss. Queste interazioni rompono la simmetria rotazionale nello spazio dello spin, quindi l'ordine magnetico non pu essere escluso utilizzando la diseguaglianza di Bogoliubov. Comunque riscrivendo l'intrazione spin orbita in termini di una teoria di Gauge SU(2) siamo in grado di dire che l'ordine magnetico assente se le costanti di accoppiamento delle interazioni Rashba e Dresselhauss sono uguali.

Indice

Capitolo 2

Introduction

Phase transitions are the manifestation of violation of the thermodynamic stability conditons like the convexity of the Energy or, equivalently, the convexity of the thermodynamics potential with respect their extensive variables and the concavity with respect the intensive variables. In such cases homogeneous states of the system are not possible and equilibrium manifestes between many phases. The transition liquid-vapour is a classic example where, below the critical point, two portions of the system have different comprexibility and density in equilibrium between them. The Equilibrium conditions are given by the equality of the chemical potentials of the two phases, furthermore the equation $\mu_1(P,T) = \mu_2(P,T)$ is a line where we have coexistence of the two phases. Now by variation of the pressure or volume there are transitions between these phases. This is an example of first order phase transition, indeed one defines a transition of the first order if the internal Energy of the system changes in a discontinuous way at a certain temperature, that is the transition is accompanied by a release or an assimilation of latent heat. If T is increased, the coexistence line terminates in the critical point, where the transition between the two phases is continuous. Beyond the critical point, there is no transition between the two phases, there is no singularity in any physical quantity upon going from one phase to the other. This is a second order phase transition. One defines the second order phase transition if it does not involve latent heat and the Internal Energy changes continuously with the temperature but the first derivative of the Energy diverges at the transition temperature called critical temperature T_c. The most important examples for materials undergoing second-order transitions are ferromagnets, superfluids, and superconductors. Furthermore such transition can usually be characterized by an order parameter, this is a thermodynamic quantity that is zero in one phase (the disordered or symmetric phase) and non-zero and non-unique in the other (the ordered) phase, indeed by a microscopic point of view one can define an observable such that its thermal expectation value can be considered as an order parameter, in particular if it is not vanishing and is not unique then the symmetry of the Hamiltonian and the Gibbs potential are spontaneously broken. In general one speaks of a

spontaneous symmetry breakdown if the symmetry group in field space reduces to a subgroup when passing from the disordered high-temperature phase to the ordered low-temperature phase.

An important property of second-order phase transitions is the divergence, at the critical temperature T_c, of the length scale, over which the system behaves coherently. Indeed while the thermodynamic average of the order parameter is zero in the disordered phase, its fluctuations are non-zero, hence if the critical point is approached, the spatial correlations of the order parameter fluctuations become long-ranged and this is accompanied by a divergence of the size of thermal fluctuations. As a consequence, many physical observables show, near T_c, a power type behaviour in the temperature difference $|T - T_c|$ from the critical point. More precisely they behave like $|T - T_c|^p$ where the power p is called a critical exponent of the associated observable.

In order to describe correctly a second-order phase transition, a model must have the following properties. At T_c, the fluctuations must occur on arbitrarily large length scales. In the neighborhood of T_c, a correlation length which diverges for $T \to T_c$ should be the only relevant length scale of the system, making the correlation functions of the model at the critical point scale independent. For example close to the critical point their typical length scale, the correlation length ζ, diverges as:

$$\zeta \propto |t|^{-\nu} \tag{2.1}$$

with $t = \frac{T-T_c}{T_c}$. In addition to the long-range correlations in space there are analogous long-range correlations of the order parameter fluctuations in time. The typical time scale for a decay of the fluctuations is the correlation (or equilibration) time τ_c. As the critical point is approached the correlation time diverges as:

$$\tau_c \propto |t|^{-z\nu} \tag{2.2}$$

The divergencies (2.1) and (2.2) are responsible for the so-called critical phenomena. At the phase transition point, correlation length and time are infinite and the system is scale-invariant. Then to the critical point the correlation length is the only relevant length scale, therefore the physical properties must be unchanged if we rescale all lengths in the system by a common factor, and at the same time adjust the external parameters in such a way that the correlation length retains its old value. This gives rise to the homogeneity relation for the singular part of the free energy density:

$$f(t, h) = b^{-d} f(t d^{\frac{1}{\nu}}, b^{y_B})$$

Here y_B is another critical exponent whereas d is the spatial dimensionality. The scale factor b is an arbitrary positive number. Analogous homogeneity relations for other thermodynamic quantities can be obtained by differentiating f. If follows that in the vicinity of a second-order phase transition all thermodynamic potentials are generalized homogeneous functions. In addition to the critical exponents ν, and z defined above, a number of other exponents is in common use. They describe the dependence of the order parameter and its correlation

on the distance from the critical point and on the conjugate field h to the order parameter. In particular for the specific heat at zero external field h one has that $C \propto |t|^{-\alpha}$ the order parameter $M \propto (-t)^{\beta}$ whereas the susceptivity $\chi \propto |t|^{-\gamma}$ and the critical isotherm $h \propto sign(M)|M|^{\delta}$ at $t = 0$. The set of corresponding critical exponents completely characterizes the critical behavior near a particular phase transition. Indeed one of the most remarkable features of continuous phase transitions is universality, that is, the fact that the critical exponents are the same for entire classes of phase transitions which may occur in very different physical systems. These universality classes are determined only by the symmetries of the order parameter and by the space dimensionality of the system. The mechanism behind universality is, again, the divergence of the correlation length, therefore, to the critical point, the relevant characteristics of the system are the averages over large volumes hence the microscopic details of the Hamiltonian are unimportant.

The phase transition described above have critical temperature strictly positive and the order parameter is the thermal average of an observable, but is possible to define phase transitions at zero temperature that describe the change in the ground state structure of the system as function of a parameter in the Hamiltonian operator (for example a coupling constant). These are Quantum Phase Transition. A quantum phase transition is a non-analyticity of the ground state properties of the system as a function of a control parameter g. If this singularity arises from a simple level crossing in the many-body ground state, then we have a first order quantum phase transition, without diverging correlations and associated critical singularities. The situation is different for continuous transitions, where a higher-order singularity in the ground state energy occurs, where an infinite number of many-body eigenstates are involved, and the thermodynamic limit is required to obtain a sharp transition. Near a phase transition the relevant physics is described by long-wavelength order parameter quantum fluctuations that it is the quantum expectation value on the ground state of an operator.

In the study of quantum system new emergent states of the matter can be described if one consider systems with a highly degenerate ground state. These new states of the matter can be described in terms of topological quantum order (TQO) where one does not define any order parameter or spontaneous symmetry breking, but they are intuitively associated with insensivity to any local perturbation. In essence, this new order is associated with robustness against local perturbations, and hence cannot be described in principle by local order parameter. Thus, the underlying order remains hidden to ordinary local probes. Indeed, this new order exhibits nonlocal correlations that potentially can lead to novel physical consequences, indeed the characteristic signature of the novel phase is a finite ground state degeneracy that depends on the topology of the system, where can exist charge fractionalization (with respect to that of the constituent particles) and/or fractional statistics of the quasiparticles (Anyons). In more precise terms when a system is in a topological phase it has a set of orthonormal pseudo-ground states $|a_i >$ with $a = 1, 2, ..., N_g$, which includes the absolute ground state of the system. These pseudo-ground states

satisfy, for each $|a>$ and $|a'>$, the following condition:

$$\delta E_0 = max_{(a,a')}|E_a - E_{a'}| \sim O(e^{-\frac{L}{\zeta}})$$

where L is the system size and ζ is the correlation length of the system, which is finite in the limit $L \to \infty$, that is these ground states are degenerate exactly in the thermodynamics limit. Furthermore these states are separated from the rest of the spectrum by an energy gap that remains non-zero in the thermodynamics limit. In a topological phase, one has degeneration of the ground state V_0 which depends only on the topological configuration of the system, genus, number of boundaries, its topology and boundary conditions, in particular the correlation functions on the ground state are invariant under smooth deformation of the spacetime manifold in which the system lives. Furthermore, for any local operator Q and for each $|a>, |b> \in V_0$ one has

$$< a|Q|b >= q_0\delta_{a,b} + O(e^{-\frac{L}{\zeta}}) \tag{2.3}$$

with q_0 is a constant independent from $|a>$ and $|b>$, that is any local operator cannot cause transitions between states belonging to V_0, at most, the state of the system can acquire an overall phase. This condition is naturally satisfied if degenerate states are distinguished only by a non-local topological order parameter.

A system that satisfies the properties listed above is described by a topological quantum field theory (TQFT), that is a field theory where the correlators or the expectation value are independent from the metric tensor. In particular, the low-energy and long distances physical properties are described by an effective theory in which the degrees of freedom are entirely topological, they depend only on the global properties of the system (with no dynamical degrees of freedom nor geometry/metric dependence). The first and classical example of topologically ordered system is a quantum Hall fluid. This effect, realized for two dimensional electronic systems in a strong magnetic field, is characterized by a gap between the ground state and the excited states, a vanishing longitudinal resistivity $\rho_{xx} = 0$ and the quantization of the Hall resistivity, precisely to values of $\rho_{xy} = \frac{1}{\nu}\frac{h}{e^2}$, with ν being an integer (IQHE), whereas in the FQHE $\nu = \frac{1}{n}$ with n odd. Indeed if one neglects Coulombian interaction then the system can be considered as a gas of free electrons in a magnetic field, in this case the eigenstates of the single particle Hamiltonian are a discrete set of degenerate levels equally spaced called Landau levels. If the electrons are confined to a surface of area A pierced by magnetic flux $B \cdot A$, then there are $N_g = BA/\Phi_0 = BA\frac{e}{hc}$ degenerate states in each Landau level, that is the degree of degeneration is equal to the number of elementary quantum flux $\Phi_0 = \frac{hc}{e}$. In the absence of disorder, these single-particle states are all precisely degenerate. When the chemical potential lies between the ν^{th} and $(\nu+1)^{th}$ Landau levels, the Hall conductance takes the quantized value $\sigma_{xy} = \nu\frac{e2}{h}$ while $\rho_{xx} = 0$. The two-dimensional electron density is $n = \nu\frac{eB}{hc}$. In the presence of a periodic potential and/or disorder as for example impurities, the Landau levels broaden

into bands. When the chemical potential lies in the region of localized states between the centers of the ν^{th} and $(\nu+1)^{th}$ Landau bands, the Hall conductance again takes the quantized value $\sigma_{xy} = \nu\frac{e2}{h}$ while $\rho_{xx} = 0$ and the electronic density will be close but not necessarily equal to $\nu\frac{eB}{hc}$. This is known as the Integer quantum Hall effect because ν is an integer. Neglecting Coulomb interactions is justified when an integer number of Landau levels is filled, so that the energy splitting between Landau levels is much larger than the scale of the Coulomb energy, whereas if the electron density is such that a Landau level is only partially filled then the Coulomb interactions may be important and the degeneration of the Landau levels is broken by electron-electron interaction. In this case there is a gap between the ground state and the exciting states as in the IQHE but only a fraction of the Landau level is filled. In this case we have the Fractionary Quantum Hall Effect and a its theorical description is given by Laughlin.

In this work we give, in the chapter three, some mathematical concept on the phase transitions. In particular we define the thermodynamic potentials and the thermodynamic limit. We prove that, under certain conditions, the thermodynamics potentials exist and are uniques. We give a classification of the phase transitions and the connection between phase transitions and Spontaneous Symmetry Breaking concept. An important part of the second chapter is devoted to the study of some methods used in Statistical Mechanics in order to prove the existence or the absence of phase transitions in specific models. These are the Bogoliubov and the indetermination inequality used in order to prove that a specific system does not exhibit a phase transition. We devoted particular attention to the problem of the existence of a phase transition in particular at the Infrared Bounds methods and the Reflection Positivity concept.

We dedicate the fourth chapter to some applications of the methods studied in the third chapter. Here we give a proof of the Mermin and Wagner theorem for a generic model of Strongly Correlated Electronic System, furthermore we extend the theorem at the d-band Hubbard model with tensorial order parameter. In the specific case we study the possible orbital order in a model of TMO (Transition Metal Oxides) system, in particular we define the order parameter as the expectation value of the electric quadrupole momentum obtaining that in a rotational symmetric model the order is absents.

In the fifth chapter we study the problem of the existence of phase transitions in TMO models, in the specific case we consider the d-band Hubbard model where an infraband off-site Coulombian repulsion is introduced, obtaining that, under particular conditions, the orbital order can exist in this model at low temperature in two and three dimensional systems. In this chapter we study possible Charge Density Wave (CDW) and Superconductivity Lond Range Order (LRO) in these systems.

In the Chapter six we introduce the spin orbit interaction in Strongly Correlated Electronic Systems as a $SU(2)$ Gauge theory in the Pauli Lagrangian density. We decsribe how the charge is conserved and spin current is covariantly conserved with this approach. In a system defined a lattice we introduce

the spin orbit interaction by an Hamiltonian (Kogut Susskind approach) lattice $SU(2)$ Gauge theory. In particlar we study the non degenerate Hubbard model with Rashba and Dresselhaus interaction obtainig some rigorous result.

Capitolo 3

Mathematical tools in Phase Transitions

3.1 Thermodynamic Potentials and the Thermodynamic Limit.

Let H the Hamiltonian and $\{|a>\}$ the eigenvectors of the quantum system, one defines a Partition function as $Z(T,N,V,\partial V) = Tr(e^{-\frac{H}{k_B T}})$ with T the temperature, k_B the Boltzmann constant whereas N and V are respectively the number of particle an the volume of the system. For a classical system the trace is replaced by integration on the phase space, hence the partition function is $Z(T,N,V,\partial V) = \int d\mu e^{-\frac{H}{k_B T}}$ where $d\mu$ is the Lebesgue measure on the phase space. Furthermore one defines $dP = \frac{1}{Z} e^{-\frac{H}{k_B T}} d\mu$ as a probability measure of realization of a microscopic state (Gibbs measure), for a finite size systems this is a conditioned probability and depends on the boundary conditions ∂V of the system. Formally one can define a Thermodynamic limit where the system has infinite size at constant density. Hence one defines the thermodynamic limit as $\lim_{N\to\infty,V\to\infty}()$ under the condition that $\lim_{N\to\infty,V\to\infty} \frac{N}{V} = \rho$ where ρ is the density of the system. More formally the ensembles which we have considered describe systems enclosed in a bounded region $\Lambda \in \mathbb{R}^d$ of $\Lambda \in \mathbb{Z}^d$, then let $(L_1,...,L_d) \in \mathbb{R}^d$ (resp.$\in \mathbb{Z}^d$) and $\Lambda_L = \{x \in \mathbb{R}^d \;\; 0 \leq x_i \leq L_i\}$ or (if lattice systems are considered) $\Lambda_L = \{x \in \mathbb{Z}^d \;\; |0 \leq x_i \leq L_i\}$, furthermore let $\Lambda_{nL} = \{x \;\; |n_i L_i \leq x_i \leq (n_i+1)L_i\}$ then the family of regions $\{\Lambda_{nL}\}_{n\in\mathbb{Z}^d}$ forms a partitions of $\mathbb{R}^d$ or $\mathbb{Z}^d$. For each $\Lambda \in \mathbb{R}^d$ (or $\in \mathbb{Z}^d$) one define:

- $N^+(\Lambda)_L$ the number of sets Λ_{nL} such that $\Lambda_{nL} \bigcap \Lambda = \varnothing$
- $N^-(\Lambda)_L$ the number of sets Λ_{nL} such that $\Lambda_{nL} \subset \Lambda$

then the sets Λ tend to infinity in the sense of Van Hove if:

$$\lim_{N_L^- \to \infty} \frac{N_L^-}{N_L^+} = 1 \tag{3.1}$$

Let $|\Lambda|$ be the measure of $\Lambda \in \mathbb{R}^d$ and $\partial\Lambda_\rho = \{x \in \mathbb{R}^d \ \ |d(x, \partial\Lambda) \leq \rho\}$ where $d(x, \partial\Lambda)$ is a distance between a point x and $\partial\Lambda$ the contour of the set Λ, then the Van Hove convergence to infinity is equivalent to :

$$\lim_{|\Lambda| \to \infty} \frac{|\partial\Lambda_\rho|}{|\Lambda|} = 0$$

We will restrict our study from now on to quantum lattice systems, hence the system is defined on $\Lambda \in \mathbb{Z}^d$. Now we introduce some basic objects of thermodynamics and statistical mechanics, in particular the so called thermodynamic functions. Let $H_\Lambda : \mathbb{V} \to \mathbb{V}$ the selfadjoint Hamiltonian of the system with $\mathbb{V}$ the Hilbert space, furthermore the operator $e^{-\beta H_\Lambda}$ is a Trace class operator, hence if $O : \mathbb{V} \to \mathbb{V}$ an observable then one defines:

- **The equilibrium state:** The expectetion value of O is

$$< O >= \frac{1}{Z_\Lambda} \mathrm{Tr}(O e^{-\beta H_\Lambda}),$$

  then one defines $< \cdot >$ as equilibrium state and it is unique and it is invariant under all symmetry operators of the Hamiltonian, hence for Hamiltonians commuting with the traslations operator this state is traslation-invariant. This means that finite size systems do not have phase transitions or symmetry breaking. Furthermore the equilibrium state has the KMS (Kubo-Martin-Schwinger) property

$$< A(t)B^+(t') >=< B^+(t')A(t + i\beta) >=< B^+(t' - i\beta)A(t) >$$

  indeed

$$< A(t)B^+(t') >= \mathrm{Tr}\left(e^{-\beta H} A(t) B^+(t')\right) = \mathrm{Tr}\left(e^{-\beta H} e^{\beta H} B^+(t') e^{-\beta H} A(t)\right) =$$

$$= \left(e^{-\beta H} e^{i(-i\beta)H} B^+(t') e^{-i(-i\beta)H} A(t)\right) =< B^+(t' - i\beta)A(t) > .$$

  This periodicity in the imaginary time caracterizes the equilibrium states.

- **Energy density:** $u_\Lambda = \frac{1}{Z_\Lambda |\Lambda|} Tr(H_\Lambda e^{-\beta H_\Lambda})$

- **Helmotz free energy density:** $f_\Lambda(T, ..) = \frac{F(T, |\Lambda|, ...)}{|\Lambda|} = -\frac{1}{\beta} \frac{1}{Z_\Lambda |\Lambda|} \ln Z_\Lambda$

- **Gibbs free energy density:** If one introduce an external field h in the Hamiltonian such that $H \to H + \sum_{x \in \Lambda} h(x) O(x)$ where $O(x)$ is an observable, then the Partition function depends on $h(x)$. By differentiation respect to this parameter of the Helmotz free energy one has

$\frac{<O(x)>_h}{|\Lambda|} = \frac{\partial}{\partial h(x)} f_\Lambda(T,h)$. Then the order parameter $\phi_h(x) = \frac{<O(x)>_h}{|\Lambda|}$ depends by external field, hence one defines the Gibbs free energy as the Legendre transformation with respect to h that is

$$G_\Lambda(T,\phi_h) = g_\Lambda(T,\phi_h)|\Lambda| = |\Lambda| f(T,h) - \sum_{x\in\Lambda} h(x) < O(x) > .$$

By differentiation of $g_\Lambda(T,\phi_\Lambda)$ with respect to the order parameter one has:

$$h(x) = \frac{\partial}{\partial \phi_h(x)} g_\Lambda(T,\phi_h(x)). \tag{3.2}$$

In general one cosiders the Hamiltonian operators such that $H_\Lambda = \sum_{X\subset\Lambda} \Phi(X)$ where $\Phi(X)$ is a $|X|$ particles potential interaction and/or hopping in a subset X of the lattice Λ with finite range r, that is $\Phi(X) = 0$ if $diam(X) = sup_{x,y\in X}|x-y| > r$. Now we will prove a theorem due Griffiths Robinson and Ruelle:

Theorem 1: If the Hamiltonian is traslation invariant then the thermodynamic limit (Van Hove) of the thermodynamic potentials exist and they are finite.

Lemma1 Let A and B be two bounded and selfadjint operators and $||\cdot||$ the norm, then:

$$|\ln(Tr(e^A)) - \ln(Tr(e^B))| \leq ||A-B|| \tag{3.3}$$

proof: One defines the self-adjoint operator $O = tA + (1-t)B$ and $f(t) = \ln Tr(e^{O(t)})$ then:

$$|\ln(Tr(e^A)) - \ln(Tr(e^B))| = |f(1) - f(0)| = |\int_0^1 dt \frac{d}{dt} f(t)| =$$

$$= |\frac{1}{Tr(e^{O(t)})} Tr(\frac{d}{dt} O(t) e^{O(t)})| \leq ||\frac{d}{dt} O(t)||$$

where the inequality is due at the Eq.(8.2). Now if one defines two Hamiltonian with two interactions Φ_1 and Φ_2 then by Eq.(3.3) with $A = -\beta H_1$ and $B = -\beta H_2$, one has the following inequality for the free energy:

$$|F_\Lambda(T,\Phi_1,..) - F_\Lambda(T,\Phi_2..)| \leq ||\Phi_1 - \Phi_2||. \tag{3.4}$$

Furthermore by the Peierls-Bogoliubov theorem the free energy is a convex functions in Φ.

Proof of the theorem 1: In order to prove the theorem 1 one considers systems of increasing size $L_n = 2^n$ with $n \in \mathbb{N}$, hence $|\Lambda_n| = 2^{nd}$ where d is the dimensionality of the system. Correspondingly, the Free energy density is $f_n = -\frac{1}{\beta|\Lambda_n|} \ln(Tre^{-\beta H_{\Lambda_n}})$, hence the prove is obtained if one show that the sequence $\{f_n\}_{n\in\mathbb{N}}$ is a Couchy sequence, indeed in $\mathbb{R}$ any Couchy sequence is

convergent. For this, one divides the volume Λ_n into 2^d subdomains Λ_{n-1} and provide each domain with an inside margin of width r (the range of interaction in the Hamiltonian). This provide that each pair of internal subregions do not interact. Furthermore, in each sublattice, the Hamiltonian is $H_{\Lambda_{n-1}} = H^{<}_{\Lambda_{n-1}} + H^{>}_{\Lambda_{n-1}}$, where respectively $H^{<}_{\Lambda_{n-1}}$ and $H^{>}_{\Lambda_{n-1}}$ are the Hamiltonian operators in the internal and the margin of Λ_{n-1}, hence $H_{\Lambda_n} = \sum_{i=1}^{2^d}\{H^{(i)<}_{\Lambda_{n-1}} + H^{(i)>}_{\Lambda_{n-1}}\}$ (the index (i) indicates the $i-$sublattice). Then by inequality Eq.(3.3) one has:

$$|f_n - f_{n-1}| = |\frac{1}{\beta|\Lambda_n|}\ln(Tre^{-\beta H_{\Lambda_n}}) - \frac{1}{\beta|\Lambda_{n-1}|}\ln(Tre^{-\beta H_{\Lambda_{n-1}}})| =$$

$$= \frac{1}{\beta|\Lambda_n|}|\ln(Tre^{-\beta H_{\Lambda_n}}) - 2^d\ln(Tre^{-\beta H_{\Lambda_{n-1}}})|$$

but using Eq.(8.1) one has

$$2^d\ln(Tre^{-\beta H_{\Lambda_{n-1}}}) = \ln(Tre^{-\beta H_{\Lambda_{n-1}}})^{2^d} \geq \ln(Tre^{-2^d\beta H_{\Lambda_{n-1}}})$$

then

$$|f_n - f_{n-1}| \leq \frac{1}{2^{nd}}||H_{\Lambda_n} - 2^d H_{\Lambda_{n-1}}||$$

hence by traslational invariance of the Hamiltonian the theorem is proved.

3.2 Phase transitions and Spontaneous Symmetry Breaking

The phase transitions are formally the singular points of the free energy of the system that arise by thermodynamic limit, indeed, as we said any finite size system does not have phase transition and the free energy is an analytic function. This definition arises by thermodynamic considerations and the phase transitions can be classified according to the type of singular point of the free energy. In particular one defines:

Discontinuos or the first order phase transitions. If we define the chemical potential as $\mu = \frac{\partial}{\partial|\Lambda|}F(T, |\Lambda|, h, ...)$ where h is an external field, then the condition for a first-order phase transition is that the chemical potentials, of the two phases, must be equals

$$\Delta\mu = \mu_1(T, h, ...) - \mu_2(T, h, ...) = 0$$

whereas

$$\frac{\partial}{\partial T}\Delta\mu(T, h, ...) \neq 0 \qquad \frac{\partial}{\partial h}\Delta\mu(T, h, ...) \neq 0 \qquad \frac{\partial}{\partial ...}\Delta\mu(T, h, ...) \neq 0$$

so that the chemical potentials or the free energies cross at the transition. The phase with the lower chemical potential is stable and the other phase is metastable. By a microscopic point of view one has coexistence of phases if the thermodynamic limit of the Gibbs state is not unique but there are many equilibrium states sensible to the boundary conditions.

Continuous phase transitions. A transition is continuous when the chemical potentials of both phases are equal and when their first derivatives are also equal:

$$\Delta\mu = \mu_1(T, h, ...) - \mu_2(T, h, ...) = 0$$

and

$$\frac{\partial}{\partial T}\Delta\mu(T, h, ...) = 0 \quad \frac{\partial}{\partial h}\Delta\mu(T, h, ...) = 0 \quad \frac{\partial}{\partial ...}\Delta\mu(T, h, ...) = 0$$

so that the chemical potentials or the free energies have a common tangent at the transition. There is no latent heat in this type of transition and the Free Energy has a singular point in the second derivative (susceptibility χ), more precisely the susceptibility has a divergence to critical point. Instead of continuous transitions, some authors write about second order phase transitions. The phase transition can be studied by a point of view of the changing of symmetries of the system. Indeed, in a transition the number of local minimum states of the thermodynamic potentials is not constant with the temperature variations, that is, there is a unique infinite-volume Gibbs state for $T > T_c$ and two or more translation-invariant Gibbs measures for $T < T_c$ where one has coexistence of two or more phases. More precisely the Hamiltonian is invariant under a transformations belonging to a group $\mathcal{G}$, hence for each $U \in \mathcal{G}$ one has $[H, U] = 0$, whereas the equilibrium state does not have this symmetry, in particular there are many degenerate ground states and they are invariant under a subgroup of $\mathcal{G}$. Therefore there is an observable O such that $< U^+OU >=< O >= 0$ for $T > T_c$ whereas $< U^+OU > \neq < O > \neq 0$ for $T < T_c$. Since a symmetry is either absent or present, the two phases must be described by different functions of thermodynamic variables, which cannot be continued analytically across the critical point. Because of the reduction in symmetry, an additional parameter is needed to describe the thermodynamics of the low-temperature phase. This parameter is called the order parameter that, generally, is connected to the expectation value of the observable O. An example of this fact is th ferromagnetic transition in the isotropic Heisenberg model defined on the lattice $\Lambda \subset \mathbb{Z}^d$. If we consider interaction between spins relative at nearest sites, then the Hamiltonian operator of the system is:

$$H = -\sum_{x\in\Lambda,\delta} \vec{S}(x) \cdot \vec{S}(x + \delta)$$

where δ is an unit vector on lattice. The Hamiltonian is invariant for rotations in the spin space, whereas if one turn on an external magnetic field $\vec{B}$ this breaks explicitely this symmetry and the spins are all polarized in the direction of the field. Now, if the system has finite size and we turn off the magnetic field, then for each finite temperature we have that the magnetisation is zero always. On the other hand, if one turn off $\vec{B}$ after the thermodynamic limit then, below critical temperature, there is a spontaneous magnetisation $\vec{M} = \lim_{|\Lambda|\to\infty} \sum_{x\in\Lambda} \frac{<\vec{S}(x)>}{|\Lambda|} \neq 0$ and the equilibrium state has a preferred direction in space. Now we describe this fact in more precise terms. Then we

consider a finite size system described by Hamiltonian H_Λ invariant under spatial traslations and the unitary transformations $U \in \mathcal{G}$ where $\mathcal{G}$ is a group, then $[U, H] = 0$. Let O be an observable and if an external field h is introduced the Hamiltonian becomes $H_\Lambda \to H_\Lambda(h) = H_\Lambda - h\sum_{x\in\Lambda} O(x)$ then for each finite size lattice one has:

$$< O(x) >_{\Lambda,h} = \frac{Tr(O(x)e^{-\beta H_\Lambda(h)})}{Z_\Lambda(h)} =< O(x) >_{\Lambda,h} \neq 0 \tag{3.5}$$

furthermore one has always

$$\lim_{h\to 0} < O(x) >_{\Lambda,h} = 0$$

but, if there is a phase transition, a critical temperature T_c exists such that for $T < T_c$ one has:

$$\lim_{h\to 0} \lim_{|\Lambda|\to+\infty} < O(x) >_{\Lambda,h} \neq 0.$$

that is the infinite volume limit and vanishing external field limit does not commute for $T < T_c$. This because the Free energy has the first derivative discontinuous below critical temperature.

Now we consider some example.

Group $\mathbb{Z}^2$: A classical example is the forromagnetic Ising model:

$$H(\sigma, h) = -\sum_x \sigma(x)\sigma(x+\delta)$$

where $\sigma(x) : \Lambda \to [-1, 1]$ and Λ a two or more dimensional lattice. The symmetry group $\mathbb{Z}^2$ corresonds to the replacement $\sigma(x) \to -\sigma(x)$. As it is easy to prove for each finite size lattice, if one introduces an external field $H \to H(h) = H - h\sum_x \sigma(x)$ then $\lim_{h\to 0} < \sigma(x) >_{\Lambda,h} = 0$, but it is possible to prove that:

$$\lim_{h\to 0^+} \frac{\partial}{\partial h}(\lim_{|\Lambda|\to\infty} f_\Lambda(T, h)) = m > 0$$

$$\lim_{h\to 0^-} \frac{\partial}{\partial h}(\lim_{|\Lambda|\to\infty} f_\Lambda(T, h)) = -m < 0$$

Then below the critical temperature two phase coexist, sublattices with $< \sigma(x) >= 1$ and sublattices where $< \sigma(x) >= -1$. Therefore for $T > T_c$ the Gibbs potential has an unique ground state where $< \sigma(x) >= 0$, whereas at $T < T_c$ there are two equilibrium states sensible to the boundary conditions.

Continuous group: Let $\mathcal{G}$ a group such that for each $g(\theta) \in \mathcal{G}$, $g = e^{-i\theta_a T_a}$ with $a = 1, ..., n$, θ_a are the parameters and T_a are the group generators. The n matrices T_a fulfil the following commutation rules:

$$[T_a, T_b] = i f_{abc} T_c$$

where the group structure constants f_{abc} are completely antisymmetric under permutation of the indices. In a quantum representation $g(\theta) \to U(\theta) = e^{-i\theta_a G_a}$ where G_a (the charge operators) are the quantum representations of the group generators such that $[G_a, G_b] = if_{abc}G_c$. We can do the following considerations:

1. if $A(x)$ is a scalar representation of $\mathcal{G}$ then $U^+A(x)U = A(x)$ from which

$$[A(x), G_a] = 0 \tag{3.6}$$

for each a. Hence there are not reason for which $< A(x) >_\Lambda = 0$

2. if $A_i(x)$ a $\mathcal{G}$-vectorial representation then $U^+A_i(x)U = (e^{-i\theta_a T_a})_{ij}A_j(x)$. If we consider an infinitesimal $\mathcal{G}$-transformation $U = \hat{1} - i\theta_a G_a$ we obtain:

$$U^+A_i(x)U = A_i(x) - i\theta_a(T_a)_{ij}A_j(x)$$

in adjoint representation $(T_a)_{ij} = if_{abc}$ hence

$$[G_a, A_b(x)] = if_{abc}A_c(x). \tag{3.7}$$

Hence if U is an infinitesimal transformation we compute

$$< A_i(x) >_\Lambda = \frac{1}{Z_\Lambda}Tr(e^{-\beta H_\Lambda}A_i(x)) = \frac{1}{Z_\Lambda}Tr(e^{-\beta H_\Lambda}U^+A_i(x)U) =$$

$$= \frac{1}{Z_\Lambda}Tr(e^{-\beta H_\Lambda}A_i(x)) + i\theta_a\frac{1}{Z_\Lambda}Tr(e^{-\beta H_\Lambda}[G_a, A_i(x)]) =$$

$$= < A_i(x) >_\Lambda - \theta_a f_{aij}\frac{1}{Z_\Lambda}Tr(e^{-\beta H_\Lambda}A_j(x))$$

then we have $< A_i(x) >_\Lambda = 0$ for each finite size lattice.

3. if $B_{ij}(x)$ a 2-rank tensorial representation of $\mathcal{G}$ then

$$U^+B_{ij}(x)U = (e^{-i\theta_a T_a})_{ik}(e^{-i\theta_a T_a})_{jl}B_{kl}(x)$$

and the commutation rules with the generators are:

$$[G_a, B_{ij}(x)] = if_{aik}B_{kj}(x) + if_{ajl}B_{il}(x), \tag{3.8}$$

This representation is reducible, but it is possible to prove that $< B_{ij}(x) >_\Lambda = 0$ for each lattice Λ such that $|\Lambda| < \infty$ considering the irreducible representations.

These considerations can be generalized to k-rank tensorial representation of the group $\mathcal{G}$.

An important consequence of the spontaneous symmetry breaking is the correlation between operators relative to infinite spaced sites of lattice. Indeed, if SSB occurs one has Long Range Order, that is

$$\lim_{|x|\to\infty}\lim_{|\Lambda|\to\infty} < A(x)A(0) >_\Lambda = m \neq 0.$$

In a lattice system invariant under translations the correlation function dependes only by the coordinate difference of the sites on lattice, that is $< A(x)A(y) >= G(x-y) =< A(x-y)A(0) >$ and if $g(k)$ is the Fourier transformate then $g(k) =< A(k)A(-k) >$. Indeed one can write:

$$g(k) = \sum_{x\in\Lambda} e^{-ik\cdot x} < A(x)A(0) >= \sum_{x\in\Lambda} e^{-ik\cdot x} < A(x+y)A(y) >=$$

$$= \sum_{x\in\Lambda} e^{-ik\cdot(x-y)} < A(x)A(y) >= \sum_{x\in\Lambda,q,q'} \frac{e^{-ik\cdot(x-y)}e^{iq\cdot x}e^{iq'\cdot y}}{|\Lambda|} < A(q)A(q') >$$

from which:

$$g(k) = \sum_{q} e^{i(k+q)\cdot y} < A(k)A(q) >$$

Now, the first side of the previous equation is independent by y then we sum on y and divide by $|\Lambda|$ both side, obtaining

$$g(k) = \frac{1}{|\Lambda|}\sum_{y} g(k) =< A(k)A(-k) > .$$

Now we will prove the theorem:

Theorem: Let $M(x,y) =< O(x)O(y) >$ a square matrix of order $|\Lambda|$, if $M(x,y)$ has an eigenvalue of the order of $|\Lambda|$ then the system has Long Range Order.
Proof: The matrix $M(x,y)$ is an Hermitian matrix hence it is diagonalizable, furthermore, if its eigenvalues are $\{\lambda_i\}_{i=1}^{|\Lambda|}$ and $f_i(x)$ are the eigenvectors then:

$$M(x,y) = \sum_{i=1}^{|\Lambda|} \lambda_i f_i(x) f_i^*(y)$$

now the eigenvectors are normalized $||f_i||^2 = \sum_{x\in\Lambda} |f_i(x)|^2 = 1$ therefore they have a normalization constant $\sim O(\frac{1}{\sqrt{|\Lambda|}})$, furthermore if $\lambda_j = O(|\Lambda|) = \alpha|\Lambda|$ then we write:

$$M(x,y) = \frac{\alpha|\Lambda|}{|\Lambda|} f_j(x) f_j^*(y) + \sum_{i=1, i\neq j}^{|\Lambda|} \lambda_i f_i(x) f_i^*(y) \tag{3.9}$$

hence $\lim_{|x-y|\to\infty} \lim_{|\Lambda|\to\infty} < O(x)O(y) >= \alpha f_j(x) f_j^*(y) \neq 0$.

Theorem: For traslational invariant Hamiltonian the plane waves are eigenvectors of $M(x,y)$ and its Fourier coefficients are the eigenvalues.
Proof: The secolar equation is $\sum_y M(x-y)e^{ik\cdot y} = \lambda e^{ik\cdot x}$ hence by replacement $x' = x - y$ one obtains:

$$\sum_{y} M(x-y)e^{ik\cdot y} = e^{ik\cdot x}\sum_{x'} M(x')e^{-ik\cdot x'}$$

from which $\lambda = g(k)$. In this basis the Eq.(3.9) can be rewritten as:

$$< O(x)O(0) >_\Lambda = \sum_k \frac{1}{|\Lambda|} e^{ik\cdot x} g(k) = \frac{e^{ik^*\cdot x} g(k^*)}{|\Lambda|} + \sum_{k\neq k^*} \frac{1}{|\Lambda|} e^{ik\cdot x} g(k)$$

therefore in the thermodynamics limit

$$\lim_{|\Lambda|\to\infty} < O(x)O(0) >_\Lambda = \alpha e^{ik^*\cdot x} + \int \frac{d^d k}{(2\pi)^d} e^{ik\cdot x} g(k).$$

Therefore an Hamiltonian H has Long Range Order for the observable $O(x)$ if exist a vector of the reciprocal lattice k_j such that $g(k_j) = O(|\Lambda|)$, that is, the correlator has a divergence for some vector of the reciprocal lattice.

In the following theorem we prove that the Spontaneous Symmetry Breaking is equivalent to the Long Range Order condition. Indeed if we define the fluctuations of the order parameter as $(\Delta\phi))^2 =< (\phi - < \phi >)^2 >$ one has that $(\Delta\phi)^2 \geq 0$ hence $| < \phi > |^2 \leq < \phi^2 >$ and defining the order parameter $A = \sum_{x\in\Lambda} \frac{e^{iq^*\cdot x}}{|\Lambda|} A(x)$, in the thermodynamic limit one has:

$$(\sum_{x\in\Lambda} \frac{e^{iq^*\cdot x}}{|\Lambda|} < A(x) >)^2 \leq \frac{1}{|\Lambda|} \sum_{x\in\Lambda|} e^{iq^*\cdot x} < A(x)A(0) > \tag{3.10}$$

that is the maximum of the eigenvalue of the matrix $M(x-y)$ then one can write:

$$\lim_{h\to 0} \lim_{|\Lambda|\to\infty} (< A(x) >_{\Lambda,h})^2 \leq$$

$$\leq \lim_{|x|\to\infty} \lim_{|\Lambda|\to\infty} < A(x)A(0) >_{\Lambda,h=0} . \tag{3.11}$$

Therefore if the second side of the Eq.(3.11) is zero then also the order parameter vanishes. On the other hand if the order parameter is non-vanish then also the correlator is non-vanishing.

Theorem: One has spontaneous symmetry breaking if and only if

$$\lim_{|x|\to\infty} \lim_{|\Lambda|\to\infty} < O(x)O(0) >_\Lambda = \alpha \neq 0 \tag{3.12}$$

3.3 Inequalities

In the theory of the phase transitions the use of inequalities between traces and/or expectation value of operators has a natural application. In particular it is possible to find upper and/or lower bounds of the order parameters or correlators which allow to obtain rigorous results on absence or existence a Long Range Order in thermodynamic systems. Therefore we derive some of this inequalities by defining an opportune inner product and using the Schwartz inequality.

3.3.1 Indetermination Inequality

Theorem: Let $A, B : \mathcal{H} \to \mathcal{H}$ two arbitrary operators on Hilbert space $\mathcal{H}$, furthermore let $H : \mathcal{H} \to \mathcal{H}$ the Hamiltonian operator and $|0>$ the its ground state then

$$| < 0|[A, B]|0 > |^2 \leq < 0|[A^+, A]_+|0 >< 0|[B^+, B]_+|0 > \tag{3.13}$$

where $[,]$ and $[,]_+$ are, respectively, the commutator and the anticommutator between the two operators.
Proof: One defines an inner product between the operators A and B as $(A, B) =< 0|A^+B|0 >$ then one has:

$$| < 0|A^+B|0 > |^2 \leq < 0|A^+A|0 >< 0|B^+B|0 >$$

but

$$| < 0|[A^+, B]|0 > |^2 = | < 0|A^+B|0 > - < 0|B^+A|0 > |^2 \leq$$
$$\leq < 0|A^+A|0 >< 0|B^+B|0 > + < 0|AA^+|0 >< 0|BB^+|0 > +$$
$$+2\sqrt{< 0|A^+A|0 >< 0|BB^+|0 >< 0|AA^+|0 >< 0|B^+B|0 >}$$

by using $2\sqrt{ab} \leq |a| + |b|$ one proves the theorem.

3.3.2 Two point Duhamel function and Bogoliubov inequality

The order parameter is the first derivative of the Helmholtz Free energy respect to the external field h. The second derivative of $f(T, h)$ gives the susceptivity χ, then it is:

$$\chi = -\frac{\partial^2}{(\partial h)^2} f(T, h) = \frac{1}{\beta} \lim_{|\Lambda| \to \infty} \frac{1}{|\Lambda| \mathrm{Tr}(e^{-\beta H + \beta h O})} \frac{\partial}{\partial h} \mathrm{Tr}(e^{-\beta H + \beta h O} O)$$

Now, one knows that in general $\frac{d}{dh} e^{H(h)} \neq \frac{dH(h)}{dh} e^{H(h)}$, this because $\frac{dH(h)}{dh}$ and $H(h)$, in general, do not commute. Therefore one has:

$$\frac{d}{dh} e^{H(h)} = \int_0^1 dx e^{(1-x)H(h)} \frac{dH(h)}{dh} e^{xH(h)}. \tag{3.14}$$

By using Eq.(3.14) the susceptivity is the thermodynamic limit of the following function:

$$\chi = \frac{1}{|\Lambda|} \int_0^1 \frac{dx}{Z_\Lambda} \mathrm{Tr}(e^{-\beta(1-x)H(h)} O e^{-\beta x H(h)} O) \tag{3.15}$$

Then one defines the two points Duhamel function as

$$(A, B) = \int_0^1 \frac{dx}{Z} \mathrm{Tr}(e^{-(1-x)\beta H} A e^{-x\beta H} B), \tag{3.16}$$

it is easy to verify thet the Eq.(3.16) defines an inner product between two operators, then by the Schwartz inequality one obtains:

$$|(A^+, B)|^2 \leq (A^+, A)(B^+, B). \tag{3.17}$$

Now we give two important properties of the two points Duhamel function:

Lemma: Let $A : \mathcal{H} \to \mathcal{H}$ an operator, then:

$$(A^+, A) \leq \frac{1}{2} < A^+A + AA^+ > . \tag{3.18}$$

Proof: Indeed, writing explicitely the trace in Eq.(3.16) and inserting the identity operator $\hat{1} = \sum_\alpha |\alpha >< \alpha|$, where $|\alpha >$ are the eigenvectos of the Hamiltonian, one has:

$$(A^+, A) = \frac{1}{Z}\int_0^1 dx \sum_{\alpha\alpha'} e^{-(1-x)\beta E_\alpha} < \alpha|A^+|\alpha' > e^{-x\beta E_{\alpha'}} < \alpha'|A|\alpha >=$$

$$= \frac{1}{Z}\sum_{\alpha\alpha'}\int_0^1 dx e^{-\beta E_\alpha} e^{x\beta(E_\alpha - E_{\alpha'})} < \alpha|A^+|\alpha' >< \alpha'|A|\alpha >=$$

$$= \frac{1}{Z}\sum_{\alpha\alpha'} e^{-\beta E_\alpha}\frac{e^{-\beta(E_{\alpha'}-E_\alpha)} - 1}{\beta(E_\alpha - E_{\alpha'})} < \alpha|A^+|\alpha' >< \alpha'|A|\alpha >,$$

but knowing that the exponential function is a convex function one has the following uinequality

$$\frac{e^{-x\beta E_\alpha} - e^{-E_{\alpha'}}}{\beta(E_{\alpha'} - E_\alpha)} \leq \frac{\beta}{2}(e^{-\beta E_\alpha} + e^{-\beta E_{\alpha'}}),$$

then

$$(A^+, A) \leq \frac{1}{2Z}(\sum_{\alpha\alpha'} e^{-\beta E_\alpha} < \alpha|A^+|\alpha' >< \alpha'|A|\alpha > + \sum_{\alpha\alpha'} e^{-\beta E_{\alpha'}} < \alpha|A^+|\alpha' >< \alpha'|A|\alpha >) =$$

$$= \frac{1}{2} < A^+A + AA^+ > .$$

Lemma: For each A and B operators on the Hilbert space $\mathcal{H}$ the following equality holds:

$$< [A, B] >= \beta([A, H], B) \tag{3.19}$$

Proof: Writing the second side of the Eq.(3.19) in explicit way one has

$$\beta([A, H], B) = \frac{\beta}{Z}\sum_{\alpha\alpha'}\int_0^1 dx e^{-(1-x)\beta E_\alpha} < \alpha|[A, H]|\alpha' > e^{-x\beta E_{\alpha'}} < \alpha'|B|\alpha >$$

but $< \alpha|[A,H]|\alpha' >= (E_{\alpha'} - E_\alpha) < \alpha|A|\alpha' >$ hence

$$\beta([A,H],B) = \frac{1}{Z}\sum_{\alpha\alpha'} e^{-\beta E_\alpha} \int_0^1 dx e^{-x\beta(E_{\alpha'}-E_\alpha)} \beta(E_{\alpha'} - E_\alpha) < \alpha|A|\alpha' >< \alpha'|B|\alpha >$$

being, furthermore $e^{-x\beta(E_{\alpha'}-E_\alpha)}\beta(E_{\alpha'} - E_\alpha) = -\frac{d}{dx}e^{-x\beta(E_{\alpha'}-E_\alpha)}$ one obtains

$$\beta([A,H],B) = \frac{1}{Z}\sum_{\alpha\alpha'}(e^{-\beta E_\alpha} - e^{-\beta E_{\alpha'}}) < \alpha|A|\alpha' >< \alpha'|B|\alpha >=< [A,B] > .$$

Bogoliubov inequality for $T > 0$[1]: For each A and B arbitrary operators on the Hilbert space $\mathcal{H}$ the following inequality holds:

$$| < [A,B] > |^2 \leq \frac{\beta}{2} < [A^+,A]_+ > | < [B^+,[H,B]] > |, \tag{3.20}$$

proof: By Eq.(3.19) and Eq.(3.17) one has:

$$| < [A,B] > |^2 = |\beta([B,H],A)|^2 \leq (A^+,A)([H,B^+],[B,H])$$

but if one defines $C^+ = [H,B^+]$ then
$\beta([H,B^+],[B,H]) = ([B,H],C^+) = \beta < [B,C^+] >= \beta < [B,[H,B^+]] >$. Therefore by using the Eq.(3.18) the proof of the theorem is complete. The Bogoliubov inequality is a rigorous relation between two arbitrary operators A, B and the Hamiltonian H of the physical system. The its physical significance depends by choice of the operators involved, it holds at closely positive temperature, but it is possible to extend this result also at the ground state of the system ($T = 0$) where, in this case, the enegy gap play the role of the temperature. Hence we prove the following theorem:

Bogoliubov inequality for $T = 0$: Let two arbitrary operators $A, B : \mathcal{H} \to \mathcal{H}$ and $H : \mathcal{H} \to \mathcal{H}$ be the Hamiltonian of the system, if

$$\Delta = \inf_{\alpha\in(\sigma(H)-\{E_0\})} |E_\alpha - E_0| \neq 0$$

with $\sigma(H)$ is the spectrum of H and E_0 the energy on its ground state, then

$$| < 0|[A,B]|0 > |^2 \leq \frac{1}{\Delta} < 0|[A^+,A]_+|0 > | < 0|[B^+,[H,B]]|0 > |, \tag{3.21}$$

where $|0 >$ is the ground state of the Hamiltonian.
Proof: One defines the inner product as

$$(A|C) = \sum_{\alpha\in(\sigma(H)-\{E_0\})} \frac{1}{E_\alpha - E_0}(< 0|A^+|\alpha >< \alpha|C|0 > + < 0|A^+|\alpha >< \alpha|C|0 >)$$

then $(A|[H,B]) =< 0|[A^+,B]|0 >$ furthermore $(A|A) \leq \frac{1}{\Delta} < 0|[A^+,A]_+|0 >$ hence by Schwartz inequality one can write:

$$| < 0|[A^+,B]|0 > |^2 = |(A|[H,B])|^2 \leq (A|A)([H,B]|[H,B]) \leq$$

$$\leq \frac{1}{\Delta} < 0|[A^+, A]_+|0 >< 0|[[H, B]^+, B]|0 >$$

from which follows the theorem.

3.3.3 Falk Bruch Inequality

In Eq.(3.18) we give an upper bound of the two point Duhamel function, now we prove the existance of a lower bound of this function.

Theorem[2]: Let $f : [0, +\infty) \to (0, 1]$ such that $f(x \tanh x) = \frac{\tanh x}{x}$ then the following inequality holds[2]:

$$(A^+, A) \geq \frac{1}{2} < [A^+, A] > f(\frac{\beta < [A^+, [H, A]] >}{2 < [A^+, A] >}) \tag{3.22}$$

Proof: The function $f(x)$ is a convex and strictly monotone decreasing function, indeed if one define $g(x) = x \tanh x$ then $f(x) = \frac{\tanh(g^{-1}(x))}{g^{-1}(x)}$ with $f'(x) < 0$ and $f''(x) > 0$ for each $x \in [0, +\infty)$. Now we define the following variables:

$$b(A) = (A^+, A) \tag{3.23}$$

$$g(A) = \frac{1}{2} < [A^+, A]_+ > \tag{3.24}$$

$$c(A) = \beta < [A^+, [H, A]] > \tag{3.25}$$

$$h(x) = \frac{1}{Z}\mathrm{Tr}(e^{-(1-x)\beta H} A^+ e^{-x\beta H} A). \tag{3.26}$$

By differentiation of the Eq.(3.26) one has $h'(x) = \frac{\beta}{Z}\mathrm{Tr}((e^{-(1-x)\beta H}[H, A]e^{-x\beta H} A^+)$ hence

$$b(A) = \int_0^1 dx h(x) \quad g(A) = \tfrac{1}{2}(h(0) + h(1)) \quad c(A) = h'(1) - h'(0), \tag{3.27}$$

in Eq.(3.26) we write the trace in the basis $\{|\alpha >\}$ of the eigenvectors of the Hamiltonian and including the identity operator $\hat{1} = \sum_\alpha |\alpha >< \alpha|$ hence

$$h(x) = \frac{1}{Z}\sum_{\alpha\alpha'} e^{-\beta E_\alpha} e^{x\beta(E_\alpha - E_{\alpha'})} | < \alpha|A^+|\alpha > |^2$$

furthermore inserting $1 = \int dt \delta(t - \beta(E_\alpha - E_{\alpha'}))$ one has that $h(x) = \int d\mu(t) e^{xt}$ where

$$d\mu(t) = dt \frac{1}{Z}\sum_{\alpha\alpha'} e^{-\beta E_\alpha} | < \alpha|A^+|\alpha > |^2 \delta(t - \beta(E_\alpha - E_{\alpha'})). \tag{3.28}$$

The Eq.(3.28) defines a definite positive measure. The proof of the theorem is besed on the Jensen inequality that involves probability measures and convex

function, that is if $d\omega$ is a probability measure and $\phi(t)$ a convex function one has:

$$f(\int d\omega(t)\phi(t)) \leq \int d\omega(t)\phi(t). \tag{3.29}$$

Then one define a new measure $d\nu(t) = \frac{1}{2}(e^t + 1)d\mu(t)$ from which:

$$b(A) = \int d\nu(t)\frac{2}{t}\tanh\frac{t}{2} \quad g(A) = \int d\nu(t) \quad c(A) = 4\int d\nu(t)\frac{t}{2}\tanh\frac{t}{2},$$

hence $d\omega(t) = \frac{d\nu(t)}{g(A)}$ is a probability measure, furthermore being $f(x)$ convex one has:

$$g(A)f(\frac{c(A)}{4g(A)}) = g(A)f(\int d\omega\frac{t}{2}\tanh\frac{t}{2}) \leq g(A)\int d\omega f(\frac{t}{2}\tanh\frac{t}{2}) =$$

$$= g(A)\int d\omega\frac{2}{t}\tanh\frac{t}{2} = b(A)$$

Corollary: Let $b \geq gf(\frac{c}{4g})$ with $f : [0, +\infty) \to (0, 1]$ a function such that $f(x\tanh x) = \frac{\tanh x}{x}$. If there are two quantities B and C such that $b \leq B$ and $c \leq C$ then

$$g \leq \frac{1}{2}\sqrt{BC}\coth(\sqrt{\frac{C}{4B}}) \tag{3.30}$$

Proof: We define G such that $B = Gf(\frac{C}{4G})$, if we suppose that $g \geq G$ hence $\frac{c}{4g} \leq \frac{C}{4G}$, but $f(x)$ is strictly decreasing then $b > B$ and this is in contrast with the ipothesis. Now if one defines $\frac{C}{4G} = x\tanh x$ then $\frac{B}{G} = \frac{\tanh x}{x}$ hence the inequality in Eq.(3.30).

3.3.4 Reflection Positivity

In this section we consider certain interactions which satisfy a positivity property called reflection positivity. This concept was introduced in quantum field theory Osterwalder and Schrader[3] and it has continued to play an important role, in particular in the theory of the phase transitions[4, 6, 7, 8, 10]. This property can only be formulated for lattices which have a certain reflection invariance. For simplicity we only consider simple, cubic lattices. In the language of a mathematical physicist reflection positivity expresses the existence of a self adjoint transfer matrix. In more general case let H a many-body Hamiltonian defined on a lattice and $\mathcal{M}$ is a set of all relevant operators of the system, and we assume that this set is an algebra with the operations of addition, complex scalar multiplication and operator product. In several cases, this algebra can be written as the direct product of two subalgebras and an isomorphism Θ between these subalgebras can also be introduced. More precisely we consider an arbitrary Hermitean polynomial Hamiltonian $H : \mathcal{H} \to \mathcal{H}$, wehre the Hilbert space has the form of tensorial product of two subspace $\mathcal{H} = \mathcal{H}_+ \otimes \mathcal{H}_-$ furthermore let $\mathcal{M}_\pm$ the subalgebras $\mathcal{M}_\pm = \{F \ \ |F : \mathcal{H}_\pm \to \mathcal{H}_\pm\}$ and Θ an isomorphism between $\mathcal{M}_+$ and $\mathcal{M}_-$ such that for each $F \in \mathcal{M}_-$

- $\Theta^2 = \hat{1}$
- $< F\Theta(F)^* > \geq 0$

then the Gibbs state $< \cdot >$ is called reflection positive. Here * is the complex conjugation. In Classical and Quantum Lettice systems this propriety is used to prove the existence of the Long Range Order, in these case one assumes periodic boundary conditions so that the lattice $\Lambda \subset \mathbb{Z}^d$ is equivalent to a d-dimensional torus . If the number of sites along a specified direction is even, then it exists a plane P orthogonal to this direction that divides the lattice Λ in two sublattices Λ^+ and Λ^- such that $\Lambda = \Lambda^+ \cup \Lambda^-$, and $\Lambda^+ \cap \Lambda^- = 0$. For instance, for a direction along the x-axis, we have

$$\begin{aligned} \Lambda &= \{x \in \mathbb{Z}^d \ \ | -L+1 \leq x_i \leq L, i = 1...d\}, \\ P &= \{x \in \mathbb{R}^{d-1} \ \ | x_1 = \frac{1}{2}\}, \\ \Lambda^+ &= \{x \in \mathbb{Z}^d \ \ | -L+1 \leq x_1 \leq 0\}, \\ \Lambda^- &= \{x \in \mathbb{Z}^d \ \ | 1 \leq x_1 \leq L\}, \end{aligned} \tag{3.31}$$

L being the number of lattice sites.
Thus, it is possible to define an idempotent one to one mapping θ between Λ^+ and Λ^- such that:

$$\theta(x)_k = \{ \begin{array}{ll} x_k & \text{if } k \neq 1 \\ 1 - x_1 & \text{if } k = 1 \end{array} \tag{3.32}$$

and the ensemble Λ_P, a sublattice of sites of Λ, that lies on a plane located on the left of P plane and parallel to it,

$$\Lambda_P = \{x \in \Lambda \ \ | x_1 = 0\}. \tag{3.33}$$

Therefore, P is a empty ensemble whereas Λ_P is not empty.
Next, we define a mapping χ between operators on the two sublattices such that

$$\Theta(O(x)) = G^+ O(\theta(x)) G,$$

for any operator $O(x)$, with $x \in \Lambda^+$, $\theta(x) \in \Lambda^-$; G is a suitable unitary operator. The reflection positivity condition corresponds to the definition of the definite positive inner product between two operators relative to two sublattices. More precisely, the Hilbert space of the Hamiltonian model is the tensorial product of two subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$ associated with two sublattices and for each $A : \mathcal{H}^+ \to \mathcal{H}^+$, $\Theta(A) : \mathcal{H}^- \to \mathcal{H}^-$, hence for each pair of operators $A, B : \mathcal{H}^+ \to \mathcal{H}^+$ one can define an positive inner product between A and B as:

$$(A|B) =< A\Theta(B) > .$$

Therefore, by the Schwartz inequality one has that for each $A, B \in \mathcal{M}^+$, where $\mathcal{M}^+$ and $\mathcal{M}^-$ the corresponding subalgebras operators to the two subblettices, the following inequality:

$$| < A\Theta(B) > | \leq (< A\Theta(A) >)^{\frac{1}{2}} (< B\Theta(B) >)^{\frac{1}{2}}. \tag{3.34}$$

Lemma: For each $A \in \mathcal{M}^+$ one has $\mathrm{Tr}(A\Theta(A)) \geq 0$.
Proof: Indeed

$$\mathrm{Tr}(A\Theta(A)) = \mathrm{Tr}_{\Lambda_+}(A) Tr_{\Lambda_-}(\Theta(A)) = |\mathrm{Tr}_{\Lambda_+}(A)|^2 \geq 0$$

Theorem: If the Hamiltonian of the system has the form:

$$H = A \otimes \hat{1} + \hat{1} \otimes \Theta(A)^* - \sum_{i=1}^{p} B_i \otimes \Theta(B_i)^* \,, \tag{3.35}$$

where $A, B_i \in \mathcal{M}^+$ then the Gibbs state is reflection positive.
Proof: We consider $F \in \mathcal{M}^+$ and compute the thermal expectation value:

$$< F\Theta(F) >= \frac{1}{Z}\mathrm{Tr}(e^{-\beta H} F\Theta(F)) =$$

$$= \frac{1}{Z}\mathrm{Tr}(e^{-\beta(A\otimes\hat{1}+\hat{1}\otimes\Theta(A)^* - \sum_{i=1}^{p} B_i\otimes\Theta(B_i)^*)} F\Theta(F)^*).$$

The Hamiltonian, by redefinition of A, can be transformed as follows:

$$H = A \otimes \hat{1} + \hat{1} \otimes \Theta(A)^* + \frac{1}{2}\sum_{i=1}^{p}(B_i - \Theta(B_i)^*)^2 \tag{3.36}$$

then, by using the Trotter formula, one has

$$< F\Theta(F) >= \lim_{n\to\infty} a_n$$

where the sequence a_n is:

$$a_n = \frac{1}{Z}\mathrm{Tr}(F\Theta(F)^*\{e^{-\beta\frac{A}{n}} e^{-\beta\frac{\Theta(A)^*}{n}} \prod_{i=1}^{p} e^{-\beta\frac{(B_i - \Theta(B_i)^*)^2}{2n}})\}^n) \tag{3.37}$$

but using the Hubbard Stratonovic transformation

$$e^{-F^2} = \int_{-\infty}^{+\infty} \frac{dq}{\sqrt{4\pi}} e^{-\frac{q^2}{4} + iqF} \tag{3.38}$$

we write:

$$a_n = \frac{1}{Z}\mathrm{Tr}(F\Theta(F)^*\{e^{-\beta\frac{A}{n}} e^{-\beta\frac{\Theta(A)^*}{n}} \int_{\mathbb{R}^p} \frac{d^p q e^{-\frac{\sum_i q_i^2}{4}}}{(4\pi)^{\frac{p}{2}}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_i B_i} e^{-i\sqrt{(\frac{\beta}{2n})}q_i \Theta(B_i)^*}\}^n)$$

and, observing that $(\int dq(..))^n = \prod_{i=1}^n \int dq_i (...)_i = \int d^n q \prod_i (...)_i$, we have:

$$a_n = \frac{1}{Z}\mathrm{Tr}(F\Theta(F)^* \int d\mu \prod_{l=1}^{n} e^{-\beta\frac{A}{n}} e^{-\beta\frac{\Theta(A)}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_i B_i} e^{-i\sqrt{(\frac{\beta}{2n})}q_i \Theta(B_i)^*})$$

where the measure $d\mu$ is defined as

$$d\mu = \frac{d^{np}q}{(4\pi)^{\frac{np}{2}}} \prod_{i=1}^{p}\prod_{l=1}^{n} e^{-\frac{q_{il}^2}{4}} \tag{3.39}$$

then

$$a_n = \frac{1}{Z}\int d\mu \mathrm{Tr}(F\Theta(F)^* \prod_{l=1}^{n} e^{-\beta\frac{A}{n}} e^{-\beta\frac{\Theta(A)}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_i B_i} e^{-i\sqrt{(\frac{\beta}{2n})}q_i\Theta(B_i)^*}) =$$

$$= \frac{1}{Z}\int d\mu \{\mathrm{Tr}_{\Lambda_+}(F\prod_{l=1}^{n} e^{-\beta\frac{A}{n}} \prod_{i=1}^{p} e^{-i\sqrt{(\frac{\beta}{2n})}q_i B_i})\}^2 \geq 0$$

where we used tha condition that each operator in $\mathcal{M}_+$ commute with any operator in $\mathcal{M}_-$.

Gaussian Domination theorem: Let an Hamiltonian operator of the form (3.35) with the additional condition that the all B_i operators are real (that is $B_i^* = B_i$) then one has:

$$Z(h) = \mathrm{Tr}(e^{-\beta(A\otimes\hat{1}+\hat{1}\otimes\Theta(A)^*+\frac{1}{2}\sum_{i=1}^{p}(B_i-\Theta(B_i)-h_i)^2)}) \leq Z(h=0) \tag{3.40}$$

where h_i with $i = 1, ..., p$ are real number, physically it is an external field. **Proof:** one follows the same procedure used in the previous theorem. Indeed by Trotter formula one writes $Z(h)$ as limit of a sequence $\{a_n\}_{n=0}^{+\infty}$ where the general term a_n is:

$$a_n = \mathrm{Tr}((e^{-\beta\frac{A}{n}} e^{-\beta\frac{\Theta(A)}{n}} \prod_{i=1}^{p} e^{-\beta\frac{(B_i-\Theta(B_i)-h_i)^2}{2n}}))^n))$$

from which, using the Hubberd Stratonovic transformation, after some step one has:

$$a_n = \int d\mu \prod_{l=1}^{n} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}h_i} Tr(e^{-\beta\frac{A}{n}} e^{-\beta\frac{\Theta(A)}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_i B_i} e^{-i\sqrt{(\frac{\beta}{2n})}q_i\Theta(B_i)}) =$$

$$= \int d\mu \prod_{l=1}^{n} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}h_i} Tr^{(+)}(e^{-\beta\frac{A}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}B_i}) \prod_{j=1}^{n} Tr^{(-)}(e^{-\beta\frac{\Theta(A)}{n}} \prod_{i=1}^{p} e^{-i\sqrt{(\frac{\beta}{2n})}q_{ij}\Theta(B_i)}). \tag{3.41}$$

Now an inner product can be defined $(f|g) = \int d\mu f(q)g^*(q)$, hence if we define the two function f and g as

$$f(q) = \prod_{l=1}^{n} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}h_i} \mathrm{Tr}^{(+)}(e^{-\beta\frac{A}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}B_i})$$

$$g(q) = \prod_{j=1}^{n} \mathrm{Tr}^{(-)}(e^{-\beta\frac{\Theta(A)}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_{ij}\Theta(B_i)}) = \prod_{l=1}^{n} \mathrm{Tr}^{(+)}(e^{-\beta\frac{A}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}B_i})$$

then using the Schwartz inequality we have that $a_n \leq |a_n| = |(f|g)| \leq \sqrt{(f|f)(g|g)}$, but it is easy to prove that $(f|f) = (g|g)$ from which

$$a_n \leq (f|f) = \int d\mu \prod_{l=1}^{n} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}h_i} Tr^{(+)}(e^{-\beta\frac{A}{n}} \prod_{i=1}^{p} e^{i\sqrt{(\frac{\beta}{2n})}q_{il}B_i}). \tag{3.42}$$

Now following step by step backward the procedure one proves that the second side of the Eq.(3.42) is equal to $Z(h = 0)$. Therefore the ineqality (3.40) is proved. We notice that the index i in Eq.(3.40) can be an enumeration of operators but it can indicate also the sites of the lattice. Then, in this case, the Hamiltonian is:

$$H = H_+ \otimes \hat{1} + \hat{1} \otimes \Theta(H_+) - \sum_{x\in\Lambda, i=1}^{p} (B_i(x)\Theta(B_i(x)))^2 \tag{3.43}$$

Gaussian Domination theorem II: Let H be an Hamiltonian operator of the type:

$$H(h) = A + \Theta(A)^* + \sum_{a=1}^{n}(B_a - \Theta(B_a) - h_a)^2 - \sum_{b=1}^{m}(D_b - \Theta(D_b))^2 \tag{3.44}$$

where the operators $\{B_a\}_{a=1}^n$ are real hence $B_a^* = B_a$ whereas the operators $\{D_b\}_{b=1}^m$ are purely imaginary, that is $D_b^* = -D_b$, then one has the following inequality:

$$Z(h) = \mathrm{Tr}(e^{-\beta H(h)}) \leq \mathrm{Tr}(e^{-\beta H(h=0)}) = Z(0). \tag{3.45}$$

Proof: The proof follows the same steps of the previous theorem, but the Hubbard Stratonovic Eq.(3.38) for imaginary operators is:

$$e^{D^2} = \int_{-\infty}^{+\infty} \frac{dq}{\sqrt{4\pi}} e^{-\frac{q^2}{4}+qD}. \tag{3.46}$$

In Classical and Quantum systems defined on lattice the Gaussian domination theorem has an important corollary that we will use.

Corollary 1: Let H be an Hamiltonian operator of a system defined on lattice $\Lambda \subset \mathbb{Z}^d$, let G be an unitary operator such that G^+HG has the form (3.43) and $\{h_{il}(x) \quad | x \in \Lambda, i = 1, ..., p, \quad l = 1, ..., d\}$ with $h_{il}(x) \in \mathbb{R}$, furthermore let $\Theta(O(x)) = O(\theta(x))$. If one defines the divergence on lattice as $\partial_l h_{il}(x) = \sum_l h_{il}(x + \delta_l) - h_{il}(x)$, then the following inequality holds:

$$\frac{\mathrm{Tr}(e^{-\beta(G^+HG - \sum_{x\in\Lambda i=1}^{p}\sum_{l=1}^{d}\partial_l h_{il}(x)B_i(x))})}{\mathrm{Tr}(e^{-\beta H})} \leq e^{\frac{\beta||h||^2}{2}} \tag{3.47}$$

where $l = 1, ..., d$ whereas $||h||^2 = \sum_{x\in\Lambda i=1}^{p} |h_i(x)|^2$ in which $h_i(x) = \sum_{l=1}^{d} h_{il}(x)$.
Proof: The proof of the theorem uses the result of the Gaussian Domination theorem. The first step is to fix the reflection plane P orthogonal to x_1 axis, therefore the Hamiltonian has the form (3.36) and contains a term with the external field $h_i(x)$ as follows:

$$G^+HG = H_+(h)\otimes\hat{1} + \hat{1}\otimes\Theta(H_+(h)) + \frac{1}{2}\sum_{x\in\Lambda_P, i=1}^{p}(B_i(x) - \Theta(B_i(x))^*)^2 -$$

$$- \sum_{x\in\Lambda_P,i}\sum_{l=1}^{d} h_{il}(x)(B_i(x) - B_i(x-\delta_l)))^*) + \frac{1}{2}\sum_{x\in\Lambda,i}\sum_{l=1}^{d}|h_{il}(x)|^2 - \frac{1}{2}\sum_{x\in\Lambda,i}\sum_{l=1}^{d}|h_{il}(x)|^2 =$$

$$= H'_+(h)\otimes\hat{1} + \hat{1}\otimes\Theta(H'_+(h)) + \frac{1}{2}\sum_{x\in\Lambda_P,i=1}^{p}(B_i(x) - \Theta(B_i(x))^* - h_{i1}(x))^2 - \frac{1}{2}\sum_{x\in\Lambda,i}\sum_{l=1}^{d}|h_{il}(x)|^2.$$

The Hamiltonian has the same form of Eq.(3.36) hence we can write:

$$Tr(e^{-\beta(G^+HG - \sum_{x\in\Lambda i=1}^{p}\sum_{l=1}^{d}\partial_l h_{il}(x)B_i(x))}) = e^{\frac{\beta}{2}||h||^2}Z(h)$$

where the partition function is defined as in Eq.(3.40). Then by the Gaussian domination theorem one has:

$$|Z(h)|^2 \leq Z(h_{(+)})Z(h_{(-)}) \tag{3.48}$$

with

$$h_{(-)i}(x) = \{ \begin{array}{cc} h_i(x) & \text{if } x\in\Lambda_- - \Lambda_P \\ 0 & \text{if } x\in\Lambda_P \\ h_i(\theta(x)) & \text{if } x\in\Lambda_+ \end{array} ,$$

and similarly

$$h_{(+)i}(x) = \{ \begin{array}{cc} h_i(x) & \text{if } x\in\Lambda_+ \\ 0 & \text{if } x\in\Lambda_P \\ h_i(\theta(x)) & \text{if } x\in\Lambda_- - \Lambda_p \end{array} .$$

We notice that $h_{(\pm)i}(x)$ have a number of equal zero components larger than $h_i(x)$, this property allows us to state that if the inequality Eq.(3.48) is true, then $Z(h)$ is maximum when $h_i(x) = 0$ for each $x \in \Lambda$.
Indeed, let us suppose that $Z(h)$ is maximum for a specified value $h = h_{max}$; if this maximum value is assumed at more than one point of the lattice we may select the point with the largest number of h's components equal to zero. Then, by inequality Eq.((3.48)), we know that there is an other point of maximum for $Z(h)$ with larger number of vanishing components in contradiction with the hypothesis. Therefore, h_{max} must be identically zero, therefore the inequality in Eq.(3.47) holds.
Now we shift the external field as $h_i(x) \to \lambda h_i(x))$, where λ is a constant, therefore, in Eq.(3.47), the first side is a function of λ and $f(\lambda) \leq e^{\frac{\lambda^2\beta}{2}\sum_{x\in\Lambda,il=1}^{p}(h_{il}(x))^2}$.

Performing a Taylor expansion of both sides of the Eq.(3.47) and noticing that$f(0) = 1$ and $\frac{d}{d\lambda} f(\lambda)|_{\lambda=0} = 0$, we get:

$$f(0) + \frac{\lambda^2}{2} f''(0) + O(h^3) \leq 1 + \frac{\lambda^2 \beta}{2} \sum_{x \in \Lambda, il=1}^{p} (h_{il}(x))^2 + O(h^4)$$

$$(\frac{dO}{d\lambda}, \frac{dO}{d\lambda}) \leq \beta \sum_{x \in \Lambda, il=1}^{p} h_{il}^2(x)\,, \tag{3.49}$$

where $O(\lambda) = -\beta H + \lambda\beta \sum_{x\in\Lambda, i=1}^{p} \sum_{l=1}^{d} \partial_l h_{il}(x) B_i(x)$. The Eq.(3.49) holds for h such that any its component is real. Now we observe that for each A and B complex we have:

$$(A, B) = (\mathrm{Re}A, \mathrm{Re}B) + (\mathrm{Im}A, \mathrm{Im}B) \tag{3.50}$$

where $\mathrm{Re}P$ and $\mathrm{Im}P$ are, respectively, the Real part and Imaginary part of the operator P. Therefore the inequality Eq.(3.49) holds separately for Real and Imaginary part of the involved quantitities. The choice of the h function is arbitrary and depeds by physical system, typically the Eq.(3.47) is used to obtain an upper bound on the susceptivity $\chi_{ij}(q) = (B_i(q), B_j(-q))$, in this case we choose $h_{il}(x) = h_i(e^{-iq\cdot(x-\delta_l)} - e^{-iq\cdot x})$, hence $O(\lambda) = -\beta H + 2\lambda\beta \sum_{i=1}^{p} h_i B_i(q) E_-(q)$ where $E_-(q) = \sum_{l=1}^{d}(1 - \cos q_l)$ and h_i are constants, furthermore, by Eq.(3.49), we have the following inequality:

$$2\beta E_-(q) \sum_{ij=1}^{p} h_i h_j (B_i(q), B_j(-q)) \leq |\Lambda| \sum_{i=1}^{p} h_i^2,$$

but taking $h_i = \delta_{i1}$ or $h_i = \delta_{i2}$ or...$h_i = \delta_{ip}$ we have:

$$(B_i(q), B_i(-q)) \leq \frac{|\Lambda|}{2\beta E_-(q)}. \tag{3.51}$$

In Eq.(3.51) the two point Duhamel function is computed using the Hamiltonian $G^+ H G$ hence, returning, to H we write:

$$(G^+ B_i(q) G, G^+ B_i(-q) G) \leq \frac{|\Lambda|}{2\beta E_-(q)}. \tag{3.52}$$

The plane P is arbitrary, furthermore the Schwartz inequality (3.34) can be used an arbitrary number of times hence one can obtain an its disseminates version (a type of Holder inequality).

Chessboard estimation: Under the hypoyhesis of the previous theorem, given
$A : \mathcal{H} \to \mathcal{H}$ an osservable and T_x the traslation operator such that $T_x^+ A(y) T_x = A(x + y)$ then for each $x \in \Lambda$ the following inequality holds:

$$| < \prod_{x\in\Lambda} A(x) >_\Lambda | \leq \prod_{x\in\Lambda} (< \prod_{y\in\Lambda} (T_y^+ A(x) T_y) >_\Lambda)^{\frac{1}{|\Lambda|}}. \tag{3.53}$$

Proof: We do reference to the convention (3.31), (3.32) and (3.33), with periodic boundary condition and, for convenience, we take $L_i = 2^p$ for each $i = 1, ..., d$ where $p \in \mathbb{N}$. As the first step we consider two reflection planes, the plane P_1 is defined as in Eq.(3.32) whereas P_2 is shifted of 2^{p-2} sites respect to P_1, hence they divide the lattice in four sublattices and the operator algebra in four subalgebras. Now if we consider four operators belonging to the four subalgebras $A_1(1), A_2(2), A_3(3), A_4(4)$ and the correspondent shifted operators $A_i(1), A_i(2), A_i(3), A_i(4)$ with $i = 1, ..., 4$. Then the iterated Schwartz inequality gives the following result:

$$| < A_1(1)A_2(2)A_3(3)A_4(4) >_\Lambda | = | < A_1(1)A_2(2)\Theta_1(A_3(2))\Theta_1(A_4(1)) >_\Lambda | \leq$$

$$\leq (< A_1(1)A_2(2)\Theta_1(A_1(1))\Theta_1(A_2(2)) >_\Lambda)^{\frac{1}{2}}(< A_3(2)A_4(1)\Theta_1(A_3(2))\Theta_1(A_4(1)) >_\Lambda)^{\frac{1}{2}} =$$

$$= (< A_1(1)\Theta_1(A_1(1))A_2(2)\Theta_1(A_2(2)) >_\Lambda)^{\frac{1}{2}}(< A_3(2)\Theta_1(A_3(2))A_4(1)\Theta_1(A_4(1)) >_\Lambda)^{\frac{1}{2}} \leq$$

$$\leq (< A_1(1)\Theta_1(A_1(1))\Theta_2(A_1(1))\Theta_2(\Theta_1(A_1(1))) >_\Lambda)^{\frac{1}{4}} \times$$

$$\times (< A_2(2)\Theta_1(A_2(2))\Theta_2(A_2(2))\Theta_2(\Theta_1(A_2(2))) >_\Lambda)^{\frac{1}{4}} \times$$

$$\times (< A_3(2)\Theta_1(A_3(2))\Theta_2(A_3(2))\Theta_2(\Theta_1(A_3(2))) >_\Lambda)^{\frac{1}{4}} \times$$

$$\times (< A_4(1)\Theta_1(A_4(1))\Theta_2(A_4(1))\Theta_2(\Theta_1(A_4(1))) >_\Lambda)^{\frac{1}{4}}.$$

But being for example $\Theta_1(A_1(1)) = A_1(2)$, $\Theta_2(A_1(1)) = A_1(4)$ and $\Theta_2(\Theta_1(A_1(1))) = A_1(3)$, hence we have that:

$$| < A_1(1)A_2(2)A_3(3)A_4(4) >_\Lambda | \leq (< A_1(1)A_1(2)A_1(3)A_1(4) >_\Lambda)^{\frac{1}{4}} \times$$

$$\times (< A_2(1)A_2(2)A_2(3)A_2(4) >_\Lambda)^{\frac{1}{4}} (< A_3(1)A_3(2)A_3(3)A_3(4) >_\Lambda)^{\frac{1}{4}} \times$$

$$\times (< A_4(1)A_4(2)A_4(3)A_4(4) >_\Lambda)^{\frac{1}{4}}.$$

This procedure can be iterated and in general one can consider a generic reflection mapping $\theta^{(l)}$ with respect to P_l plane as:

$$\theta^{(l)}(x)_k = \{ \begin{array}{ll} x_k & \text{if } k \neq 1 \\ 2l - 1 - x_1 & \text{if } k = 1 \end{array} \tag{3.54}$$

we can take l such that $\leq l < 2^p$, that is a plane for each bond between two sites on lattice obtaining the inequality:

$$| < \prod_{i=1}^{2^p} A_i(x_i^{(1)}) >_\Lambda | \leq \prod_{i=1}^{2^p} (< \prod_{j=1}^{2^p} A_j(x_i^{(1)}) >_\Lambda)^{\frac{1}{2^p}}. \tag{3.55}$$

In Eq.(3.55) we considered all the planes P_i with $i = 1, ..., 2^p$ orthogonal to the $x^{(1)}$ direction, hence repeating the argument in the other $d - 1$ directions one has

$$| < \prod_{i=1}^{|\Lambda|} A_i(x_i) >_\Lambda | \leq \prod_{i=1}^{|\Lambda|} (< \prod_{j=1}^{|\Lambda|} A_i(x_j) >_\Lambda)^{\frac{1}{|\Lambda|}},$$

if one has a single operator $A(x)$ depending by site on lattice one has the result in Eq.(3.53). The Eq.(3.53) is used in the Infrared method and in the Peierls Argument in order to estimete the Contour weight.

3.4 Infrared Bound Method

If in a translation-invariant model there is a phase transition then we can prove the existence rigorously if some inequality is fulfilled, in particular if there is a k^* belonging to the first zone of Brillouin such that the correspondent Fourier component deverge in the thermodynamic limit, in such case the Fourier transformate, in the thermodynamics limit, has the form:

$$g(k) =< B(k)B(-k) >= g'(k) + m^2\delta(k-k^*)$$

hence the system has Long Range Order with order parameter $m^2 = \lim_{|\Lambda|\to\infty} < (\sum_{x\in\Lambda} B(x))^2 >$. The goal of the Infrared Bound Method is to prove that $m^2 > 0$ at low temperature. Therefore, in a general theory, we consider a system with Hamiltonian H where H is invariant under transformation $U = e^{i\theta_a Q_a}$ belonging a Group $\mathcal{G}$ where Q_a with $a = 1, ..., N$ are the generators of the group, furthermore $\{Q_a\}$ fulfil the following commutation rules:

$$[Q_a, Q_b] = if_{abc}Q_c.$$

We suppose that, for example, B_a is a vectorial order parameter, hence:

$$[Q_a, B_a] = if_{abc}B_c.$$

We suppose that the Fourier Transformate of the correlator

$$g(k) \leq f(k) \tag{3.56}$$

and that there exist an wave vector k^* such that $\lim_{k\to k^*} f(k) = +\infty$. This is a condition to prove the existence of the phase transition, now we find another condition. If the B_a operator is bounded then we have the condition:

$$\sum_{x\in\Lambda,a=1}^{N} \frac{< B_a(x)B_a(x) >}{|\Lambda|} = \frac{1}{Z|\Lambda|}\sum_{x\in\Lambda,a=1}^{N} Tr(e^{-\beta H}B_a(x)B_a(x)) =$$

$$= \frac{1}{Z|\Lambda|}\sum_{x\in\Lambda,a=1}^{N}\sum_{\alpha} e^{-\beta E_\alpha} < \alpha|B_a(x)B_a(x)|\alpha >= \frac{1}{Z}\sum_{\alpha} e^{-\beta E_\alpha}||B_a(x)|\alpha > ||^2 \leq ||B||^2.$$

then there exist a positive constant M such that the Parseval identity holds:

$$\sum_{x\in\Lambda,a=1}^{N} \frac{< B_a(x)B_a(x) >}{|\Lambda|} = \sum_{a=1}^{N} < (B_a(0))^2 >= M, \tag{3.57}$$

where we used the translation-invariant of the Hamiltonian and the quantity $||B||$ is the norm of the $B_a(x)$ operator. The Eq.(3.57) is an example of sum rule and it together with the Eq.(3.56) forms a pair of conditions necessary to

prove the existance of the phase transition. Indeed by the Eq.(3.57) one can write

$$M = \sum_{x\in\Lambda,a=1}^{N} \frac{< B_a(x)B_a(x) >}{|\Lambda|} = \sum_{k\in BZ,a=1}^{N} \frac{1}{|\Lambda|} < B_a(k)B_a(-k) >=$$

$$= \frac{1}{|\Lambda|}\sum_{a=1}^{N} < B_a(k^*)B_a(-k^*) > + \sum_{k\in BZ,k\neq k^* a=1}^{N} \frac{1}{|\Lambda|} < B_a(k)B_a(-k) >$$

that, in the thermodynamics limit, one can rewrite as $M = m^2 + \int \frac{d^dk}{(2\pi)^d} g(k)$, but by Eq(3.56) one has:

$$M \leq m^2 + \int \frac{d^dk}{(2\pi)^d} f(k).$$

Therefore one has phase transition if $M - \int \frac{d^dk}{(2\pi)^d} f(k) > 0$ at low temperature. Now the reflection positivity property and the Gaussian domination theorem or Chessboard estimate can be used to obtain the function $f(k)$. As the first example, we do reference to the Eq.(3.52) from which we notice that the susceptivity of the vectorial observable $\Phi_i(x) = G^+B_i(x)G$ has a divergence in $q = 0$. Then we compute the double commutator $[G^+B_i(-q)G, [H, G^+B_i(q)G]]$ and we estimate its upper bound, that is, we find the Function $C(q)$ such that $| < [G^+B_i(-q)G, [H, G^+B_i(q)G]] > | \leq C(q)$, hence by inequality (3.30) one has

$$< \Phi_i(q)\Phi_i(-q) > \leq \sqrt{\frac{C(q)}{2E_-(q)}} \coth(\beta\sqrt{\frac{C(q)E_-(q)}{2}})$$

but using the inequality $\coth x \leq 1 + \frac{1}{x}$ one has:

$$< \Phi_i(q)\Phi_i(-q) > \leq \sqrt{\frac{C(q)}{2E_-(q)}} + \frac{1}{\beta E_-(q)}, \tag{3.58}$$

in particular in the ground state of the Hamiltonian ($T \to 0$) then

$$< 0|\Phi_i(q)\Phi_i(-q)|0 > \leq \sqrt{\frac{C(q)}{2E_-(q)}} \tag{3.59}$$

In this case the sum rule of the Eq.(3.57) corresponds to $\sum_{q\in BZ,i=1}^{p} \frac{1}{|\Lambda|} < \Phi_i(q)\Phi_i(-q) >= M$, therefore one has Long Range Order if the following inequality holds:

$$M - \int \frac{d^dk}{(2\pi)^d} \sqrt{\frac{C(q)}{2E_-(q)}} > 0, \tag{3.60}$$

whereas we can estimate the critical temperature by:

$$M - \int \frac{d^dk}{(2\pi)^d} \sqrt{\frac{C(q)}{2E_-(q)}} - \frac{1}{\beta}\int \frac{d^dk}{(2\pi)^d} \frac{1}{E_-(q)} > 0. \tag{3.61}$$

Example[10]: As example we consider the Antiferromagnetic Heisenberg model, the Hamiltonian is

$$H = j \sum_{x\in\Lambda,\delta} \vec{S}(x)\cdot\vec{S}(x+\delta) \tag{3.62}$$

where δ is a unit vector on lattice. The invariance Group is $SU(2)$ and the spin components are the generators, the order parameter is the staggered magnetization

$$M(T) = \lim_{h\to 0} \sum_{x\in\Lambda} \frac{e^{iQ\cdot x}}{|\Lambda|} < S_3(x) >_h .$$

The sum rule is easly obtained observing that

$$\sum_{x\in\Lambda} \frac{1}{|\Lambda|} S^2(x) = \sum_{q\in BZ} \vec{S}(q)\cdot\vec{S}(-q) = s(s+1)$$

where s is the spin of the single site on lettice. Now we know that the S_i are not all reals but we have two real components (S_1 and S_3) and one purely imaginary (S_2). In Eq.(3.62) the interaction is restrict to nearest lattice sites, hence the lattice is bipartite, $\Lambda = \Lambda_A \bigcup \Lambda_B$ with:

- $\Lambda_A = \{x \in \Lambda \;\; (-1)^{|x|} = 1\}$
- $\Lambda_B = \{x \in \Lambda \;\; (-1)^{|x|} = -1\}$

Then we define the transformation operator $G = \prod_{x\in\Lambda_B} e^{-i\pi S_2(x)}$, that is a rotation around Y axis of angle π of the sites belonging Λ_B sublattice. Therefore the transformed Hamiltonian is:

$$G^+HG = j \sum_{x\in\Lambda,\delta} S_2(x)S_2(x+\delta) - j \sum_{x\in\Lambda,\delta} (S_1(x)S_1(x+\delta)+S_3(x)S_3(x+\delta)) \tag{3.63}$$

Now by introducing the external field h we observe that the Hamiltonian exhibits the Reflection Positivity propriety, indeed if we do refernce to the convenction Eq.(3.31), (3.32) and (3.33), then Hamiltonian (3.63) can be rewritten as:

$$G^+HG =$$

$$= H_- + \Theta(H_-) + j \sum_{x\in\Lambda_P} S_2(x)\Theta(S_2(x)) - j \sum_{x\in\Lambda_P} (S_1(x)\Theta(S_1(x)) + S_3(x)\Theta(S_3(x))), \tag{3.64}$$

where

$$H_- = j \sum_{x,x+\delta\in\Lambda_-} S_2(x)S_2(x+\delta) - j \sum_{x,x+\delta\in\Lambda_-} (S_1(x)S_1(x+\delta) + S_3(x)S_3(x+\delta))$$

Therefore by inequality (3.52) one has:

$$(GS_i(q)G^+, GS_i(-q)G^+) \leq \frac{1}{2\beta E_-(q)},$$

then

$$(S_i(q), S_i(-q)) \leq \frac{1}{2\beta(1+\cos q)} \quad \text{for each } i = 1, 2, 3. \tag{3.65}$$

The susceptivity diverge at the $q = Q = (\pi, ..., \pi) \in \mathbb{R}^d$ and this is a signal of a phase transition. Now, we must compute the upper bound $C(q)$ to the doubble commutator $[S_j(-q)[H, S_j(q)]]$, hence

$$[H, S_j(q)] = i\epsilon_{ijk} \sum_{x\in\Lambda,\delta} e^{-iq\cdot x} \left(e^{-iq\cdot\delta} - 1\right) S_i(x) S_k(x+\delta)$$

from which

$$[S_j(-q)[H, S_j(q)]] = -2\sum_{\delta}(1 - e^{-iq\cdot\delta})(1 - e^{iq\cdot\delta}) \sum_{x\in\Lambda}\sum_{i=1}^{3} S_i(x) S_i(x+\delta)$$

therefore

$$| < [S_j(-q)[H, S_j(q)]] > | \leq 4s(s+1)\sum_{i=1}^{d}(1 - \cos q_i) = \frac{1}{\beta} C(q). \tag{3.66}$$

then by the Falk-Bruch inequality we have that the correlation function has an upper bound, hence

$$g(q) = \sum_{i=1}^{3} < S_i(q) S_i(-q) > \leq \sqrt{\frac{3s(s+1)E_-(q)}{2E_+(q)}} \coth\left(2\beta\sqrt{\frac{2}{3}s(s+1)E_-(q)E_+(q)}\right)$$

Now if we define $M^2 = \frac{<S_j(Q)S_j(-Q)>}{|\Lambda|}$ then

$$s(s+1) = M^2 + \int_{BZ} \frac{d^4q}{(2\pi)^4} g(q),$$

therefore there is spontaneous magnetization if the following inequality holds

$$s(s+1) - \int_{BZ} \frac{d^4q}{(2\pi)^4} \sqrt{\frac{3s(s+1)E_-(q)}{2E_+(q)}} \coth\left(2\beta\sqrt{\frac{2}{3}s(s+1)E_-(q)E_+(q)}\right) > 0 \tag{3.67}$$

whereas the Ground State is ordered if

$$\sqrt{\frac{2s(s+1)}{3}} > \int_{BZ} \frac{d^4q}{(2\pi)^4} \sqrt{\frac{E_-(q)}{E_+(q)}} \tag{3.68}$$

Inequalities like Eqs.(3.67) and (3.68) and their generalizations[11, 12, 13] allow us to conclude that the Antiferromagnetic Heisenberg model supports a staggered spontaneous magnetization at low temperature in three or higher dimensions, whereas in two dimensional systems the Ground state is ordered if $s > 1/2$. For $s = 1/2$ there is not an exact proof of the existence of a quantum order of the system.

Capitolo 4

Mermin and Wagner Theorem

The phase transitions can be absent if the fluctuations amplitude diverge for each temperature. The quantum fluctuation, due to the Heisenberg indetermination principles, can destroy the order in the ground state of the Hamiltonian. The dimensionality of the system play a very important role on the amplification of the thermal and quantum fluctuation of the order parameter. Indeed a theorem due to Mermin and Wagner[35, 34] states that a continuous symmetry can only be spontaneously broken in a dimension larger than two. For a discrete symmetry this lower critical dimensionality is one. For example the antiferromagnetic Heisenberg model with $SU(2)$ symmetry can not be ordered at the one an two dimension at any finite temperature. Alternatively, for the models with discrete symmetry as the Ising model where the symmetry corresponds to reversing all the spins, the symmetry is spontaneously broken in the low-temperature phase below a critical point in dimension two or higher, but no transition occurs in dimension one.

The Mermin-Wagner theorem has been restated by Coleman in the framework of field theory. One can establish this property by showing that the spontaneous breakdown of a continuous symmetry would lead to a Goldstone boson. But in a two-dimensional space-time it is not possible to construct a massless scalar field operator. Indeed the correlator is

$$< 0|\phi(x,t)\phi(0)|0 >= \int_0^{+\infty} \frac{dq}{2\pi q} \cos(qx) e^{iqt} \tag{4.1}$$

and it is an infrared divergent integral. No subtraction procedure may be devised to circumvent this difficulty without spoiling the fundamental properties of field theory, for instance, positivity of the Hilbert space metric. A massless scalar field theory is undefined in a two-dimensional world due to severe infrared divergences. In the statistical language, fluctuations overcome energy in destroying long-range order in this dimension. A simple argument reveals the

nature of this phenomenon. Let us use a discrete classical Heisenberg model on a lattice of side L. Compare the two configurations where the orientation of the spin is allowed to vary along the direction, for example, of the X axis, the energies are, respectively, proportional respectively to $E_a = -L^d$ (spins parallel to X axis) and to $E_b = -L^{d-1}\sum_{i=1}^{L}\cos(\frac{\theta}{L}i)$ if the angle between the spins and the X axis is $(\theta/L)i$. The relative weight of these configurations is given by the Boltzmann factor $e^{-\beta(E_a-E_b)} \approx e^{-\frac{\beta\theta^2}{2}L^{d-2}}$, For $d > 2$ one can see that the (b) configuration has a negligible weight in the thermodynamic limit and for sufficiently low temperature, meaning that order is favored. For $d = 2$ averaging over fluctuations will destroy the order where all the spins are parallel to X axis.

Same consideration can be done for the quantum fluctuation on the ground state, therefore one can exclude that the countinuous symmetry can be broken sponteneously in one dimensional systems. The Mermin and Wagner theorem has a general validity, the unique restriction is that the interaction must be short ranged. In which that follows we will consider itinerant electron systems.

4.1 T-finite Mermin and Wagner theorem

We consider an Hamiltonian operator having the form

$$H = \sum_{xy\in\Lambda,a=1}^{N} t(|x-y|)\psi^{+}(x)\psi(y) + \lambda\sum_{x\in\Lambda} f(\psi^{+}(x)\psi(x)) \tag{4.2}$$

where $\Lambda \in \mathbb{Z}^d$ is a d-dimensional lattice, the field $\psi(x)$ is

$$\psi(x) = \begin{pmatrix} c_1(x) \\ . \\ . \\ . \\ c_n(x) \end{pmatrix} \tag{4.3}$$

with the anticommutation rules $[c_a(x), c_b^{+}(y)]_+ = \delta_{xy}\delta_{ab}$ and $[c_a(x), c_b(y)]_+ = 0$. The Hamiltonian is invariant under a countinuous Group $\mathcal{G}$. The more general continuous Symmetry Group of physical interest is the $U(n)$ Group. The $U(n)$ Group is composed by $n \times n$ Unitary matrices and any element of $U(n)$ is $g = e^{-i\sum_{a=1}^{N}\theta_a T_a}$ where θ_a are the parameter, whereas $\{T_a\}_{a=0}^{N}$ with $T_0 = \hat{1}$ and $N = n^2$ are the generators of the group, they fulfil the following commutation rules

$$[T_a, T_b] = if_{abc}T_c$$

Here the constant f_{abc} are the structure constant of the Group, they are completely antisymmetric under permutations of any pairs of the indices. In a quantum representation $g \to U$ such that $U = e^{-i\sum_{a=1}^{N}\theta_a Q_a}$ the charge

$$Q_a = \sum_{x\in\Lambda}\psi^{+}(x)T_a\psi(x)$$

are the quantum representation of the generators. It is easy to prove that:

$$[Q_a, Q_b] = if_{abc}Q_c.$$

Hence we suppose $[H, Q_a] = 0$ for each $a = 1, ..., N$, furthermore the following commutation rules are fulfilled:

$$\begin{aligned}[Q_a(x), \psi(y)] &= -\delta_{xy}T_a\psi(x) \\ [Q_a(x), \psi^+(y)] &= \delta_{xy}\psi(x)T_a \end{aligned} \tag{4.4}$$

Mermin and Wagner Theorem: Let the Hamiltonian (4.2) where the hopping is short ranged $\sum_{x\in\Lambda} t(x)|x|^2 \leq \infty$, if one defines an order parameter as the expectation value of the vectorial bounded operator

$$O_a = \sum_{x\in\Lambda} \frac{e^{-ik^*\cdot x}}{|\Lambda|} O_a(x) = \frac{O_a(k^*)}{|\Lambda|},$$

where k^* is a particular vector wave belonging to the first zone of Brillouin. Then there is not Long Range Order for any finite temperature.
Proof: The proof of the theorem follows three step:

1. One introduces an external field h, then $H \to H(h) = H + V_h = H + h\sum_{x\in\Lambda} e^{-ik^*\cdot x}O_a(x)$.
2. One obtains an upper bound of the order parameter, that is $M(T, h, \Lambda) \leq f(T, h, \Lambda)$ that after the thermodynamic limit became $M(T, h) \leq f(T, h)$.
3. If the $\lim_{h\to 0} f(T, h) = 0$ one proves that the order is absent.

In Eq.(4.2) the term $\sum_x f(\psi^+(x)\psi(x))$ commute with $Q_a(x) = \psi^+(x)T_a\psi(x)$ whereas the Hopping term commute with total charge $Q_a = \sum_x Q_a(x)$. In order to obtain the function $f(T, h, \Lambda)$ we use the Bogoliubov inequality Eq.(3.20) with an appropriate definition of the operators A and B, in particular their commutator must be the order parameter whereas the operator B must be connected to the generators of the invariance Group. Therefore, if we want study the 1-component of the order parameter then we take: $A = f_{1Nj}O_j(k^*-k)$ whereas $B = Q_N(k)$. The order parameter is a vectorial operator under $\mathcal{G}$ hence the following commutation rules are fulfilled:

$$[A, B] = \sum_{xy\in\Lambda} e^{-i((k^*-k)\cdot x+k\cdot y)} f_{1Nj}[O_j(x), Q_N(y)] =$$

$$= -if_{1Nj}f_{jNk}\sum_{xy\in\Lambda} e^{-i(q\cdot x+k\cdot y)}O_k(x)\delta_{xy}$$

but using the Fiertz identity Eq.(8.12) one has that $-f_{1Nj}f_{jNk} = -f_{j1N}f_{jNk} = n\delta_{1k}$ hence:

$$[A, B] = inO_1(k^*) \tag{4.5}$$

Then $| < [A,B] > |^2 = n^2|\Lambda|^2|M_1|^2 = n^2| < O_1(k^*) > |^2$ is the 1-component of the order parameter. Now it is necessary to compute the double commutator $[B^+,[H,B]$, but we notice that $[f(\psi^+(x)\psi(x)),B] = 0$ then we must compute only $[B^+,[H_t+V_h,B]$ where H_t is the hopping term in the Hamiltonian (4.2). Therefore we write:

$$[H_t,B] = -\sum_{xx'y\in\Lambda} t(x-y)e^{-ik\cdot x'}[Q_N(x'),\psi^+(x)\psi(y)] =$$

$$= -\sum_{xx'y\in\Lambda} t(x-y)e^{-ik\cdot x'}(\psi^+(x)[Q_N(x'),\psi(y)] + [Q_N(x'),\psi^+(x)]\psi(y)) =$$

from which by using the Eq.(4.4) one has:

$$[H_t,B] = -\sum_{xy\in\Lambda} t(x-y)(e^{-ik\cdot x} - e^{-ik\cdot y})\psi^+(x)T_N\psi(y).$$

Furthermore:

$$[B^+,[H_t,B]] = -\sum_{xx'y\in\Lambda} t(x-y)(e^{-ik\cdot x} - e^{-ik\cdot y})e^{ik\cdot x'}[Q_N(x'),\psi^+(x)T_N\psi(y)] =$$

$$= -\sum_{xx'y\in\Lambda} t(x-y)(e^{-ik\cdot x} - e^{-ik\cdot y})e^{ik\cdot x'}(\Psi^+(x)T_N[Q_N(x'),\psi(y)] + [Q_N(x'),\psi^+(x)]T_N\psi(y)]) =$$

$$= -\sum_{xy\in\Lambda} t(x-y)(e^{-ik\cdot x} - e^{-ik\cdot y})(e^{ik\cdot x} - e^{ik\cdot y})\psi^+(x)(T_N)^2\psi(y) =$$

$$= -2\sum_{xy\in\Lambda} t(x-y)(1-\cos k\cdot(x-y))\psi^+(x)(T_N)^2\psi(y)$$

Therefore its expectation value is

$$| < [B^+,[H_t,B]] > | \leq 2\sum_{xy\in\Lambda} t(x-y)(1-\cos k\cdot(x-y))| < \psi^+(x)(T_N)^2\psi(y) > |$$

but knowing that $1-\cos x \leq \frac{x^2}{2}$ and $(k\cdot(x-y))^2 \leq k^2(x-y)^2$ one has

$$| < [B^+,[H_t,B]] > | \leq k^2\sum_{xy\in\Lambda} t(x-y)(x-y)^2| < \psi^+(x)(T_N)^2\psi(y) > |, \quad (4.6)$$

Now one defines an inner product as $(A|B) =< A^+B >$, hence by Schwartz inequality one has:

$$< \Psi^+(x)(T_N)^2\psi(y) > \leq < \psi^+(x)(T_N)^2\psi(x) >$$

hence, if the group $\mathcal{G}$ is the $SU(2)$ group the $T_b = \frac{\sigma_b}{2}$ with σ_b is a Pauli matrix, then $(T_b)^2 = \frac{1}{4}$ and the expectation value of the $\psi^+(x)\psi(x)$ is smaller then 4

(the field operator $\psi(x)$ has only two component). However, in general $(T_N)^2$ is an hermitean matrix $M = (m_{ij})_{ij=1}^n$, therefore

$$< \psi^+(x)(T_N)^2\psi(x) >= \sum_{ij=1}^{n} m_{ij} < \psi_i^+(x)\psi_j(x) >\leq \lambda_{max} \sum_{ij} < \psi_i^+(x)\psi_j(x) >\leq$$

$$\leq \lambda_{max} \sum_{ij} \sqrt{< \psi_i^+(x)\psi_i(x) >< \psi_j^+(x)\psi_j(x) >} = \lambda_{max} N^2,$$

where λ_{max} is the max of the eigenvalue of the matrix M, furthermore by hipothesis $\sum_{x\in\Lambda} t(x)x^2 \leq \alpha$ with α independent by number of sites on lattice. Hence the Eq.(4.6) can be rewritten as:

$$| < [B^+, [H_t, B]] > | \leq k^2|\Lambda|\alpha n^2\lambda_{max} = \rho n^2|\Lambda|k^2. \tag{4.7}$$

By the same procedure we compute:

$$< [B^+, [V_h, B]] >= h < O_1(k^*) >= h|\Lambda|M_1 \tag{4.8}$$

Now we compute the quantity $< [A^+, A]_+ >$ obtaining:

$$< [A^+, A]_+ >= 2f_{1Nj}f_{1Nk} < O_j(k-k^*)O_k(k^*-k) >\leq$$

$$\leq 2\sqrt{f_{1Nj} < O_j(k-k^*)O_j(k^*-k) > f_{1Nk} < O_k(k-k^*)O_k(k^*-k) >} =$$

$$= 2f_{1Nj} < O_j(k-k^*)O_j(k^*-k) >$$

but let $f_{max} = \max_{(2\leq j\leq N-1)}\{f_{1Nj}\}$ and $||O||$ the norm of the operator $O_j(x)$ then:

$$\sum_k < [A^+, A]_+ >\leq 2f_{max} \sum_{x\in\Lambda,k} e^{-i(k-k^*)\cdot x} < O_j(x)O_j(0) >\leq 2f_{max}N|\Lambda|^2||O||^2. \tag{4.9}$$

Therefore by Bogoliubov inequality (3.20), the Eq.(4.7), (4.8), (4.9) and summing on k one has:

$$\sum_k \frac{n^2}{|\Lambda|} \frac{|M_1|^2}{k^2 + h\frac{|M_1|}{\rho}} \leq \beta f_{max} N||O||^2\rho$$

and in the thermodynamics limit:

$$n^2|M_1|^2 \int \frac{d^dk}{(2\pi)^d} \frac{1}{k^2 + h\frac{|M_1|}{\rho}} \leq \beta f_{max} N||O||^2\rho \tag{4.10}$$

then the order parameter $|M_c|^2$ is smaller of the function $f(T,h)$ defined as:

$$f(T,h) = \{ \begin{array}{ll} \frac{\beta f_{max}N||O||^2\rho}{n^2 \frac{2}{\sqrt{\frac{h|M_1|}{\rho}}} \arctan \frac{\pi}{\sqrt{\frac{h|M_1|}{\rho}}}} & \text{if } d = 1 \\ \\ \frac{\beta f_{max}N||O||^2\rho}{n^2\pi \ln(1+\frac{\rho\pi}{h|M_1|})} & \text{if } d = 2. \end{array} \tag{4.11}$$

hence $\lim_{h\to\infty} f(T,h) = 0$ in $d = 1,2$ We proved the Mermin and Wagner theorem in a generic Hamiltonian of itinerant electrons, but one can generalize it to the Hamiltonian of the form:

$$H = -\sum_{xy\in\Lambda i=1}^{N} j(x-y)B_i(x)B_i(y) + \sum_{x\in\Lambda} F(x) \tag{4.12}$$

where the operators $B_i(x)$ with $i = 1,...,N$ are vectorial observable under $\mathcal{G}$ and the operator $F(x)$ is a scalar.

4.1.1 Tensorial order parameters and Nematicity in the Hubbard model

Until now we considered order parameters where the component are vector under transformation belonging to group $\mathcal{G}$. But we can extend the theorem if tensorial order parameters are considered. Indeed during the past decade the nematic Fermi fluids have received a great deal of attention[14]. The term nematic comes from the classical liquid crystal terminology, and refers to a phase that breaks a continuous rotational symmetry, but remaining invariant under other symmetry operations, such as inversion and translation. When a lattice is introduced, the underlying symmetry of the system becomes discrete, so that the nematic order breaks a discrete rotational symmetry. The interest towards these systems has been triggered by interesting and unconventional transport measurements observed in two-dimensional electron systems at high magnetic fields[15, 16], strontium ruthenate materials,[17] in several high temperature superconductors[18, 19], and also in Fe-based superconductors[20, 21], Furthermore, among the heavy-fermion systems, it is found that CeB_6 exhibits non-magnetic quadrupole order[22], and the hidden-order phase in URu_2Si_2 is expected to be a quadrupole or higher-rank multipole ordered phase[23, 24]. The multiorbital Hubbard models have been adopted to investigate the orbital polarized state, usually studied within a mean-field approximation[30, 31]. In this picture, the microscopic models includes the three t_{2g} orbital manifold in presence of an on-site intraorbital, an on-site interorbital, and a nearest-neighbor intraorbital interaction as well as the spin-orbit coupling[32].

Since we are primarily interested in d-band materials, we will start from a suitable mathematical description of electrons belonging to these orbitals. It is well-known that the five real d-states $|d_\alpha>$ are given by

$$|d_{x^2-y^2}>= \frac{1}{\sqrt{2}}(|2,2>+|2,-2>) \;\; |d_{xy}>= \frac{1}{\sqrt{2}i}(|2,2>-|2,-2>)$$

$$|d_{xz}>= \frac{1}{\sqrt{2}}(|2,1>+|2,-1>) \;, \;\; |d_{yz}>= \frac{1}{\sqrt{2}i}(|2,1>-|2,-1>)$$

$$|d_{3z^2-r^2}>= |2,0>, \tag{4.13}$$

where, $|l,m>$ denotes a state with angular momentum l, its third component being m.

If we define the annihilation and creation operators $d_{\sigma\alpha}$, $d^+_{\sigma\alpha}$ of electrons having spin σ in the α orbital, the model Hamiltonian on a periodic lattice Λ is:

$$H = \sum_{x,y\in\Lambda,\alpha,\sigma} t(x-y)d^+_{\sigma,\alpha}(x)d_{\sigma,\alpha}(y)+$$

$$+U\sum_{x,\alpha} n_{\uparrow\alpha}(x)n_{\downarrow\alpha}(x) + \frac{1}{2}(U' - \frac{J}{2})\sum_{x,a\neq b} n_a(x)n_b(x) - J\sum_{x,a\neq b} S^i_a(x)S^i_b(x) + H_{so}, \tag{4.14}$$

where a and b denote the orbitals like in Eq.(4.13), $t(x-y)$ are the hopping amplitudes between x and y sites on the lattice Λ, U is the on-site intra-orbital Coulomb repulsion, and $U' - \frac{J}{2}$ is the on-site inter-orbital Coulomb repulsion whereas J is the Hund coupling constant between electronic spin at different orbital a and b. The last term in the Hamiltonian is the SOI, whose explicit expression is $H_{so} = \eta\sum_{x\in\Lambda}\vec{L}_x\cdot\vec{S}_x$. Defining a multi-component field operator by:

$$\psi(x) = \begin{pmatrix} d_{x^2-y^2}(x) \\ d_{xy}(x) \\ d_{xz}(x) \\ d_{yz}(x) \\ d_{3z^2-r^2}(x) \end{pmatrix}. \tag{4.15}$$

Now by using the propriety of the Pauli matrices the Hund term can be rewritten as:

$$H_J = -J\sum_x(\psi^+(x)\frac{\sigma^i}{2}\psi(x))^2 + \frac{3}{2}J\sum_x\psi^+(x)\psi(x) - \frac{3}{4}J\sum_{x,a}(n_a(x))^2$$

therefore the Hamiltonian in Eq.(4.14) can be rewritten as:

$$H = \sum_{x,y\in\Lambda} t(x-y)\psi^+(x)\psi(y)+$$

$$+\frac{1}{2}(U-U'-J)\sum_{x,a}(n_a(x))^2+\frac{1}{2}(U'-\frac{J}{2})\sum_x(\psi^+(x)\psi(x))^2-\frac{1}{2}(U-3J)\sum_x\psi^+(x)\psi(x)+$$

$$+J\sum_x(\psi^+(x)\frac{\sigma^\alpha}{2}\psi(x))^2 + H_{so}.$$

We note that the term proportional to $(n_a(x))^2$ is not invariant under rotation hence with the constraint $U = U' + J$ we recover the rotational symmetry and the Hamiltonian is:

$$H = \sum_{x,y\in\Lambda} t(x-y)\psi^+(x)\psi(y)+$$

$$+\frac{U'}{2}\sum_x(\psi^+(x)\psi(x))^2-\frac{1}{2}(U'+\frac{3}{4}J)\sum_x\psi^+(x)\psi(x)+\frac{J}{2}\sum_x(\psi^+(x)\frac{\sigma^\alpha}{2}\psi(x))^2+H_{so} \tag{4.16}$$

Introducing the following matrices:

$$T^1 = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \quad T^2 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & \sqrt{3} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \end{pmatrix}$$

$$T^3 = \begin{pmatrix} 0 & -2i & 0 & 0 & 0 \\ 2i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 \\ 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

the components of the orbital angular momentum are $L^a(x) = \psi^+(x)T^a\psi(x)$, a=x, y, z. Moreover, it is easy to prove that

$$[L^a(x), \psi(x)] = -T^a\psi(x)$$

$$[L^a(x), \psi^+(x)] = \psi^+(x)T^a. \tag{4.17}$$

Analogously, the components of the spin operator can be written as:

$$S^a(x) = \psi^+(x)\frac{\sigma^a}{2}\psi(x),$$

implying that

$$[S^a(x), \psi(x)] = -\frac{\sigma^a}{2}\psi(x)$$

$$[S^a(x), \psi^+(x)] = \psi^+(x)\frac{\sigma^a}{2}.$$

Finally, the components of the total angular momentum are $J^a = \sum_x J^a(x)$, where

$$J^a(x) = \psi^+(x)(T^a \otimes \mathbb{1} + \mathbb{1} \otimes \frac{\sigma^a}{2})\psi(x). \tag{4.18}$$

We notice that the following commutation rules are fulfilled

$$[J^a, \psi(x)] = -(T^a \otimes \mathbb{1} + \mathbb{1} \otimes \frac{\sigma^a}{2})\psi(x)$$

$$[J^a, \psi^+(x)] = \psi^+(x)(T^a \otimes \mathbb{1} + \mathbb{1} \otimes \frac{\sigma^a}{2}). \tag{4.19}$$

Using these representations, the spin-orbit coupling term is then written as

$$H_{so} = \eta \sum_x \psi^+(x)(T^a \otimes \frac{\sigma^a}{2})\psi(x)$$

where the T^a matrices act on the orbital index, whereas the Pauli matrices σ^a act on the spin index. Furthermore, it can easily be checked that the Hamiltonian in Eq.(4.14) commutes with each component of the total angular momentum. We define the order parameter as the expectation value of the quadrupole momentum defined as:

$$Q^{ij} = \int d^d x \rho(x)(n_i n_j - \frac{1}{3}\delta_{ij}), \tag{4.20}$$

where n_i is the i-component of a unit vector $n_i = \frac{x}{|x|}$ and $\rho(x)$ is a charge density. To investigate if the model Hamiltonian in Eq.(4.16) exhibits spontaneous nematic order, we start considering the case in which η is vanishing, i. e. when the spin-orbit term is absent. In this case, the total orbital angular momentum, i. e. $L^a = \sum_x L^a(x)$, as well as the total spin, i. e. $S^a = \sum_x S^a(x)$, are conserved quantities, therefore by the Wigner-Eckart theorem, we know that the matrix elements in the basis of the angular momentum L^2 and L^z of any vectorial operator A^i are proportional to the same matrix elements of the angular momentum L^i. Thus, one can write the second quantized Q^{ij} in the Eq.(4.20) as

$$Q^{ij}(x) = \psi^+(x)\left[\frac{1}{2}\left(T^i T^j + T^j T^i\right) - \frac{1}{3}\delta^{ij}T^2\right]\psi(x), \tag{4.21}$$

and we may define the nematic order parameter as the expectation value of the quadrupole momentum operator:

$$\Delta^{ij} = \frac{1}{|\Lambda|}\sum_{x\in\Lambda} < Q^{ij}(x) >, \tag{4.22}$$

where $|\Lambda|$ denotes the number of lattice sites of the Λ lattice.

It is important to remark that the Hamiltonian (4.16) has the same form of the Eq.(4.2) and the order parameter (4.22) is a tensor under transformation belonging to the $SU(2)$ group, therefore under rotation it transforms like the product of two vectors and fulfils the following commutation rules:

$$[L^a, Q^{ij}] = i\epsilon^{aik}Q^{kj} + i\epsilon^{ajk}Q^{ik}. \tag{4.23}$$

Now, let us suppose that there is a nematic symmetry breaking around the third axis; in this case the nematic order parameter is

$$\Delta_n = \frac{1}{|\Lambda|}\sum_x < Q_{x^2-y^2}(x) >=$$

$$= \frac{1}{|\Lambda|}\sum_x (2\sqrt{3} < (d^+_{x^2-y^2}(x)d_{3z^2-r^2}(x) + d^+_{3z^2-r^2}(x)d_{x^2-y^2}(x)) > + 3 < (n_{xz}(x) - n_{yz}(x)) >).$$

We notice that Δ_n is the sum of the two terms: the first one is related to the anisotropy between the $X-Y$ plane and Z axis, whereas the second one to the charge anisotropy between X and Y axis. It is well-known from classical electrodynamics that if we write the electric potential of a charge distribution as

the sum of electric multipoles, then the interaction energy between the charge distribution and an external electric field may be easily written considering that the charge density interacts with the external electric potential, the dipole with the electric field, and the quadrupole momentum with the gradient of the electric field. Therefore, the symmetry breaking Hamiltonian which we has to add to the Hamiltonian in Eq.(4.16) is of the form $H_{int} \sim -\partial^i E^j Q^{ij}$, i. e. $H_{int} = -\lambda^{ij} Q^{ij}$. If we introduce an electric field with gradient on the $X - Y$ plane, then the symmetry-breaking Hamiltonian is:

$$H_\lambda = -\lambda \sum_x Q_{x^2-y^2}(x).$$

Now, we may finally apply the Bogoliubov's inequality to prove the absence of nematic order. To this end, we define $B(k) = \sum_x e^{-ik\cdot x} L^3(x)$ and $A(-k) = \sum_x e^{ik\cdot x} Q^{xy}$, so that $< [A(-k), B(k)] >= -i|\Lambda|\Delta_n$, and

$$| < [A(-k), B(k)] > |^2 = |\Lambda|^2 |\Delta_n|^2.$$

The upper bound of the expectation value of the anticommutator between A and A^+ is:

$$< [A, A^+]_+ >= \sum_{x,y\in\Lambda} e^{-ik\cdot(x-y)} < [Q^{xy}(x), Q^{xy}(y)]_+ >,$$

and summing on all wave vectors k belonging to the first Brillouin zone we can write:

$$\sum_k < [A, A^+] >= |\Lambda| \sum_x < [Q^{xy}(x), Q^{xy}(x)]_+ >= 2|\Lambda| \sum_x < Q^{xy}(x) Q^{xy}(x) > .$$

Since by Eq.(4.20) the order parameter operator Q^{xy} may be written as $Q^{xy} = \psi^+(x)\Gamma^{xy}\psi(x)$ with $\Gamma^{xy} = \frac{1}{2}(T^x T^y + T^y T^x)$, we have that:

$$\sum_k < [A, A^+]_+ >= |\Lambda| (\Gamma^{xy})_{ij} (\Gamma^{xy})_{kl} \sum_x < (\psi_i^+(x)\psi_j(x)\psi_k^+(x)\psi_l(x)) > .$$

Introducing the following operator $O_{ij}(x) = \psi_i(x)\psi_j^+(x)$, and defining an inner product between two operators as $(A|B) =< A^+ B >$, then the second term in the previous equation is

$$| < (\psi_i^+(x)\psi_j(x)\psi_k^+(x)\psi_l(x)) > |^2 \leq < \psi_i^+(x)(1-n_j(x))\psi_i(x) >< \psi_k^+(x)(1-n_l(x))\psi_k(x) >\leq$$

$$\leq < n_i(x) >< n_k(x) >\leq 1,$$

where we used the condition that the matrix elements of the operators $n_i(x)$ and $1 - n_i(x)$ are smaller of 1. Then we proved that

$$\sum_k < [A^+, A] >\leq |\Lambda|^2 N^4 \max_{1\leq i,j\leq N} (\Gamma_{ij}^{xy})^2 = |\Lambda|^2 \alpha$$

that is smaller then the maximum of the matrix element of Γ_{ij}^{xy}.
As the second step, we notice that

$$[B^+,[B,H]] = \sum_{x,y\in\Lambda} t(x-y)(e^{-ik\cdot x}-e^{-ik\cdot y})(e^{ik\cdot x}-e^{ik\cdot y})\psi^+(x)(T^3)^2\psi(y) - 4\lambda\sum_{x\in\Lambda} Q_{x^2-y^2}(x).$$

The expectation value of this quantity is:

$$< [B^+,[B,H]] >= 2\sum_{x,y\in\Lambda} t(x-y)(1-\cos k\cdot(x-y)) < \psi^+(x)(T^3)^2\psi(y) > -4\lambda|\Lambda|\Delta_n,$$

and its upper bound is:

$$| < [B^+,[B,H]] > | \leq \sum_{x,y\in\Lambda} t(x-y)|x-y|^2k^2| < \psi^+(x)(T^3)^2\psi(y) > |+4\lambda|\Lambda||\Delta_n|$$

implying that

$$| < [B^+,[B,H]] > | \leq |\Lambda|\rho\sigma(k^2+\lambda\frac{4|\Delta_n|}{\rho\sigma}).$$

Here, we used the inequality

$$| < \psi^+(x)(T^3)^2\psi(y) > | \leq \sum_{ij}((T^3)^2)_{ij}\sqrt{< n_i >< n_j >} \leq 2\sum_{ij}((T^3)^2)_{ij} =$$

$$= 2N^2 \max_{1\leq i,j\leq N}\{((T^3)^2)_{ij}\} = \sigma,$$

i. e. σ is connected to the maximum among the matrix elements of $(T^3)^2$; we also introduce the following notation: $\rho = \sum_x t(x)|x|^2$.
In conclusion, summing on k of the first Brillouin zone, the Bogoliubov's inequality becomes

$$|\Delta_n|^2\frac{1}{|\Lambda|}\sum_k \frac{1}{k^2+\lambda\frac{4|\Delta_n|}{\rho\sigma}} \leq \frac{\rho\alpha\sigma}{2k_BT}. \tag{4.24}$$

but performing the thermodynamics limit and remembing the Eq.(4.10) and Eq.(4.11) $\lim_{\lambda\to 0}\lim_{|\Lambda|\to\infty}|\Delta_n(\lambda,|\Lambda|)| = 0$.
Therefore, we conclude that for one- and two-dimensional multiorbital Hubbard model without spin-orbit coupling, the nematic long-range-order will not appear at any nonzero temperature, since the order parameter goes to zero as the symmetry-breaking field λ is turned off.
The SOI explicitly breaks the rotational symmetry in the real space so that the orbital angular momentum is not a conserved quantity. However, the total angular momentum commutes with the Hamiltonian. Thus, the previous conclusions still remain valid if the operators A and B in Eq.(3.20) are defined as follows: B operator has to be related to the symmetry operator for the Hamiltonian, i. e. the total angular momentum, whereas the operator A must be such that the commutator between A and B has to reproduce the order parameter.

Therefore, we define A and B in the following way: $A(k) = \sum_x e^{ik\cdot x} Q^{xy}$ and $B(k) = \sum_x e^{-ik\cdot x} J^3(x)$, respectively. With these definitions we obtain an inequality like that of Eq.(4.24), and we can state that the spontaneous quadrupole momentum is vanishing also for a multiorbital Hubbard model in the presence of a SOI, in low dimensional cases.
We notice that in the presence of SOI the results here obtained can be generalized to model Hamiltonians containing other terms such as the hopping between different orbitals or other Coulomb interactions. In the first case, the angular momentum is not conserved. Nevertheless, if this hopping term commutes with total angular momentum we can recover the results previously shown, otherwise the rotational symmetry is explicitly broken and the previous conclusions are no more valid. To prove this conclusion, we introduce the hopping term by means of a mixing matrix M such that H_t may be written as:

$$H_t = \sum_{x,y\in\Lambda} t(x-y)\psi^+(x) M \psi(y).$$

The commutator of this term with the total angular momentum is:

$$[J^a, H_t] = \sum_{x,y\in\Lambda} t(x-y)\psi^+(x)[T^a + \frac{\sigma^a}{2}, M]\psi(y),$$

so that if $[T^a + \frac{\sigma^a}{2}, M] = 0$ then the rotational symmetry is preserved and the conclusions of the present paper still hold, whereas if $[T^a + \frac{\sigma^a}{2}, M] \neq 0$ the symmetry is broken and we cannot exclude the existence of the nematic order.

To generalize the previous results at k-rank tensorial order parameter it is necessary to describe it in terms of its spherical component, indeed the cartesian tensor Q^{ij} or, in general, $Q^{i_1\cdots i_k}$ is reducible (it is the sum of object that they transform itself in different way under transformation belonging $\mathcal{G}$ group, in this case rotations). One defines irreducible k-rank tensor if it transform itself as the irreducible representation of the rotations. Hence if $U = e^{-i\theta_a J_a}$ is a rotation of angle $\vec{\theta}$ then one defines the irreducile k-representation of the rotations the matrices $D^{(k)}_{mm'}(\vec{\theta}) =< k, m|e^{-i\theta_a J_a}|k, m' >$ where $k(k+1)$ are the eigenvalue of the J^2 whereas m are the eigenvalue of the J_z, therefore $T^{(k)}_q$ with $-k \leq q \leq k$ is a irriducible k-rank tensor if under rotations one has:

$$U^+ T^{(k)}_q U = \sum_{q'} D^{(k)}_{qq'} T^{(k)}_{q'}. \tag{4.25}$$

Let U a infinitesimal rotation operator then $U = 1 - i\theta_a J_a$ (on the repeated indices we intend the sum) then we write:

$$(1 + i\theta_a J_a) T^{(k)}_q (1 - i\theta_a J_a) = \sum_{q'} < k, q|(1 - i\theta_a J_a)|k, q' > T^{(k)}_{q'}$$

from which we have the following commutation rules:

$$[J_a, T^{(k)}_q] = -\sum_{q'} < k, q|J_a|k, q' > T^{(k)}_{q'}, \tag{4.26}$$

therefore

$$[J_z, T_q^{(k)}] = qT_q^{(k)} \tag{4.27}$$

$$[J_\pm, T_q^{(k)}] = \sqrt{k(k+1) - q(q\pm 1)}T_{q\pm 1}^{(k)}. \tag{4.28}$$

In this case, the tensorial order parameter can be defined as

$$\Delta = \sum_{x\in\Lambda} \frac{e^{iq^*\cdot x}}{|\Lambda|} < T_q^{(k)}(x) >$$

hence if we have an Hamiltonian like Eq. (4.2) then defining, for example, $B(q) = J_+(q) = \sum_{x\in\Lambda} e^{-iq\cdot x} J_+(x)$ and $A = T_{q-1}^{(k)}(q^* - q) = \sum_{x\in\Lambda} e^{-i(q^*-q)\cdot x} T_{q-1}^{(k)}(x)$ one has an inequality as Eq.(4.24) for the order parameter Δ.

4.2 T=0 Mermin and Wagner Theorem

The consideration done in the previous paragraph can be extended immediately to the Ground State of the system if the non-vanishing energetic gap exist, indeed if $\Delta = \inf_{E_a\in(\sigma(H)-E_0)} |E_a - E_0| \neq 0$ then the inequality (3.21) allows to obtain a inequality like (4.24) where the order parameter, now, is defined as the quantum expectation value on the Ground State of an observable, say $O(x)$, that is

$$M = \sum_{x\in\Lambda} \frac{e^{-ik^*\cdot x}}{|\Lambda|} < 0|O(x)|0 > .$$

In general we does not know the spectrum of the Hamiltonian, therefore we can not extend the previous results to the ground state, furthermore a vanishing energetic gap do not mean existence of the order. Then we need another strategy for to study the Quantum Order on the Ground State.

In general the quantum fluctuations of the order parameter are smaller then the thermal fluctuation, then there is not reason for exclude the order in the Ground state of a two dimensional system, on the other hand, in one spatial dimension the fluctuations can be amplified and the order can be absent. In relativistic field theory the Coleman theorem excludes Spontaneous Symmetry Breaking on the Ground State of a scalar field. The quantum fluctuation are due to the Heisenberg indetermination principle, hence if the operator relative to the order parameter commute with the Hamiltonian then the Ground state can be ordered in one dimensional system, an example of this is the ferromagnetic Heisenberg model where the Ground State is ordered also in one spatial dimension. Indeed the Hamiltonian is:

$$H = -\sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} \tag{4.29}$$

where the periodic boundary conditions are imposed $\vec{S}_{N+1} = \vec{S}_1$. Now we consider the state in which all spins are polarized along Z direction, that is

$|\alpha>=\otimes_{i=1}^{N}|j,j>_{(i)}$ then it is an eigenvector of the Hamiltonian with energy $E_\alpha=-Nj$, furthermore any state like

$$|\alpha'>=\otimes_{i=1}^{k-1}|j,j>_{(i)}\otimes|j,j-1>_{(k)}\otimes_{i=k+1}^{N}|j,j>_{(i)}$$

is an eigenstate with energy $E_{\alpha'}=-Nj+1$ then it is an excited state. We remark that the order parameter is the expectation value of the total spin, but it is a motion integral, hence the quantum fluctuations are absent. However, in this case, one has Spontaneous Symmetry Breaking of the discrete symmetry $\vec{S}_i\to-\vec{S}_i$. Similar consideration can not done for the antiferromagnetic Heisenberg model where the SSB is necessarily a continuous symmetry and the Ground State is disordered, indeed, in this case an ordered Ground State does not break the symmetry $\vec{S}_i\to-\vec{S}_i$.

In order to prove the Mermin and Wagner theorem in the Ground State of one dimensional system one must be use the inequality (3.13) and the reflection positivity is necessary. The strategy is the same of the T-finite theorem, but it is necessary the knowledge of the upper bound of the correlation function on the Ground state, that is an inequality like Eq.(3.59). A prototype of this considerations is the antiferromagnetic Heisenberg model where the Ground State is disordered. Indeed the Hamiltonian is:

$$H=j\sum_{x\in\Lambda,\delta}\vec{S}(x)\cdot\vec{S}(x+\delta) \tag{4.30}$$

The invariance Group is $SU(2)$ and the spin components are the generators.

Now by introducing the external field h we observe that the Hamiltonian exhibits the Reflection Positivity propriety, indeed if we do refernce to the convenction Eq.(3.31), (3.32) and (3.33), then Hamiltonian (3.63) can be rewritten as:

$$G^+HG=$$
$$=H_-+\Theta(H_-)+j\sum_{x\in\Lambda_P}S_2(x)\Theta(S_2(x))-j\sum_{x\in\Lambda_P}(S_1(x)\Theta(S_1(x))+S_3(x)\Theta(S_3(x))), \tag{4.31}$$

where

$$H_-=j\sum_{x,x+\delta\in\Lambda_-}S_2(x)S_2(x+\delta)-j\sum_{x,x+\delta\in\Lambda_-}(S_1(x)S_1(x+\delta)+S_3(x)S_3(x+\delta))+$$
$$+h\sum_{x\in\Lambda_-}(-1)^{|x|}S_3(x).$$

Therefore the inequality (3.65) are true also in presence of the external field h, hence we write

$$(S_i(q),S_i(-q))\le\frac{1}{2\beta(1+\cos q)}\quad\text{for each } i=1,2,3 \tag{4.32}$$

$$(S_2(q-Q),S_2(Q-q))\le\frac{1}{2\beta(1-\cos q)}. \tag{4.33}$$

Now, using the inequality (3.13) in which one defines $A = S_1(Q-q)$ and $S_2(q)$ (here $Q = \pi$) one has:

$$| < 0|[A, B]|0 > |^2 = | < 0|S_3(Q)|0 > |^2 = |\Lambda|^2 \Delta(|\Lambda|, h) \tag{4.34}$$

where $\Delta = \lim_{h\to 0} \lim_{|\Lambda|\to\infty} \Delta(|\Lambda|, h)$ is the order parameter. Furthermore we compute the quantity:

$$\sum_q < 0|[A, A^+]_+|0 > \leq 2|\Lambda|^2 s^2, \tag{4.35}$$

whereas by inequality (3.59) the correlator

$$< 0|[B, B^+]_+|0 > = 2 < 0|S_2(Q-q)S_2(q-Q)|0 > \leq \sqrt{\frac{2|\Lambda| < 0|[S_2(Q-q), [H, S_2(q-Q)]]|0 >}{(1-\cos q)}},$$

hence after sraightforward algebra one has:

$$| < 0|[B, B^+]_+|0 > | \leq |\Lambda| \sqrt{\frac{4j(1+\cos q)s(s+1) + 2h\Delta(|\Lambda|, h)}{1-\cos q}}. \tag{4.36}$$

Therefore by inequalities (3.13), (4.35) and (4.36) one proves easly that, in the thermodynamic limit, the following inequality is fulfilled:

$$|\Delta(h)|^2 \leq \frac{4s^2\sqrt{js(s+1)}}{I(h)} \tag{4.37}$$

with

$$I(h) = \int_{-\pi}^{+\pi} \frac{dq}{2\pi} \sqrt{\frac{1-\cos q}{1+\cos q + f(h)}} \tag{4.38}$$

where the function $f(h) = h\frac{\Delta(h)}{2js(s+1)}$ then $\lim_{h\to 0} f(h) = 0$ furthermore the integral (4.38) can be computed easly and one has:

$$I(h) = \frac{2}{\pi} \ln |\frac{\sqrt{f(h)+1}+1}{\sqrt{f(h)+1}-1}|$$

but $\lim_{h\to 0} I(h) = \infty$ then the order is absent.

In order to study the itinerant electronic systems we prove the following equality for the $T = 0$ susceptivity:

$$\lim_{\beta\to\infty} \beta(\phi(q), \phi(-q)) = \int_0^{+\infty} \frac{d\omega}{\omega} \sum_{\alpha\in\sigma(H)} \delta(\omega - E_\alpha + E_0)(| < 0|\phi(q)|\alpha > |^2 + | < 0|\phi(-q)|\alpha > |^2) \tag{4.39}$$

indeed

$$\beta(\phi(q), \phi(-q)) = \int_0^1 \frac{dx}{Z} \mathrm{Tr}(e^{-(1-x)\beta H}\phi(q)e^{-x\beta H}\phi(-q)) =$$

$$= \int_0^1 \frac{dx}{Z} \sum_{\alpha\alpha'} e^{-\beta E_\alpha} e^{x\beta(E_\alpha - E_{\alpha'})} < \alpha|\phi(q)|\alpha' >< \alpha'|\phi(-q)|\alpha >=$$

$$= \frac{1}{Z} \sum_{\alpha\alpha'} \frac{e^{-\beta E_{\alpha'}} - e^{-\beta E_\alpha}}{E_\alpha - E_{\alpha'}} < \alpha|\phi(q)|\alpha' >< \alpha'|\phi(-q)|\alpha >$$

hence, we have

$$\lim_{\beta\to\infty} \beta(\phi(q), \phi(-q)) =$$

$$= \lim_{\beta\to\infty} \frac{1}{Z} \sum_{\alpha\alpha'} (e^{-\beta E_{\alpha'}} \frac{| < \alpha|\phi(q)|\alpha' > |^2}{E_\alpha - E_{\alpha'}} - e^{-\beta E_\alpha} \frac{| < \alpha|\phi(q)|\alpha' > |^2}{E_\alpha - E_{\alpha'}}) =$$

$$= \lim_{\beta\to\infty} \frac{1}{Z} \sum_{\alpha\alpha'} (e^{-\beta E_{\alpha'}} \frac{| < \alpha|\phi(q)|\alpha' > |^2}{E_\alpha - E_{\alpha'}} + e^{-\beta E_\alpha} \frac{| < \alpha'|\phi(-q)|\alpha > |^2}{E_{\alpha'} - E_\alpha})$$

and inserting inside at the sum the quantity $1 = \int_{-\infty}^{+\infty} d\omega \delta(\omega - E_\alpha + E_{\alpha'})$ the Eq.(4.39) is evident.

T=0 Mermin and Wagner Theorem: Let the $\mathcal{G}$-invariant Hamiltonian in Eq.(4.2) defined on a one dimensional lattice, then the Ground State is disordered, that is, if one defines the order parameter as

$$\Delta_a = \lim_{h\to 0} \lim_{|\Lambda|\to\infty} \sum_{x\in\Lambda} \frac{e^{-iq^*\cdot x}}{|\Lambda|} < 0|Q_a(x)|0 > \tag{4.40}$$

then is is vanish. Here q^* is a vector belonging to the first zone of Brillouin and $Q_a(x)$ is a $\mathcal{G}$-vector operator.
Proof: If the non-vanishing energy gap exist then by Bogoliubov inequality Eq.(3.21) the conclusions on systems at T-finite hold also in this case. Hence we suppose that there are gapless excitations on the energetic spectrum, that is exist a energetic band $E_\alpha(q)$ such that $\lim_{q\to 0} E_\alpha(q) = E_0$ (if there is SSB this is a Goldstone mode). The term $E_\alpha(q)$ is given by Hopping term in the Hamiltonian Eq.(4.2). Indeed if we write the Hopping term using the Fourier components then we have: $H_t = \sum_q \frac{E_\alpha(q)}{|\Lambda|} n_\alpha(q)$ with $n_\alpha(q) = c_\alpha^+(q)c_\alpha(q)$ and $E_\alpha(q) = \sum_x t_\alpha(x) e^{-iq\cdot x}$, hence if one considers an Hoppong such that $t(x) \neq 0$ for each $x = 1, ..., N < |\Lambda|$

$$E(q) = 2t^{(1)} \cos q + \sum_{l=1}^{N} t^{(l)} \cos ql \tag{4.41}$$

whereas if we consider the Hopping only between nearest sites then the dispersion law is

$$E(q) = 2t \cos q \tag{4.42}$$

furthermore if $t > 0$ the the minimum of the band is for $q = \pi$. If there is a Goldstone mode then $E(\pi) = -|E_0| + \frac{\Delta}{|\Lambda|}$, hence

$$E(q) = |E_0| \cos q + \frac{\Delta}{|\Lambda|} \tag{4.43}$$

therefore by Eq(4.39) one has that

$$\lim_{\beta \to \infty} \beta(Q_a(q), Q_a(-q)) \leq \frac{1}{|E_0|(1 + \cos q)} \tag{4.44}$$

In Eq.(4.43) the quantity $\frac{\Delta}{|\Lambda|}$ is a gap for finite size lattice, indeed, in this case, the Goldstone mode is a low lying excitation. There are many models where inequality Eq.(4.44) can be proven rigorously using the Reflection Positivity as the antiferromagnetic Heisenberg model. Now, the susceptivity diverge for $q = \pi$ therefore in Eq.(4.40) we take $q^* = \pi$. Furthermore we use the indetermination inequality Eq.(3.13) where we take $A = f_{1aN} Q_a(q)$ and $B = Q_N(Q - q)$ and following the standard Mermin and Wagner strategy the theorem can be easly proved.

We remark that if $t < 0$ then the Eq.(4.43) must be replaced by $E(q) = \frac{\Delta}{|\Lambda|} \cos q + |E_0|(1 - \cos q)$ and the susceptivity diverge for $q = 0$ then in Eq.(4.40) we must take $q^* = 0$, but in this case the order parameter commute with the Hamiltonian therefore the quantum fluctuations are absent and the Ground State can be ordered.

Capitolo 5

Existence of Phase Transitions in Strongly Correlated Electronic Systems

5.1 Orbital Order in t_{2g} band of the TMO

The Transition metals are the elements that, in their compound, have partially filled d orbitals. The properties of transition-metal (TM) compounds are a topic of longstanding interest, and many their compounds show an orbital ordering[48], that is an Long Range Order on the orbital occupation[66]. In these compounds the electrostatic interaction (Crystal Field Theory) removes partially the degeneration of the d orbitals, in particular this gives rise to two sets of orbital energy levels. The doubly degenerate e_g set consists of the axial orbitals $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ and the triply degenerate t_{2g} set consisting of the interaxial d_{xy}, d_{xz} and d_{yz} orbitals. The Jahn-Teller effect reduce further the degeneration[67]. Now we consider an Hubbard model for t_{2g} orbitals on a d-dimensional hypercubic lattice $\Lambda \subset \mathbb{Z}^d$, confining the analysis to the half filled case, i. e. three electrons on the t_{2g} orbitals. We will adopt the following model Hamiltonian:

$$H = -t \sum_{x,\delta} \psi^+(x)\psi(x+\delta) + U \sum_{x,a} (n_{\uparrow a}(x) - \frac{1}{2})(n_{\downarrow a}(x) - \frac{1}{2}) +$$

$$+U' \sum_{x,a>b} (n_a(x) - 1)(n_b(x) - 1) + V \sum_{x,\delta,a} (n_a(x) - 1)(n_a(x+\delta) - 1)\,, \quad (5.1)$$

where $a, b = xy, xz, yz$ denote the t_{2g} orbitals, δ is a unit vector on the lattice and

$$\psi(x) = \begin{pmatrix} d_{xy}(x) \\ d_{xz}(x) \\ d_{yz}(x) \end{pmatrix},$$

is a spinor field operator, $d_{xy}(x)$, $d_{xz}(x)$, $d_{yz}(x)$ being the annihilation operators for electrons in the t_{2g} manifold. The U term is the on-site intra-orbital Coulomb interaction, the U' term describes the on-site inter-orbital Coulomb interaction, and finally the V term corresponds to the off-site intra-orbital Coulomb interaction, furthermore we assume that U=U' and, without to lose generality, the hopping amplitude t is a real and positive constant.
Then, we define the nematic order parameter as

$$\Delta_N = \frac{1}{2|\Lambda|} \sum_x < (n_{xz}(x) - n_{yz}(x)) >,$$

and the staggered nematic order parameter as

$$\Delta_{NS} = \frac{1}{2|\Lambda|} \sum_x e^{iQ\cdot x} < (n_{xz}(x) - n_{yz}(x)) > .$$

with $Q = (\pi, ..., \pi) \in \mathbb{R}^d$.
To prove that a staggered nematic order (SNO) may exist within the model Hamiltonian of Eq.(5.1), we start by defining the following operators:

$$I^a(x) = \psi^+(x) \frac{T^a}{2} \psi(x)\,,$$

with $a = x, y, z$ and

$$T^a = \begin{pmatrix} 0 & 0 \\ 0 & \sigma^a \end{pmatrix},$$

where σ^a are the ordinary Pauli matrices and

$$T^2 = (T^x)^2 + (T^y)^2 + (T^z)^2 = \frac{3}{4} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \equiv \frac{3}{4} T^0\,.$$

We note that the $I^a(x)$ operators fulfil a genuine SU(2) isospin algebra, that is:

$$[I^+(x), I^-(y)] = 2\delta_{x,y} I^z(x)\,,$$

$$[I^z(x), I^\pm(y)] = \pm\delta_{x,y} I^\pm(x)\,, \tag{5.2}$$

where $I^\pm(x) = I^x(x) \pm i I^y(x)$ hence the eigenvalue of the operator $\hat{I}^2$ are $I = \frac{1}{2}, 1$.
It is worth stressing that the Hamiltonian Eq.(5.1) is invariant under the global U(1) transformation generated by I^z operator.

The order parameter can be then rewritten in term of $I^z(x)$ as

$$\Delta_{NS} = \frac{1}{|\Lambda|}\sum_x e^{iQ\cdot x} < I^z(x) >= \frac{I^z(Q)}{|\Lambda|}\,.$$

Using $I^a(x)$ operators, the off-site Coulomb term of the Hamiltonian can be written as follows:

$$H_V = V\sum_{x,\delta}(n_{xy}(x)-1)(n_{xy}(x+\delta)-1)+$$

$$+\frac{V}{2}\sum_{x,\delta}(n_{xz}(x)+n_{yz}(x)-2)(n_{xz}(x+\delta)+n_{yz}(x+\delta)-2)+2V\sum_{x,\delta}I^z(x)I^z(x+\delta)\,. \tag{5.3}$$

The existence of SNO will be accomplished if we show that[59]

$$\lim_{|x|\to\infty}\lim_{|\Lambda|\to\infty} < I^z(x)I^z(0) >= \lim_{|\Lambda|\to\infty} < (\sum_x \frac{e^{iQ\cdot x}I^z(x)}{|\Lambda|})^2 >\neq 0\,. \tag{5.4}$$

5.1.1 Sum Sule and Symmetries.

We remark that the Hamiltonian is invariant under rotation of angle $\pi/2$ around the three axis X, Y, Z of the real space, hence the three orbitals are three degenerates states, furthermore if we write the Hamiltonian as

$$H = H^{(0)} + 2V\sum_{x,\delta} I^z(x)I^z(x+\delta)$$

with $U = U'$ then $H^{(0)} = H_t + H_{int}$ has a complete rotational invariance in the isospin space, in particular for the H_{int} this symmetry is also a gauge symmetry, that is if we define $U = \prod_{x\in\Lambda} e^{-i\theta_a(x)I^a(x)}$ then $U^+H_{int}U = H_{int}$ (this is do not true for the hopping term). Now we consider the correlator $G^z(\delta) =< 0|I^z(x)I^z(x+\delta)|0 >$ in the ground state $|0>$ between two nearest sites x and $x+\delta$, it is independent from δ direction. In terms of Fourier component it is (BZ is the first Brillouin zone):

$$G^z(\delta) = \sum_{q\in BZ}\frac{e^{iq\cdot\delta}}{|\Lambda|} < 0|I^z(q)I^z(-q)|0 >$$

Now isolating the mode $q = Q = (\pi, ..., \pi)$ and performing the thermidynamic limit we have:

$$G^z(\delta) = -\frac{1}{|\Lambda|} < 0|I^z(Q)I^z(-Q)|0 > + \int_{BZ}\frac{d^dq}{(2\pi)^d}e^{iq\cdot\delta} < 0|I^z(q)I^z(-q)|0 >=$$

$$= -\Delta_{NS} - \int_{BZ}\frac{d^dq}{(2\pi)^d}(-\frac{1}{d}\sum_{i=1}^{d}\cos q_i) < 0|I^z(q)I^z(-q)|0 >$$

If we consider the set $B^+ = \{q \in BZ \ \mid \ \sum_{i=1}^{d} \cos q_i \leq 0\}$ then we have

$$\Delta_{NS} \geq -G^z(\delta) - \int_{B^+} \frac{d^d q}{(2\pi)^d} (-\frac{1}{d} \sum_{i=1}^{d} \cos q_i) < 0|I^z(q) I^z(-q)|0 > \qquad (5.5)$$

indeed the integrand function is non negative in B^+ hence $\int_{BZ} ... \leq \int_{B^+} ...$
At this point it is necessary to obtain an upper bound of the function $G^z(\delta)$, therefore we write the energy in the ground state as

$$E_0 = -t \sum_{x,\delta} < 0|\psi^+(x)\psi(x+\delta)|0 > + < 0|H_{int}|0 > +2Vd|\Lambda|G^z(\delta)$$

but $< 0|A^+ B|0 >$ is an inner product between the operators A and B, hence using the Schwartz inequality one can write that

$$< 0|\psi^+(x)\psi(x+\delta)|0 > \leq < 0|\psi^+(x)\psi(x)|0 >$$

where we used the traslational invariance of the ground state. Then we conclude that

$$E_0 \geq -3td|\Lambda| + < 0|H_{int}|0 > +2Vd|\Lambda|G^z(\delta)$$

Now we consider the excited state $|\alpha >$ such that for each site the isospin is polarized in $\pm I^z$ direction (the sign $\pm$ depends from the sublattice), that is $I^z(x)|\alpha > = e^{iQ\cdot x} I|\alpha >$. In this state the energy is higher or equal at the ground state energy, furthermore it is easy compute an upper bound of this energy. Indeed, the state $|\alpha >$ is obtained from the ground state by rotation of angle $\theta_a(x)$ dependent by the site of the lattice around an opportune axis a in the isospin space, that is $|\alpha > = \prod_{x\in\Lambda} e^{-i\theta_a(x) I^a(x)}|0 > = U|0 >$. Furthermore by Schwartz inequality we write

$$< \alpha|H_t|\alpha > \leq | < \alpha|H_t|\alpha > | \leq t \sum_{x,\delta} | < 0|U^+\psi^+(x)UU^+\psi(x+\delta)U|0 > | \leq$$

$$\leq td \sum_x < 0|U^+\psi^+(x)\psi(x)U|0 > = td \sum_x < \alpha|\psi^+(x)\psi(x)|\alpha > = 3td|\Lambda|$$

then we have

$$E_\alpha \leq 3td|\Lambda| + < 0|H_{int}|0 > -2VI^2 d|\Lambda|$$

from which

$$G^z(\delta) \leq 3\frac{t}{V} - I^2$$

but knowing that $I^2 \geq \frac{1}{4}$ one has that the condition Eq.(5.5) can be rewritten as

$$\Delta_{NS} \geq \frac{1}{4} - 6\frac{t}{2V} - \int_{B^+} \frac{d^d q}{(2\pi)^d} (-\frac{1}{d} \sum_{i=1}^{d} \cos q_i) < 0|I^z(q) I^z(-q)|0 > \qquad (5.6)$$

then there is SNO long range order if the second side of the previous equation is strictly positive.

5.1.2 Existence of the Long Range Order.

In order to prove the existence of the SNO we do reference to the conventions Eq.(3.31), (3.32) and (3.33) and we use the Infrared Bound Method.
Now, we notice that the hopping term of the Hamiltonian acts on an antisymmetric Fock space, which does not have the form of tensor product $\mathcal{H}^+ \otimes \mathcal{H}^-$. Indeed, the field operators defined on $\mathcal{H}^+$ does not commute with all field operators defined on $\mathcal{H}^-$. Therefore, by means of a Jordan Wigner[60] transformation we introduce two new operators $\rho^+(x)$ and $\rho(x)$ defined as follows:[61]

$$\rho(x) = \prod_{y\in\Lambda^+} e^{i\pi\psi^+(y)\psi(y)}\psi(x)\,, \tag{5.7}$$

$$\rho^+(x) = \psi^+(x) \prod_{y\in\Lambda^+} e^{-i\pi\psi^+(y)\psi(y)}\,. \tag{5.8}$$

It can be easily checked that

$$[\rho(x),\rho^+(y)]_+ = 0 \quad [\rho(x),\rho(y)]_+ = 0 \quad [\rho^+(x),\rho^+(y)]_+ = 0\,,$$

for each $x, y \in \Lambda^+$ or $x, y \in \Lambda^-$, while

$$[\rho(x),\rho^+(y)] = 0 \quad [\rho(x),\rho(y)] = 0 \quad [\rho^+(x),\rho^+(y)] = 0\,,$$

for each $x \in \Lambda^+ \quad y \in \Lambda^-$ or $x \in \Lambda^- \quad y \in \Lambda^+$.
Now, coming back to our model Hamiltonian, we define two operators F and R, where F is the hole-particle transformation and R is an opportune gauge transformation.

Since the lattices is bipartite, hence we define:

- $\Lambda_A = \{x \in \Lambda \quad |e^{iQ\cdot x} = 1\}$
- $\Lambda_B = \{x \in \Lambda \quad |e^{iQ\cdot x} = -1\}$

If one defines a patricle-hole transformation as follows:

$$F^+\rho(x)F = \{ \begin{array}{ll} \rho(x) & \text{if } x \in \Lambda_A \\ e^{iQ\cdot x}\rho^+(x) & \text{if } x \in \Lambda_B \end{array}$$

then the hopping term of the Hamiltonian (5.1) is rewritten as:

$$F^+H_tF = -t \sum_{x\in\Lambda_A,\delta} e^{iQ\cdot(x+\delta)}\rho(x)\rho(x+\delta) - t \sum_{x\in\Lambda_B,\delta} e^{iQ\cdot x}\rho^+(x)\rho^+(x+\delta)$$

Now by U(1) Gauge transformation $R = \prod_{x\in\Lambda_B} e^{i(Q\cdot x)n(x)}$ the Hamiltonian can be rewritten as follows:

$$R^+F^+HFR = -t \sum_{x\in\Lambda_A,\delta} \rho(x)\rho(x+\delta) - t \sum_{x\in\Lambda_B,\delta} \rho^+(x)\rho^+(x+\delta) -$$

$$-V\sum_{x,\delta}(n_{xy}(x)-1)(n_{xy}(x+\delta)-1)+H_U-$$

$$-\frac{V}{2}\sum_{x,\delta}(n_{xz}(x)+n_{yz}(x)-2)(n_{xz}(x+\delta)+n_{yz}(x+\delta)-2)-2V\sum_{x,\delta}I^z(x)I^z(x+\delta)\,. \tag{5.9}$$

Then, we can write the Hamiltonian in the required form and the Gibbs states exhibit the reflection-positivity property:

$$H'=R^+F^+HRF=H^+\otimes\hat{1}+\hat{1}\otimes\chi(H^+)-$$

$$-t\sum_{x\in\Lambda_P\bigcap\Lambda_A}\rho(x)\otimes\chi(\rho(x))-t\sum_{x\in\Lambda_P\bigcap\Lambda_B}\rho^+(x)\otimes\chi(\rho^+(x))$$
$$-\sum_{x\in\Lambda_P,a}B_a(x)\otimes\chi(B_a(x))-2V\sum_{x\in\Lambda_P}I^z(x)\otimes\chi(I^z(x))\,, \tag{5.10}$$

where $[B_a(x),\chi(B_a(x))]=0$ for each $x\in\Lambda_P$, a indicates all operators in Eq.(5.9) that are defined on Λ_P and that are different from $I^z(x)$.

Now, the Reflection Positive form of the Hamiltonian allows the use of the Gaussian Domination theorem then one has that the the nematic susceptibility $\chi'(q)$ defined as

$$\chi(q)=(I^z(q),I^z(-q))',$$

has the following upper bound:

$$\chi(q)=(I^z(q),I^z(-q))'\leq\frac{|\Lambda|}{4\beta VE_-(q)}\,, \tag{5.11}$$

where $I^z(q)=\frac{1}{\sqrt{|\Lambda|}}\sum_x e^{-iq\cdot x}I^z(x)$ and $E_-(q)=\sum_{i=1}^d(1-\cos q_i)$, whereas $(,)'$ is the Duhamel function computed using the Hamiltonian H' in Eq.(5.10). Therefore we easly obtain the following inequality:

$$\chi(q)=(I^z(q),I^z(-q))\leq\frac{|\Lambda|}{4\beta VE_+(q)}\,, \tag{5.12}$$

where now $E_+(q)=\sum_{i=1}^d(1+\cos q_i)$.

In order to obtain the upper bound for the correlator we use the Falk-Bruch inequality (3.22), but we must compute the $C(q)$ function, hence:

$$[I^z(-q),[H_t,I^z(q)]]=\frac{t}{2}\sum_{x,\delta}\frac{(1-\cos q\cdot\delta)}{|\Lambda|}\psi^+(x)T^0\psi(x+\delta),$$

but by Schwartz inequality one get $<\psi^+(x)T^0\psi(x+\delta)>\leq 4$, so that

$$<[I^z(-q),[H_t,I^z(q)]]>\leq 2tE_-(q)\,, \tag{5.13}$$

with $E_-(q)=\sum_{i=1}^d(1-\cos q_i)$.

We point out that the inequality Eq.(5.13) is verified also in the ground state, i. e.

$$< 0|[I^z(-q), [H_t, I^z(q)]]|0 >\leq 2tE_-(q)\,.$$

Using this result, the correlator has the following upper bound:

$$< I^z(q)I^z(-q) >\leq \frac{1}{2}\sqrt{\frac{tE_-(q)}{2VE_+(q)}}\coth(2\beta\sqrt{2tVE_+(q)E_-(q)})\,. \tag{5.14}$$

On the other hand, in the ground state we have:

$$< 0|I^z(q)I^z(-q)|0 >\leq \frac{1}{2}\sqrt{\frac{tE_-(q)}{2VE_+(q)}}\,.$$

Hence, the susceptibility has an upper bound that diverges when $q = Q = (\pi, ..., \pi)$. This result is very important since it may suggest a possible phase transition. Indeed, let us start from Eq.(5.6) we have a SNO if

$$\Delta_{NS} \geq \frac{1}{4} - 6\frac{t}{2V} - \frac{1}{2}\sqrt{\frac{t}{2V}}\int_{B^+}\frac{d^dq}{(2\pi)^d}(-\frac{1}{d}\sum_{i=1}^{d}\cos q_i)\sqrt{\frac{E_-(q)}{E_+(q)}} > 0$$

furthermore defining $y = \sqrt{\frac{t}{2V}}$ and $\Gamma(d) = \int_{B^+}\frac{d^dq}{(2\pi)^d}(-\frac{1}{d}\sum_{i=1}^{d}\cos q_i)\sqrt{\frac{E_-(q)}{E_+(q)}}$ we have to resolve the inequality:

$$\frac{1}{4} - 6y^2 - \frac{1}{2}\Gamma(d)y > 0$$

but $\Gamma(1) = +\infty$, $\Gamma(2) = 0.65$, $\Gamma(3) = 0.35$, then the SNO exist at low temperature if:

$$d = 2) \quad \frac{t}{V} < 0.06 \tag{5.15}$$

$$d = 3) \quad \frac{t}{V} < 0.07 \tag{5.16}$$

whereas $d = 1$ the previous equation is not conclusive.

5.1.3 Consideration on e_g states and discussion of the results.

As extension of the previous results we can consider an other situation where the e_g electron are considered, in this case the infra-band off-site repulsion is:

$$H_V = V\sum_{x,\delta}\{(n_{x^2-y^2}(x)-1)(n_{x^2-y^2}(x+\delta)-1)+(n_{3z^2-r^2}(x)-1)(n_{3z^2-r^2}(x+\delta)-1)\}. \tag{5.17}$$

Furthermore now we have $\psi(x) = \begin{pmatrix} d_{x^2-y^2}(x) \\ d_{3z^2-r^2}(x) \end{pmatrix}$ whereas the isospin $I^a(x) = \psi^+(x)\frac{\sigma^a}{2}\psi(x)$ and the order parameter is $\Delta_{NS} = \sum_x \frac{e^{iQ\cdot x}}{|\Lambda|} < 0|I^z(x)|0 >$. In this case the eigenvalue of the $\hat{I}^2$ is $I = 1$ and the conditions in Eq.(5.15) and (5.16) are:

$$d = 2) \quad \frac{t}{V} < 0.44 \tag{5.18}$$

$$d = 3) \quad \frac{t}{V} < 0.31 \tag{5.19}$$

In conclusion we have shown that a half-filled multi-orbital Hubbard model may support a SNO if repulsive or attractive on-site inter-orbital and intra-orbital interactions and off-site repulsive inter-orbital interaction are considered. We find that, depending on the dimensions of the lattice where the model is defined, the SNO may or may not exist. In particular, applying the infrared bound method, we have shown that in three dimensions the order may exist at finite temperature and we get the condition for the existence of the SNO. In two and three dimensional lattices the order may exist also in the ground state, if the hopping amplitude is small enough (see Eqs.(21)-(22) and Eqs. (24)-(25)). If the existence of the nematic order is investigated within the Mermin and Wagner theorem, it has been recently proven that rotationally symmetric models cannot sustain the nematic order.[58] However, we point out that this result cannot be applied to the present case, since the intra-orbital off-site repulsion breaks the rotational symmetry of the model Hamiltonian so that the existence of the nematic order at the finite temperature cannot be excluded. We point out that the conditions Eq.(5.15) and Eq.(5.16) are sufficient but not necessary, implying that the order can exist even though they are not verified.

Now, let us comment on a potential applications of the results above presented to real systems. It is well-known that in TMO with a-axis larger than the c-axis in octahedral crystal field, if we would like to accomodate fourth electrons in d-orbitals, we face with the following problem: one electron could be used to pair one of the electrons in the lower energy (t_{2g}) set of orbitals or it could be placed in one of the higher energy (e_g) orbitals. The latter of these configurations is called high-spin because it contains four unpaired electrons with the same spin, whereas the other one is called low-spin because it contains only two unpaired electrons. We notice that a similar problem occurs when we are looking at TMO having five, six or seven electrons. On the other hand, we notice that for eight, nine and ten electrons there is only one way to write energetically satisfactory configurations. As a result, we have to worry about high-spin versus low-spin octahedral complexes only when there are four, five, six, or seven electrons in the d-orbitals. Therefore, referring to half-filled t_{2g} orbitals, the results obtained in this paper apply to elongated (a-axis lower than c-axis) TMO with seven electrons in octahedral crystal field crystal or to flattened (a-axis larger than c-axis) TMO with three electrons. Moreover, when half-filled e_g orbitals are considered, our results apply to TMO with two electrons (a-axis larger than

c-axis) or eight electrons (a-axis lower than c-axis) in the d-orbitals. We would like also point out that the Jahn-Teller effect may play an important role in TMO compounds, and it is known that in these systems this effect can lead the orbital ordering.[68] In particular, it has been recently proven that the ground state of the compass model may exhibit a SNO-like orbital ordering, similarly to the results here presented.[66] Nevertheless, we stress that the SNO order here discussed appears within the crystal field approximation, neglecting the Jahn-Teller effect, as shown in Eqs.(5.18)-(5.19).

As final remark, we notice that the conclusions of the present paper do not hold for the doped system, because in this case the particle hole-symmetry of the Hamiltonian is lost and, within the procedure here applied, the upper bound of the susceptibility cannot be inferred. Furthermore the conclusions reached are not valid for systems with anisotropic hopping.

5.2 Charge Density Wave and Superconductivity in the Multiband Hubbard model.

Now we study the Charge Density Wave in the Multiband Hubbard model, hence, doing reference to systems previous discussed, we consider an half-filled degenerate d-band Hubbard model. Therefore the Hamiltonian is defined in Eq.(4.16) where now we add a rotational-symmetric off site coulombian repulsion H_V and an off site Pseudospin interaction, hence we write:

$$H = -t \sum_{x\in\Lambda,\delta} \psi^+(x)\psi(x+\delta) + H_U + H_J +$$

$$+\frac{J'}{2} \sum_{x\in\Lambda,\delta} (\eta^+(x)\eta^-(x+\delta) + \eta^-(x)\eta^+(x+\delta)) + \frac{V}{4} \sum_{x\in\Lambda} (n(x)-N)(n(x+\delta)-N) \tag{5.20}$$

where the field $\psi(x)$ is defined in Eq.(4.15) (in the d-band case $N = 5$), whereas

$$\eta^+(x) = \sum_\alpha c^+_{\alpha\uparrow}(x)c^+_{\alpha\downarrow}(x) \quad \eta^-(x) = \textstyle\sum_\alpha c_{\alpha\downarrow}(x)c_{\alpha\uparrow}(x) \tag{5.21}$$

$$\eta^z(x) = \frac{1}{2}(\psi^+(x)\psi(x) - N) \tag{5.22}$$

are the generators of the pseudospin SU(2) algebra (α is the band index). Is evident that they fulfils the SU(2) algebra, indeed:

$$[\eta^z(x), \eta^\pm(y)] = \pm\eta^\pm(x)\delta_{xy}$$

$$[\eta^+(x), \eta^-(y)] = 2\eta^z(x)\delta_{xy}.$$

One defines Charge Density Wave order parameter as:

$$\Delta_{CDW} = \sum_{x\in\Lambda} \frac{e^{-iQ\cdot x}}{|\Lambda|} < \eta^z(x) >= \frac{< \eta^z(Q) >}{|\Lambda|} \tag{5.23}$$

with $Q = (\pi, ..., \pi) \in \mathbb{R}^d$. The Charge Density wave LRO is a Spontaneous Symmetry Breaking of the U(1) of rotation around the third axis of the Pseudospin, we remark that for $J' \neq V$ the model is not Pseudospin SU(2)-symmetric, therefore in low dimensional systems, the Mermin and Wagner arguments are not conclusive and one can not exclude the order at finite temperature. Now by Jordan-Wigner transformations Eq.(5.7), (5.8), the Hamiltonian (5.20) is rewritten as

$$H = -t \sum_{x \in \Lambda} \rho^+(x)\rho(x+\delta) + H_U + H_J +$$

$$+ \frac{J'}{2} \sum_{x \in \Lambda, \delta} (\eta^+(x)\eta^-(x+\delta) + \eta^-(x)\eta^+(x+\delta)) + V \sum_{x \in \Lambda, \delta} \eta^z(x)\eta^z(x+\delta), \quad (5.24)$$

we remember that in a state with l orbital angular momentum one as $N = 2l+1$ electrons with definite spin.

The lattices is bipartite, hence we define:

- $\Lambda_A = \{x \in \Lambda \ \ | e^{iQ\cdot x} = 1\}$
- $\Lambda_B = \{x \in \Lambda \ \ | e^{iQ\cdot x} = -1\}$

If one defines a patricle-hole transformation as follows:

$$F^+\rho(x)F = \{ \begin{array}{ll} \rho(x) & \text{if } x \in \Lambda_A \\ e^{iQ\cdot x}\rho^+(x) & \text{if } x \in \Lambda_B \end{array}$$

then the Hamiltonian (5.20) is rewritten as:

$$F^+HF = -t \sum_{x \in \Lambda_A, \delta} e^{iQ\cdot(x+\delta)}\rho(x)\rho(x+\delta) - t \sum_{x \in \Lambda_B, \delta} e^{iQ\cdot x}\rho^+(x)\rho^+(x+\delta) + H_U + H_J -$$

$$- \frac{J'}{2} \sum_{x \in \Lambda, \delta} (\eta^+(x)\eta^+(x+\delta) + \eta^-(x)\eta^-(x+\delta)) - V \sum_{x \in \Lambda, \delta} \eta^z(x)\eta^z(x+\delta) \quad (5.25)$$

Now by U(1) Gauge transformation $R = \prod_{x \in \Lambda_B} e^{i(Q\cdot x)n(x)}$ the Hamiltonian can be rewritten as follows:

$$R^+F^+HFR = -t \sum_{x \in \Lambda_A, \delta} \rho(x)\rho(x+\delta) - t \sum_{x \in \Lambda_B, \delta} \rho^+(x)\rho^+(x+\delta) + H_U + H_J -$$

$$- \frac{J'}{2} \sum_{x \in \Lambda, \delta} (\eta^+(x)\eta^+(x+\delta) + \eta^-(x)\eta^-(x+\delta)) - V \sum_{x \in \Lambda, \delta} \eta^z(x)\eta^z(x+\delta) \quad (5.26)$$

hence doing reference to the convenctions Eq.(3.31), (3.32) and (3.33) we rewrite the transformed Hamiltonian in Reflection Positive form:

$$H' = H_- \otimes \hat{I} + \hat{I} \otimes \Theta(H_-) - t \sum_{x \in \Lambda_P \bigcap \Lambda_A} \rho(x) \otimes \Theta(\rho(x)) - t \sum_{x \in \Lambda_P \bigcap \Lambda_B} \rho^+(x) \otimes \Theta(\rho^+(x)) -$$

$$-\frac{J'}{2}\sum_{x\in\Lambda_P}(\eta^+(x)\Theta(\eta^+(x))+\eta^-(x)\Theta(\eta^-(x))-V\sum_{x\in\Lambda_P}\eta^z(x)\otimes\Theta(\eta^z(x)) \quad (5.27)$$

Therefore, by Gaussian Domination theorem Eq.(3.52) one can prove that the Charge Density Susceptivity fulfils the following inequality:

$$(\eta^z(q),\eta^z(-q))\leq\frac{|\Lambda|}{V\beta E_+(q)}. \quad (5.28)$$

By same considerations we have the upper bound for the eta-pairing Susceptivity:

$$(\eta^+(q),\eta^-(-q))+(\eta^-(q),\eta^+(-q))\leq\frac{4|\Lambda|}{J'\beta E_+(q)}. \quad (5.29)$$

In each site of the lattice we can have maximum $2N$ electrons and minimum 0 electrons hence the eigenvalue m of $\eta^z(x)$ must be such that $-N/2\leq m\leq N/2$ and the eigenvalues of $\eta^2(x)=1/2(\eta^+(x)\eta^-(x)+\eta^-(x)\eta^+(x))+(\eta^z(x))^2$ are $j(j+1)$ with $j=N/2$. Therefore we have the following sum rule:

$$\frac{1}{|\Lambda|}\sum_{q,a}<\eta^a(q)\eta^a(-q)>=\frac{N}{2}(\frac{N}{2}+1) \quad (5.30)$$

furthermore by Eq.(3.30) one has:

$$<\eta^z(q)\eta^z(-q)>\leq\frac{1}{2}\sqrt{|\Lambda|\frac{<[\eta^z(-q),[H,\eta^z(q)]]>}{VE_+(q)}} \quad (5.31)$$

but $[\eta^z(-q),[H,\eta^z(q)]]=\frac{t}{2}\sum_{x,\delta}(1-\cos q\cdot\delta)\psi^+(x)\psi(x+\delta)$ then $<[\eta^z(-q),[H,\eta^z(q)]]>\leq\frac{t}{2}E_-(q)N|\Lambda|$. Then the Eq.(5.31) became:

$$<\eta^z(q)\eta^z(-q)>\leq\frac{|\Lambda|}{2}\sqrt{\frac{tNE_-(q)}{2VE_+(q)}}. \quad (5.32)$$

Then the divergence of the susceptivity indicates a possible CDW and Superconductivity Long Range Order.

Capitolo 6

Gauge theories and Spin-Orbit Coupling.

The interactions are due to the symmetry properties of the Lagrangian density that describe the system, the electromagnetism is the more striking example of this. Indeed the Lagrangian of the matter fields with charge are global U(1) invariant and the generator of the Group, the Charge, is a motion integral. This is the principle of the conservation of the electric charge. This symmetry is not only global but local and this has the consequence of the existence of the electromagnetic interaction. Indeed if one consider the Dirac field $\psi(x)$ with Lagrangian density:

$$\mathcal{L} = \bar{\psi}(x)(i\partial\!\!\!/ - m)\psi(x) \tag{6.1}$$

where $\partial\!\!\!/ = \gamma_\mu \partial^\mu = \gamma^0\partial^0 - \gamma^i\partial^i$ and $\bar{\psi}(x) = \gamma^0\psi^+(x)$. The matrices γ^μ are the four Dirac matrices, they are square matrices of the fourth order, furthermore they fulfil the Clifford algebra:

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}\hat{I} \tag{6.2}$$

where $g^{\mu\nu}$ is the metric tensor:

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{6.3}$$

In the standard representation the Dirac matrices are defined as follows

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \quad \gamma^5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where the σ^i are the classical Pauli's matrices and $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$. The Lagrangian Eq.(6.1) is U(1) invariant, that is, performing the transformation

$\psi'(x) \to e^{-ie\theta}\psi(x)$ the Lagrangian is invariant therefore, by the Noether theorem, there is a conserved current $\partial_\mu J^\mu(x) = 0$ with $J^\mu(x) = e\bar{\psi}(x)\gamma^\mu\psi(x)$ then the charge, defined as $Q = -i\int d^4x \frac{\partial\mathcal{L}}{\partial(\partial^0\psi(x))}\psi(x) = e\int d^4x\psi^+(x)\psi(x)$, is time invariant $\dot{Q} = 0$. We remark that in a quantum theory the Charge operator is the generator of the symmetry group considered, hence one has that if $U \in U(1)$ then $U = e^{-ie\theta Q}$ and $U^+\psi(x)U = e^{-ie\theta}\psi(x)$. This symmetry is also local where the parameter θ dependents on the space-time coordinate. In order to extend the invariance property of the Lagrangian density (6.1) at the local transformation one defines a covariant derivative $\mathcal{D}_\mu$ as $\partial_\mu \to \mathcal{D}_\mu = \partial_\mu - ieA_\mu(x)$ where $A_\mu(x)$ is the electromagnetic 4-potential. The covariant derivative has the following transformation propriety:

$$\psi(x) \to \psi'(x) = U(x)\psi(x)$$

and

$$\mathcal{D}_\mu\psi(x) \to \mathcal{D}_\mu^{'}\psi'(x) = U\mathcal{D}_\mu\psi(x) = U\mathcal{D}_\mu U^+\psi'(x)$$

hence

$$\mathcal{D}_\mu^{'} = U\mathcal{D}_\mu U^+$$

whereas the transformation law of the gauge field A_μ are:

$$A'_\mu(x) = A_\mu(x) + \frac{i}{e}U\partial_\mu U^+ = A_\mu(x) - \partial_\mu\theta(x)$$

Now one defines a strength gauge field as $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and its dual $\mathcal{F}_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}F^{\rho\sigma}$ they are 2-rank antisymmetric tensors, but, whereas $F_{\mu\nu}$ is a true tensor its dual is a pseudotensor under spatial reflections. The free Lagrangian density of the Gauge field can be constructed by using both $F_{\mu\nu}$ and $\mathcal{F}_{\mu\nu}$, but it must be a true scalar function then one can not have term like $\mathcal{F}_{\mu\nu}F^{\mu\nu}$. Therefore the free Lagrangian of the Gauge field is $\mathcal{L}_A = \alpha F_{\mu\nu}F^{\mu\nu}$. The constant α must be such that the Euler-Lagrange equations for $\mathcal{L}_A$ give the Maxwell Equations. Hence, in natural units, $\alpha = -\frac{1}{4}$ and the complete Lagrangian density for the Electrodynamics is:

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(x)(i\not{\mathcal{D}} - m)\psi(x) \tag{6.4}$$

These considerations can be extended to non-Abelian Group, for example the QCD is a generalization to the $SU(3)$ Group. Therefore, given a generic Lagrangian with non hermitian matter field $\phi(x)$ and $\mathcal{G}$ a non-Abelian Group of symmetry with generators $\{T_a\}_{a=}^N$, hence $U \in \mathcal{G}$ then $U = e^{-i\theta_i T_i}$. For each generator one has a conserved current $\partial_\mu J_a^\mu = 0$ where $J_a^\mu = -i\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi(x))}T_a\phi(x)$ Charge $\{Q_a\}_{a=1}^N$ defined as $Q_a = \int d^4x J_a^0(x)$ such that $\dot{Q}_a = 0$. The extension to local Gauge transformations is done by taking

$$\partial_\mu\phi(x) \to \mathcal{D}_\mu\phi(x) = \partial_\mu\phi(x) - iA_\mu\phi(x) = \partial_\mu\phi(x) - iA_{a\mu}T_a\phi(x)$$

that is, there is a Gauge field $A_{a\mu}(x)$ for each generator of the Group. In this case the transformations property of the Gauge fields are:

$$A'_\mu(x) = UA_\mu U^+ + iU\partial_\mu U^+.$$

For non-Abelian Gauge theory the strength tensor is defined as $iF_{\mu\nu} = [\mathcal{D}_\mu, \mathcal{D}_\nu]$, hence under Gauge transformation one has that $F'_{\mu\nu} = UF_{\mu\nu}U^+$. The free Lagrangian must be a Gauge invariant, that is, a G-scalar function, hence one defines it as:

$$\mathcal{L}_{YM} = -\frac{1}{2}Tr(F_{\mu\nu}F^{\mu\nu}) \tag{6.5}$$

whereas the complete Lagrangian for a generic theory is

$$\mathcal{L} = \mathcal{L}_m(\phi(x), \mathcal{D}_\mu\phi(x)) - \frac{1}{2}Tr(F_{\mu\nu}F^{\mu\nu})$$

the interaction is hidden in the covariant derivative.

6.1 Spin Orbit Coupling and Gauge Theories in non-relativistic Field Thories.

If a charged particle is moving in a region where an electric field exist then it is subject to the action of a magnetic field, this is due to the relativistic transformations property of the electromagnetic field. Indeed if $\vec{v}$ is the velocity of the particle (in the laboratory frame) with $v \ll c$ and $\vec{E}$ is the electrostatic field in the laboratory frame then, in the rest frame of the particle, one has that $\vec{B} \approx -\vec{\beta} \times \vec{E}$. Therefore if Φ is the electrostatic potential then the magnetic field, in the particle rest frame, is $\vec{B} \approx \vec{\beta} \times \vec{\nabla}\Phi(\vec{x})$. The interaction between the magnetic field due to the motion of the particle and the its spin it is the origin of the Spin-Orbit coupling. If one consider a central potential then $\vec{\nabla}\Phi(r) = \frac{\vec{x}}{r}\frac{\partial}{\partial r}\Phi(r)$ and knowing that the spin-magnetic field interaction, in Gauss units, is $H_{so} = -\frac{e\hbar}{mc}\vec{S} \cdot \vec{B}$ one writes that

$$H_{so} = \frac{e\hbar}{m^2cr}\frac{\partial\Phi(r)}{\partial r}\vec{L} \cdot \vec{S}.$$

This result is incorrect because it does not take account of the Thomas precession of the particle rest frame. A correct way to obtain all non-relativistic terms is write the non-relativistic approximation of the Dirac Equation. Therefore by solving the Euler Lagrange equations the motion equations of the Dirac field are:

$$(i\partial\!\!\!/ - m)\psi(x) = 0 \tag{6.6}$$

But, in natural units, it is:

$$(-i\vec{\alpha} \cdot \vec{\nabla} + m\beta)\psi(x) = i\frac{\partial}{\partial t}\psi(x),$$

and definited the matrices $\beta = \gamma^0$ and

$$\alpha^i = \gamma^0\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}.$$

In appendix we give a complete derivation of the non relativistic approximation of the Dirac equation, indeed by a Foldy Wouthuysen transformation it is possible to obtain, order by order, the non relativistic equation. Then rewriting the Eq.(8.39) one has:

$$i(\frac{\partial}{\partial t}+ieA^0+ig\vec{\sigma}\cdot\vec{B})\psi = \{-\frac{1}{2m}(\vec{\nabla}-ie\vec{A}-ig\frac{\vec{\sigma}}{2}\times\vec{E})^2-\frac{e^2}{8m^3}((\vec{\sigma}\cdot\vec{B})^2+(\frac{\vec{\sigma}}{2}\times\vec{E})^2)+H'\}\psi \tag{6.7}$$

where the coupling constant g is the Bohr magneton $g = \mu_B = e/2m$ and H' is defined as

$$H' = \frac{\vec{\nabla}\cdot\vec{E}}{8m^2} - \frac{1}{8m^3}((\vec{P}-e\vec{A})^4 + e(\vec{P}-e\vec{A})^2(\vec{\sigma}\cdot\vec{B}) + e(\vec{\sigma}\cdot\vec{B})(\vec{P}-e\vec{A})^2). \tag{6.8}$$

The H' term can be rewritten as

$$H' = -\frac{1}{8m^3}((\vec{P}-e\vec{A})^4 + 2e(P^i-eA^i)(\vec{\sigma}\cdot\vec{B})(P_i-eA_i) - \nabla^2(\vec{\sigma}\cdot\vec{B})).$$

One can consider this equation as the solution of the Euler-Lagrange equation

$$\frac{\delta}{\delta\psi^+(x)}\mathcal{S}(\psi,\psi^+) = 0$$

where the functional $\mathcal{S}(\psi,\psi^+) = \int d^4x\mathcal{L}(\psi,\psi^+)$ is the Action and $\mathcal{L}(\psi,\psi^+)$ is the Pauli Schroedinger Lagrnangian density defined as:

$$\mathcal{L} = i\psi^+\mathcal{D}_t\psi - \frac{1}{2m}(\mathcal{D}_i\psi)^+(\mathcal{D}^i\psi) + \frac{g^2}{2m}\psi^+((W^0)^2 + W_iW^i)\psi + \mathcal{L}' \tag{6.9}$$

where we defined

$$\mathcal{D}_t = \mathcal{D}_0 = \frac{\partial}{\partial t} + ieA^0 + ig\frac{\sigma^a}{2}W_{a0} \tag{6.10}$$

$$\mathcal{D}^i = \partial^i - ieA^i - ig\frac{\sigma^a}{2}W_a^i \tag{6.11}$$

$$\text{in covariant notation: } \mathcal{D}^\mu = \partial^\mu + ieA^\mu + ig\frac{\sigma^a}{2}W^{a\mu} \tag{6.12}$$

with $W_{ai} = \epsilon_{iaj}E^j$, $W_{a0} = 2B_a$ and $W_\mu = \frac{\sigma^a}{2}W_{a\mu}$. The fields $G_{a\mu}$ are the components of the Gauge fields and they introduce the spin-orbit coupling in the free Schroedinger Lagrangian density $\mathcal{L} = i\psi^+\frac{\partial\psi}{\partial t} - \frac{1}{2m}(\partial_i\psi)^+(\partial^i\psi)$. The kinetic term of the Gauge fields are, for the electromagnetic potential $F^{\mu\nu} = \partial^\mu A^\mu - \partial^\nu A^\mu$ and $\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} = \frac{1}{2}(\vec{E}^2 - \vec{B}^2)$ whereas for the non abelian $SU(2)$ Gauge field it is:

$$igG_{\mu\nu} = ig\frac{\sigma^a}{2}G_{a\mu\nu} = [\partial_\mu + ig\frac{\sigma^a}{2}W_{a\mu}, \partial_\nu + ig\frac{\sigma^a}{2}W_{a\nu}] =$$

$$= ig\frac{\sigma^a}{2}(\partial_\mu W_{a\nu} - \partial_\nu W_{a\mu} - g\epsilon_{abc}W^b_\mu W^c_\nu)$$

from which:

$$G_{a\mu\nu} = \partial_\mu W_{a\nu} - \partial_\nu W_{a\mu} - g\epsilon_{abc}W^b_\mu W^c_\nu. \tag{6.13}$$

then the its component are $G_{\mu\mu} = 0$ and if we define $\mathbb{E}^i = G^{0i}$ then

$$\vec{\mathbb{E}} = \frac{\partial}{\partial t}(\frac{\vec{\sigma}}{2} \times \vec{E}) - \vec{\nabla}(\vec{\sigma}\cdot\vec{B}) + ig[\vec{\sigma}\cdot\vec{B}, \frac{\vec{\sigma}}{2} \times \vec{E}] =$$

$$= \begin{pmatrix} \frac{\dot{\vec{W}}^3}{2} - \vec{\nabla}B^3 + i\frac{g}{2}(B^-\vec{W}^+ - B^+\vec{W}^-) & \frac{\dot{\vec{W}}^-}{2} - \vec{\nabla}B^- + ig(B^3\vec{W}^- - B^-\vec{W}^3) \\ \frac{\dot{\vec{W}}^+}{2} - \vec{\nabla}B^+ + ig(B^+\vec{W}^3 - B^3\vec{W}^+) & -(\frac{\dot{W}^3}{2} - \vec{\nabla}B^3) + i\frac{g}{2}(B^+\vec{W}^- - B^-\vec{W}^+) \end{pmatrix}$$

with $\vec{W}^3 = (-E^2, E^1, 0)$, $\vec{W}^1 = (0, -E^3, E^2)$, $\vec{W}^2 = (E^3, 0, -E^1)$ and defining $G_{ij} = \epsilon_{ijk}\mathbb{B}^k$

$$\vec{\mathbb{B}} = \vec{\nabla} \times (\frac{\vec{\sigma}}{2} \times \vec{E}) - ig(\frac{\vec{\sigma}}{2} \times \vec{E}) \times (\frac{\vec{\sigma}}{2} \times \vec{E}) \tag{6.14}$$

Then the free Lagrangian density of the Yang and Mills fields is $\mathcal{L}_{SU(2)} = -\frac{1}{8}Tr(G_{\mu\nu}G^{\mu\nu})$, that, after straightforward algebra becames:

$$\mathcal{L}_{SU(2)} = -\frac{1}{2}(\partial_\mu W_{a\nu}\partial^\mu W^{a\nu} - \partial_\mu W_{a\nu}\partial^\nu W^{a\mu}) + \epsilon_{abc}\partial_\mu W_{a\nu}W^\mu_b W^\nu_c -$$

$$-\frac{g^2}{2}(W_{a\mu}W^\mu_a W_{b\nu}W^\nu_b - W_{a\mu}W^\mu_b W_{a\nu}W^\nu_b)$$

therefore the complete Lagrangian density is

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{4}G_{a\mu\nu}G^{a\mu\nu} + i\psi^+\mathcal{D}_0\psi + \frac{1}{2m}(\mathcal{D}_i\psi)^+(\mathcal{D}^i\psi) + \mathcal{L}'. \tag{6.15}$$

The Zeeman and Spin-Orbit terms are hidden in the covariant derivative $\mathcal{D}_t$ and $\mathcal{D}_i$ hence if one considers only these terms then the Lagrangian density is

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{4}G_{a\mu\nu}G^{a\mu\nu} + i\psi^+\mathcal{D}_0\psi + \frac{1}{2m}(\mathcal{D}_i\psi)^+(\mathcal{D}^i\psi). \tag{6.16}$$

The Lagrangian Eq.(6.16) is $SU(2)_{spin} \otimes U(1)_{em}$ gauge invariant then the correspondents conserved Noether Currents are:

$$j^\mu(x) = -ie\left(\frac{\partial\mathcal{L}}{\partial(\mathcal{D}_\mu\psi(x))}\psi(x) - \psi^+(x)\frac{\partial\mathcal{L}}{\partial(\mathcal{D}_\mu\psi(x))^+}\right) \text{ e.m. current} \tag{6.17}$$

$$J^{a\mu}(x) = -ig\left(\frac{\partial\mathcal{L}}{\partial(\mathcal{D}_\mu\psi(x))}\frac{\sigma^a}{2}\psi(x) - \psi^+(x)\frac{\sigma^a}{2}\frac{\partial\mathcal{L}}{\partial(\mathcal{D}_\mu\psi(x))^+}\right) \quad \text{spin current.} \tag{6.18}$$

We notice the last term in Eq.(6.15) breaks the Gauge symmetry, this because the fields $\vec{E}$ and $\vec{B}$ are physical observables hence the gauge symmetry SU(2) is not fundamental. In general, if one studies system with only spin orbit coupling,

one does not consider this term. Now by Lagrangian density Eq.(6.16) we compute:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial(\mathcal{D}_0\psi(x))} &= i\psi^+(x) \\
\frac{\partial \mathcal{L}}{\partial(\mathcal{D}_0\psi(x))^+} &= 0 \\
\frac{\partial \mathcal{L}}{\partial(\mathcal{D}_i\psi(x))} &= -\frac{1}{2m}(\mathcal{D}^i\psi(x))^+ \\
\frac{\partial \mathcal{L}}{\partial(\mathcal{D}_i\psi(x))^+} &= -\frac{1}{2m}(\mathcal{D}^i\psi(x)),
\end{aligned} \tag{6.19}$$

thus the current Eq.(6.17) is $j^\mu(x) = (\rho(x), j^i(x))$ with

$$\begin{aligned}
\rho(x) &= e\psi^+(x)\psi(x) \\
j^i(x) &= -\frac{ie}{2m}\left(\psi^+(x)\mathcal{D}^i\psi(x) - (\mathcal{D}^i\psi(x))^+\psi(x)\right)
\end{aligned} \tag{6.20}$$

whereas the Spin Current Eq.(6.18) is $J^{a\mu}(x) = (M^a(x), J^{ai}(x))$ where the components are:

$$\begin{aligned}
M^a(x) &= g\psi^+(x)\frac{\sigma^a}{2}\psi(x) = gS^a(x) \\
J^{ai}(x) &= -\frac{ig}{2m}\left(\psi^+(x)\frac{\sigma^a}{2}\mathcal{D}^i\psi(x) - (\mathcal{D}^i\psi(x))^+\frac{\sigma^a}{2}\psi(x)\right)
\end{aligned} \tag{6.21}$$

Tha quantity $M^a(x)$ is the magnetic moment density, whereas the spatial component $J^{ia}(x)$ are the component of the 3-vector Spin-Current. Furthermore the Eq.(6.17) and (6.18) can be rewritten more explicitely as follows

$$\begin{aligned}
\rho(x) &= e\psi^+(x)\psi(x) \\
j^i(x) &= -i\frac{e}{2m}\left(\psi^+(x)\partial^i\psi(x) - \partial^i\psi^+(x)\psi(x)\right) - \frac{e}{m}\psi^+(x)\psi(x)A^i(x)
\end{aligned} \tag{6.22}$$

and

$$\begin{aligned}
M^a(x) &= g\psi^+(x)\frac{\sigma^a}{2}\psi(x) \\
J^{ai}(x) &= -i\frac{g}{2m}\left(\psi^+(x)\frac{\sigma^a}{2}\partial^i\psi(x) - \partial^i\psi^+(x)\frac{\sigma^a}{2}\psi(x)\right) - \frac{g^2}{4m}\psi^+(x)\psi(x)W^{ia}.
\end{aligned} \tag{6.23}$$

Therefore one can consider:

- $\mathcal{L} = i\psi^+(x)\mathcal{D}_t\psi(x) - \frac{1}{2m}(\mathcal{D}_i\psi(x))^+(\mathcal{D}^i\psi(x))$ in this case the Lagrangian density is completely invariant under gauge transformations, then the total current is covariantely conserved $\partial_\mu j^\mu = 0$ and $\mathcal{D}_\mu \vec{J}^\mu = 0$.

- The Lagrangian density Eq.(6.9), neglecting $\mathcal{L}'$, contains a Gauge fixing term $\mathcal{L}_{Gf} = \frac{g}{2m}\psi^+(x)\left(W_\mu W^\mu\right)\psi(x)$ hence by a infinitesimal gauge transformation this term changes as:

$$\mathcal{L}_{Gf} \to \mathcal{L}'_{Gf} = \mathcal{L}_{Gf} - i\frac{g^2}{2m}\psi^+(x)[W^\mu, U^+\partial_\mu U]_+\psi(x) + O(\theta^2)$$

with $U = \hat{I} - i\theta_a(x)\frac{\sigma^a}{2}$ and $[,]_+$ the anticommutator, then it is gauge invariant if

$$\psi^+(x)[W^\mu, U^+\partial_\mu U]_+\psi(x) = 0 \tag{6.24}$$

but

$$U^+\partial_\mu U = -i\partial_\mu\theta_a(x)\frac{\sigma^a}{2} + O(\theta^2)$$

from which the Eq.(6.24) can be rewritten as

$$\partial_\mu\theta_a(x)\psi^+(x)[W^\mu, \frac{\sigma^a}{2}]_+\psi(x) = 0 \tag{6.25}$$

but $[W^\mu, \frac{\sigma^a}{2}]_+ = \frac{1}{2}W^{a\mu}$ then the gauge fixing condition is:

$$\partial_\mu\theta_a(\psi^+(x)\psi(x)W^{a\mu}) = -\theta_a\partial_\mu(\psi^+(x)\psi(x)W^{a\mu}) + \text{surface term.}$$

Now neglecting the surface term one can write the gauge fixing condition as:

$$\partial_\mu(\psi^+(x)\psi(x)W^{a\mu}) = 0 \text{ for each } a = 1, 2, 3 \tag{6.26}$$

from which

$$\partial_\mu(\psi^+(x)\psi(x)) = 0 \text{ (incompressible fluid)} \tag{6.27}$$

$$\partial_\mu W^{a\mu} = 0 \text{ then } \frac{\partial B^a}{\partial t} = 0 \tag{6.28}$$

Then by Eq.(6.28) one has Gauge invariance if the magnetic field $\vec{B}$ is time independent

In general, however the $\mathcal{L}_{Gf}$ and $\mathcal{L}'$ are of the order $\sim O(\frac{1}{m^3})$ then one neglects them in the first approximation.

6.1.1 Spin-Orbit interactions in low dimensional semiconductors

Now we consider a 2D electron gas where the spin-orbit interactions are important. In particular we study some models where we have a spin orbit interaction due to an external electric field and/or produced, for example, by nuclei in molecules or solids. As frequently discussed, the Rashba spin-orbit (RSO) interaction and Dresselhaus spin-orbit (DSO) interaction exist in two dimensional electron gas (2DEG) made of semiconductor heterostructures. The former, with strength adjustable via the gate voltage[69, 70] results from the inversion asymmetry of

the structure[71], while the latter is due to lack of bulk inversion symmetry[72]. Rashba spin-orbit coupling $H_R = (\alpha/\hbar)(\vec{P} \times \vec{\sigma})$ and the coupling coefficient α is proportional to an external electric field. The Dresselhauss interaction can be written as

$$H_D = \frac{\beta}{\hbar}(P_x\sigma^1 - P_y\sigma^2)$$

For 2D models with SO interaction of Rashba and/or Dresselhaus type, the time component of SU(2) potential (in Gauss units) is

$$A^{a0}(x) = \frac{2g_L}{e}\mu_B B^a(x)$$

with an appropriate Landé factor g_L.
The spatial components are defined as

$$\vec{A}^3(x) = 0$$

$$\vec{A}^1(x) = \frac{2mc}{e\hbar}\begin{pmatrix} -\beta \\ \alpha \\ 0 \end{pmatrix} \quad \vec{A}^2(x) = \frac{2mc}{e\hbar}\begin{pmatrix} -\alpha \\ \beta \\ 0 \end{pmatrix} \tag{6.29}$$

It can be easily checked that the substitution

$$\frac{\hat{P}^2}{2m} \to \frac{1}{2m}(\hat{\vec{P}} - \frac{e}{c}\vec{A}^a\frac{\sigma^a}{2})^2 + eA^{a0}\frac{\sigma^a}{2}$$

allows to obtain the well-known Hamiltonian with SO Rashba and Dresselhaus coupling:

$$H = \frac{\hat{P}^2}{2m} + H_R + H_D + g_L\frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{B}(x) \tag{6.30}$$

Here,

$$H_R = \frac{\alpha}{\hbar}(P_x\sigma^2 - P_y\sigma^1)$$

and

$$H_D = \frac{\beta}{\hbar}(P_x\sigma^1 - P_y\sigma^2)$$

are the Rashba and Dresselhaus terms, respectively.

6.2 Lattice Gauge Theories.

The Lattice gauge theories are the most promising method for extending, at the non-perturbative regime, the Quantum Chromodynamics. The most common approach to these theories is the Lagrangian formulation, where the action and all fields contained in it are discretized on a 4-dimensional Euclidean space.

The Hamiltonian formulation, less often pursued, offers an alternative to the Lagrangian framework with several attractive features. In this case the fields are discretized on a 3-dimensional lattice whereas the time is a continuous

variable, hence in the non-relativistic many body problems this approach has a natural application. In particular we describe the Hubbard model with spin-orbit Rashba and Dresselhauss interactions as a Lattice SU(2) gauge theory.

In a Lattice Gauge Theory the Gauge fields live on the links between two sites, then $U(x,y)$ is the gauge field living between $x,y\in\Lambda$, we remark that, in our case, Λ is a Crystal Lattice defining the structure of a solid. We start describing the Lagrangian theory and as second step we describe the Hamiltonian approach. Therefore let G a gauge transformations Group, its elements are

$$g=e^{i\theta_a T_a},$$

where $\theta_1,...,\theta_n$ are the group parameters and $T_1,...,T_n$ are the group generators. These operators fulfill the commutation rules

$$[T_a,T_b]=if_{abc}T_c,$$

where $(f_{abc})_{a,b,c=1}^n$ are the group structure constants. Let $\Lambda\otimes\mathbb{Z}$ (Λ is a spatial lattice whereas $\mathbb{Z}$ represents the discretized time) a 4-dimensional Euclidean lattice and $\psi(x)$ with $x\in\Lambda\otimes\mathbb{Z}$ the matter field then a local transformation is defined by the following relation:

$$\psi(x)\to\psi'(x)=e^{-i\theta_a(x)T_a}\psi(x). \tag{6.31}$$

The Lagrangian of the matter field contains terms like $\psi^+(x)\psi(x)$ and terms non-local as $\psi^+(x)\psi(y)$. The local terms are naturally gauge invariant whereas the non-local one break the Gauge symmetry, then, as in the continuous case, in order to restore the local invariance one introduces the link Gauge field $U(x,x+e_\mu)$, where e_μ is a unit vector along the μ direction, with $\mu=0,...,3$, and a link vector potential $A_a^\mu(x)=A_a(x,x+e_\mu)$. Therefore, for each pair of $(x,x+e_\mu)$ nearest-neighbor lattice sites we write:

$$\psi(x)^+\psi(x+e_\mu)\to\psi^+(x)U_\mu(x)\psi(x+e_\mu),$$

with

$$U_\mu(x)=U(x,x+e_\mu)=e^{iA_a^\mu(x)T_a}.$$

We remark that $U_\mu^+(x)=U_{-\mu}(x+e_\mu)$. If lattice sites (x,y) are not nearest-neighbor sites, we consider the link path ordered sequence

$$\Gamma(x_1,x_n)=\bigcup_{i=1}^{n-1}(x_i,x_{i+1}),$$

and we define $U(x,y)$ as

$$U(x,y)=\prod_{(z,l)\in\Gamma(x,y)}U(z,z+e_l)=e^{i\sum_{(z,l)\in\Gamma(x,y)}A_a^l(z)T_a}=$$

$$=Pe^{i\int_x^y dx_\mu A^{a\mu}T^a},$$

where the link gauge field is such that

$$U(x,y) \to U'(x,y) = e^{-i\theta_a(x)T_a} U(x,y) e^{i\theta_a(y)T_a}. \tag{6.32}$$

If C is a closed path, that is $C = \bigcup_{i=1}^{p}(x_i, x_{i+1})$ with $x_{p+1} = x_1$ and one defines the Wilson loop

$$W(C) = \prod_{i=1}^{p} U(x_i, x_{i+1})) = Pe^{i \oint dx_\mu A^{a\mu}(x) T^a}$$

then the trace of $W(C)$ is gauge invariant for each C, indeed under Gauge transformation one has $W(C) \to W'(C) = e^{-iT_a\theta_a(x)} W(C) e^{iT_a\theta_a(x)}$ with $x \in C$. On the other hand we know that the plaquettes, elementary square, are the most local closed contours and any closed loop is the union of elementary plaquettes.

In the Group theory two elements g, g' belonging to $\mathcal{G}$ are equivalent if and only if exists $h \in \mathcal{G}$ such that $gh = hg'$ then for each C and C' closed path on lattice one has that $W(C)$ and $W(C')$ are equivalent, but the Action for the Lattice Gauge field (Wilson Action) must be 1)invariant under gauge transformation and 2) function only of the equivalence class of $W(C)$, so a candidate for the Wilson's Action on lattice[74, 75, 76] is:

$$S = \frac{1}{2g^2} \sum_{x \in \Lambda \otimes \mathbb{Z}, \mu\nu} \text{Re Tr} \left(1 - (U_\mu(x) U_\nu(x + e_\mu) U_{-\mu}(x + e_\mu + e_\nu) U_{-\nu}(x + e_\nu))\right). \tag{6.33}$$

Now we indicate the argument of the trace with $W(P)$ that is

$$W(P) = U_\mu(x) U_\nu(x + e_\mu) U_{-\mu}(x + e_\mu + e_\nu) U_{-\nu}(x + e_\nu)$$

$W(P)$ is the Wilson loop on the plaquette $P = (x, x + e_\mu) \bigcup (x + e_\mu, x + e_\mu + e_\nu) \bigcup (x + e_\mu + e_\nu, x + e_\nu) \bigcup (x + e_\nu, x)$. The Wilson Action Eq.(6.33), in the continuous limit, must be the ordinary Action for the Yang and Mills fields where the Lagrangian is defined in Eq.(6.5). In all previous equation the we taken the lattice constant $a = 1$, but if we want study the limit for $a \to 0$ we must write $U_\mu(x) = e^{-igaA_{a\mu}(x)T_a}$ where g is the coupling constant. Indeed the continuous limit is defined as

$$\lim_{a \to 0} \sum_{x \in \Lambda \otimes \mathbb{Z}, \mu\nu} \to \lim_{a \to 0} \int \frac{d^4x}{a^4} \sum_{\mu\nu}.$$

Now, knowing that $A_{-\nu}(x + e_\nu) = -A_\nu(x)$ and $A_{-\mu}(x + e_\mu + e_\nu) = -A_\mu(x + e_\nu)$ we write

$$\text{Tr} W(P) = \text{Tr} \left(e^{-igaA_\mu(x)} e^{-igaA_\nu(x+e_\mu)} e^{igaA_\mu(x+e_\nu)} e^{igaA_\nu(x)} \right) =$$

and using the formula $e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\cdots}$ we have that

$$W(P) \approx$$

$$\approx e^{-iga(A_\mu(x)+A_\nu(x)+a\partial_\mu A_\nu(x)-\frac{iga}{2}[A_\mu(x),A_\nu(x)])}e^{iga(A_\mu(x)+A_\nu(x)+a\partial_\nu A_\mu(x)+\frac{iga}{2}[A_\mu(x),A_\nu(x)])}\approx$$

$$\approx e^{-iga^2F_{\mu\nu}(x)}\approx\left(1-igaF_{\mu\nu}-\frac{a^4g^2}{2}F_{\mu\nu}^2\right),$$

since the trace of the generator T_a is vanish then $\mathrm{Tr}(W(P))\approx\mathrm{Tr}\left(1-\frac{a^4g^2}{2}F_{\mu\nu}^2\right)$ hence we write the Action as

$$\lim_{a\to0}S=\lim_{a\to0}\left(\frac{1}{2g^2}\int\frac{d^4x}{a^4}\sum_{\mu\nu}\mathrm{Tr}(\frac{a^4g^2}{2}F_{\mu\nu}F_{\mu\nu})\right)=$$

$$=\frac{1}{4}\int d^4x\mathrm{Tr}F_{\mu\nu}F_{\mu\nu},$$

hence, in the continuous limit the Wilson Action corresponds to the Euclidean ordinary Yang and Mills Action. A suitable order parameter for a Lattice Gauge theory is the expectation value of the Wilson loop, hence one considers a closed loop (closed link sequence) C and the order parameter is

$$<W(C)>=\frac{1}{Z}\int\prod_{(x',\nu)\in\Lambda\otimes\mathbb{Z}}DU_\mu(x)\prod_{(x,\mu)\in C}U_\mu(x)e^{-S}=\frac{1}{Z}\int DUW(C)e^{-S}$$

where we used the equality $W(C)=\prod_{(x,\mu)\in C}U_\mu(x)$ and Z is the Partition function defined as $Z=\int DUe^{-S}$, furthermore $DU=\prod_{(x',\nu)\in\Lambda\otimes\mathbb{Z}}DU_\mu(x)$ is the Haar measure on the group that has the proprieties:

$$1)\int DU=1$$

$$2)DU=DU'=D(g^+Ug)\text{ for each }g\in\mathcal{G}$$

that is D is invariant for transformation belonging to the Group $\mathcal{G}$. (6.34)

The propriety 1) is a normalization condition, whereas the second one states that the measure on the Group space must be invariant under Group transformations, therefore for each gauge non-invariant function $f(U)$ one has $\int DUf(U)=0$, hence

$$\int DUU_{ij}U_{kl}^+=\mathrm{const}\delta_{il}\delta_{jk}$$

indeed $\mathrm{Tr}(UU^+)$ is gauge invariant whereas $U_{ij}U_{kl}^+$ with $i\neq l$ and $j\neq k$ is gauge dependent, furthermore $\mathrm{Tr}(UU^+)=\mathrm{Tr}\hat{I}=N$ then

$$\int DUU_{ij}U_{kl}^+=\frac{1}{N}\delta_{il}\delta_{jk}$$

$$\int DUU_{ij}=0 \tag{6.35}$$

In the Hamiltonian approach[77] the time is a continuous variable hence we distinguish between plaquettes with a temporal link and those without. Therefore we have

$$\sum_{x,\mu\nu}(...)=\sum_{x,0,0}(...)+\sum_{x,0,i}(...)+\sum_{x,i,0}(...)+\sum_{x,i,j}(...)$$

and we study the system in the temporal gauge hence if $A_0 = 0$ then $U_0(x) = \hat{I}$, furthermore we take $x \in \Lambda \otimes \mathbb{Z} \to (x,t) \in \Lambda \otimes \mathbb{Z}$ where we separated the spatial coordinate by time, hence we can write the Action as

$$S = \frac{1}{2g^2}\left(\sum_{x\in\Lambda, t\in\mathbb{Z}i} \text{Re Tr}(1 - U_i(x,t)U_i^+(x,t+a)) + \text{Re Tr}(1 - U_i(x,t+a)U_i^+(x,t))\right) +$$

$$+\frac{1}{2g^2}\sum_{x\in\Lambda, t\in\mathbb{Z}ij} \text{Re Tr}\left(1 - U_i(x,t)U_j(x+e_i,t)U_i^+(x+e_j,t)U_j^+(x,t)\right) \quad (6.36)$$

where $a = t_{i+1} - t_i$, but

$$(U_i(x,t+a) - U_i(x,t))\left(U_i^+(x,t+a) - U_i^+(x,t)\right) =$$

$$= 2 - U_i(x,t)U_i^+(x,t+a) - U_i(x,t+a)U_i^+(x,t),$$

therefore the Action Eq.(6.36) can be rewritten as

$$S = \frac{1}{2g^2}\sum_{x\in\Lambda, t\in\mathbb{Z}, i} \text{Re Tr}\left(U_i(x,t+a) - U_i(x,t)\right)\left(U_i^+(x,t+a) - U_i^+(x,t)\right) +$$

$$+\frac{1}{2g^2}\sum_{x\in\Lambda, t\in\mathbb{Z}ij} \text{Re Tr}\left(1 - U_i(x,t)U_j(x+e_i,t)U_i^+(x+e_j,t)U_j^+(x,t)\right). \quad (6.37)$$

In the time continum limit one has $\lim_{a\to 0}\sum_{t\in\mathbb{Z}}(...) = \lim_{a\to 0}\int \frac{dt}{a}(...)$ then one has the form $\lim_{a\to 0} S = \int dt L$ wehre L is the Lagrangian defines as

$$L =$$

$$= \frac{1}{2g^2}\sum_{x\in\Lambda} \text{Re Tr}\left(\sum_i \dot{U}_i(x,t)\dot{U}_i^+(x,t) + \sum_{ij}\left(1 - U_i(x,t)U_j(x+e_i,t)U_i^+(x+e_j,t)U_j^+(x,t)\right)\right) \quad (6.38)$$

where the first term is the kinetic part whereas the second one is the potential function. In Eq.(6.38) the matrix elements of the spatial link gauge field are the generalized coordinates, then the conjugate canonical moments are:

$$(P_a(x,t)_{ij} = \frac{\partial L}{\partial(\dot{U}_a(x,t))_{ij}}$$

$$(P_a^+(x,t))_{ij} = \frac{\partial L}{\partial(\dot{U}_a^+(x,t))_{ij}} \quad (6.39)$$

but the kinetic part of the Lagrangian can be rewritten as

$$L_{\text{kin}} = \frac{1}{2g^2}\sum_{x\in\Lambda, a}\left((\dot{U}_a(x,t))_{ij}(\dot{U}_a^+(x,t))_{ji} + (\dot{U}_a^+(x,t))_{ij}(\dot{U}_a(x,t))_{ji}\right) =$$

$$= \frac{1}{g^2} \sum_{x\in\Lambda,a} (\dot{U}_a(x,t))_{ij} (\dot{U}^*_a(x,t))_{ij}$$

hence

$$(P_a(x,t))_{ij} = \frac{1}{g^2}(\dot{U}^*_a(x,t))_{ij} \qquad (P^*_a(x,t))_{ij} = \frac{1}{g^2}(\dot{U}_a(x,t))_{ij}.$$

The Hamiltonian is

$$H = \sum_{x\in\Lambda,a} \Big((P_a(x,t))_{ij} (\dot{U}_a(x,t))_{ij} + (P^*_a(x,t))_{ij} (\dot{U}^*_a(x,t))_{ij} \Big) - L =$$

$$= g^2 \sum_{x\in\Lambda,a} (P^*_a(x,t))_{ij} (P_a(x,t))_{ij} - \frac{1}{2g^2} \sum_{x\in\Lambda,ij} \text{Re Tr} \left(1 - U_i(x,t) U_j(x+e_i,t) U^+_i(x+e_j,t) U^+_j(x,t)\right)$$

furthermore taking

$$P^*_a(x,t))_{ij} (P_a(x,t))_{ij} = \frac{1}{2} \left(P^*_a(x,t))_{ij} (P_a(x,t))_{ij} + P_a(x,t))_{ij} (P^*_a(x,t))_{ij}\right) =$$

$$= \frac{1}{2} \text{Re Tr} \left(P^+_a(x,t) P_a(x,t)\right)$$

here $\cdot^*$ the complex conjugation. The Hamiltonian can be write as follows

$$H = \frac{g^2}{2} \sum_{x\in\Lambda,i} \text{Re Tr} \left(P^+_i(x,t) P_i(x,t)\right) - \qquad (6.40)$$

$$- \frac{1}{2g^2} \sum_{x\in\Lambda,ij} \text{Re Tr} \left(1 - \left(U_i(x,t) U_j(x+e_i,t) U^+_i(x+e_j,t) U^+_j(x,t)\right)\right)$$

Now, the matrix elements $(P_a(x,t))_{ij}$ and $(U_a(x,t))_{ij}$ are canonically conjugate variables hence their Poisson Brakets is:

$$\{(U_a(x,t))_{ij}, (P_b(x',t))_{kl}\} = \delta_{xx'}\delta_{ab}\delta_{ik}\delta_{jl}$$

$$\{(U^*_a(x,t))_{ij}, (P^*_b(x',t))_{kl}\} = \delta_{xx'}\delta_{ab}\delta_{ik}\delta_{jl} \qquad (6.41)$$

we remember that the Piosson Brakets are defined as

$$\{A,B\} = \sum_{x\in\Lambda,aij} \left(\frac{\partial A}{\partial (U_a(x,t))_{ij}} \frac{\partial B}{\partial (P_a(x,t))_{ij}} - \frac{\partial B}{\partial (U_a(x,t))_{ij}} \frac{\partial A}{\partial (P_a(x,t))_{ij}} \right) +$$

$$+ \sum_{x\in\Lambda,aij} \left(\frac{\partial A}{\partial (U^*_a(x,t))_{ij}} \frac{\partial B}{\partial (P^*_a(x,t))_{ij}} - \frac{\partial B}{\partial (U^*_a(x,t))_{ij}} \frac{\partial A}{\partial (P^*_a(x,t))_{ij}} \right) \qquad (6.42)$$

hence, in a most compact way, we can write:

$$\{A,B\} = g^2 \sum_{x\in\Lambda,a} \text{Tr} \left(\frac{\partial A}{\partial U_a(x,t)} \frac{\partial B}{\partial \dot{U}^+_a(x,t)} - \frac{\partial B}{\partial U_a(x,t)} \frac{\partial A}{\partial \dot{U}^+_a(x,t)} \right) + \text{h.c.}$$

In order to quantize this system one must identify the independents degree of freedom, a way is eliminate the $\dot{U}$ (or $P_i(x,t)$ variables in favour of the generators of gauge transformation and impose the opportune constraints. Indeed if one considers the Gauge transformation $U_i(x) \to U_i^{'}(x) = e^{-ig\theta_a(x)T_a} U_i(x) e^{ig\theta_a(x+e_i)T_a}$ with $i,j = 1,...,3$ the Lagrangian (6.38) is invariant, then there is a conserved charge $E_a(t)$ for each generator, indeed, for an infinitesimal Gauge transformation, we have

$$U_i^{'}(x,t) = U_i(x) - ig\left(\theta_a(x) T_a U_i(x,t) - \theta_a(x+e_i) U_i(x,t) T_a\right)$$

hence

$$\begin{aligned}
\delta U_i(x,t) &= -ig \sum_{x' \in \Lambda, a} \theta_a(x') \left(\delta_{x',x} T_a U_i(x,t) - \delta_{x',x+e_i} U_i(x,t) T_a\right) \\
\delta U_i^{+}(x,t) &= ig \sum_{x' \in \Lambda, a} \theta_a(x') \left(\delta_{x',x} U_i^{+}(x,t) T_a - \delta_{x',x+e_i} T_a U_i^{+}(x,t)\right)
\end{aligned} \tag{6.43}$$

then, by the Noether theorem, the conserved charge is

$$\begin{aligned}
E(t) &= \sum_{x \in \Lambda} \left(\frac{\partial L}{\partial (\dot{U}_i(x,t))_{kl}} (\delta U_i(x,t))_{kl} + (\delta U_i^{+}(x,t))_{kl} \frac{\partial L}{\partial (\dot{U}_i^{+}(x,t))_{kl}} \right) = \\
&= \frac{1}{g^2} \sum_{x \in \Lambda, i} \mathrm{Tr}\left(\dot{U}_i^{+}(x,t) \delta U_i(x,t) + \delta U_i^{+}(x,t) \dot{U}_i(x,t) \right)
\end{aligned} \tag{6.44}$$

such that $\frac{dE}{dt} = 0$ that is $E(t)$ is time independent. Now inserting the Eq.(6.43) in the Eq.(6.44) one has:

$$\begin{aligned}
E = -\frac{i}{g} \sum_{x \in \Lambda, ai} \theta_a(x) \{ &(\mathrm{Tr}\left(\dot{U}_i^{+}(x,t) T_a U_i(x,t) - U_i^{+}(x,t) T_a \dot{U}_i(x,t) \right) - \\
&- \mathrm{Tr}\left(U_i(x-e_i,t) T_a \dot{U}_i^{+}(x-e_i,t) - \dot{U}_i(x-e_i,t) T_a U_i^{+}(x-e_i,t) \right) \}
\end{aligned} \tag{6.45}$$

but, being all θ_a independents, by $\dot{E} = 0$ one has $\dot{E}_a = 0$ for each $a = 1,...,N$ with

$$\begin{aligned}
E_a = -\frac{i}{g^2} \sum_{x \in \Lambda, i} \{ &\mathrm{Tr}(\dot{U}_i^{+}(x,t) T_a U_i(x,t) - U_i^{+}(x,t) T_a \dot{U}_i(x,t)) + \\
&+ \mathrm{Tr}(\dot{U}_{-i}^{+}(x,t) T_a U_{-i}(x,t) - U_{-i}^{+}(x,t) T_a \dot{U}_{-i}(x,t)) \} = \sum_{x \in \Lambda, i=-3}^{3} E_{ai}(x)
\end{aligned} \tag{6.46}$$

where $E_{ai}(x) = -\frac{i}{g} \mathrm{Tr}(\dot{U}_i^{+}(x,t) T_a U_i(x,t)) + \mathrm{h.c.}$ is the charge on the link $(x, x+e_i)$, whereas $E_{a,-i}(x)$ on the link $(x-e_i, x)$. Now we write the Hamiltonian Eq.(6.40) in terms of the plaquette variables $U_i(x)$... and charges $E_{ai}(x)$. As

the first step, using the Eq.(8.12), we note that if A, B, C, D are four $N \times N$ matrices then

$$\sum_a \mathrm{Tr}(AT_aB)\mathrm{Tr}(CT_aD) = N\mathrm{Tr}(BADC) - \mathrm{Tr}(AB)\mathrm{Tr}(CD) \tag{6.47}$$

obtaining the following identity

$$\sum_a \sum_{i=1}^{3} E_{ai}(x,t)E_{ai}(x,t) = \frac{4}{g^2}\sum_{i=1}^{3}\left(N\mathrm{Tr}(\dot{U}_i^+(x,t)\dot{U}_i(x,t)) - (\mathrm{Tr}(U_i^+(x,t)\dot{U}_i(x,t))^2\right) \tag{6.48}$$

but, being $U_i(x) = e^{-igA_i(x,t)}$, we can write

$$\dot{U}_i(x,t) = -ig\int_0^1 d\tau e^{-i(1-\tau)gA_i(x,t)}\dot{A}_i(x,t)e^{-i\tau gA_i(x,t)}$$

hence

$$\mathrm{Tr}(U_i^+(x,t)\dot{U}_i(x,t)) = -ig\mathrm{Tr}(\dot{A}_i(x,t)) = -ig\dot{A}_{ai}(x,t)\mathrm{Tr}(T_a) = 0.$$

Therefore the Eq.(6.48) becames

$$\sum_{a=1}^{N}\sum_{i=1}^{3} E_{a,i}(x,t)E_{ai}(x,t) = \frac{4N}{g^2}\sum_{i=1}^{3}\mathrm{Tr}(\dot{U}_i^+(x,t)\dot{U}_i(x,t)) =$$

$$\frac{2N}{g^2}\sum_{i=1}^{3}\mathrm{Tr}\left(\dot{U}_i^+(x,t)\dot{U}_i(x,t) + \dot{U}_i(x,t)\dot{U}_i^+(x,t)\right) = \frac{2N}{g^2}\sum_{i=1}^{3}\mathrm{Re\ Tr}(\dot{U}_i^+(x,t)\dot{U}_i(x,t))$$

hence

$$\sum_{a=1}^{N}\sum_{i=1}^{3} E_{a,i}(x,t)E_{ai}(x,t) = \frac{2N}{g^2}\sum_{i=1}^{3}\mathrm{Re\ Tr}(P_i^+(x,t)P_i(x,t)). \tag{6.49}$$

Now, inserting the Eq.(6.49) in the Eq.(6.40), we obtain:

$$H = \frac{1}{4N}\sum_{x\in\Lambda,a=1}^{N}\sum_{i=1}^{3}(E_{a,i}(x,t))^2 - \frac{1}{2g^2}\sum_{x\in\Lambda,ij=1}^{3}\mathrm{Re\ Tr}\left(1 - \left(U_i(x,t)U_j(x+e_i,t)U_i^+(x+e_j,t)U_j^+(x,t)\right)\right). \tag{6.50}$$

Now writing the charges in terms of coordinates and canonical momenta

$$E_{ai}(x) = i\sum_{lk}\left((P_i(x,t))_{lk}(T_aU_i(x,t))_{lk} - (U_i^+(x,t)T_a)_{lk}(P_i^*(x,t)_{kl}\right)$$

the Poisson Brakets between the charges and the generalized coordinate are:

$$\{E_{ai}(x,t), U_j(x',t)\} = -ig\delta_{ij}\delta_{xx'}T_aU_i(x,t) \tag{6.51}$$

$$\{E_{ai}(x,t), U_j^+(x',t)\} = ig\delta_{ij}\delta_{xx'}U_i^+(x,t)T_a \tag{6.52}$$

with the link indices $i, j = 1, 2, 3$

but being

$$E_{a,-i}(x,t) = -\frac{i}{g^2}\mathrm{Tr}\left(U_i(x-e_i,t)T_a\dot{U}_i^+(x-e_i,t) - \dot{U}_i(x-e_i,t)T_aU_i^+(x-e_i,t)\right)$$

we have

$$\{E_{a,-i}(x',t), U_j(x,t)\} = ig\delta_{ij}\delta_{x',x+e_i}U_i(x,t)T_a \tag{6.53}$$
$$\{E_{a,-i}(x',t), U_j^+(x,t)\} = -ig\delta_{ij}\delta_{x',x+e_i}T_aU_i^+(x,t) \tag{6.54}$$

hence the Poisson Berakets

$$\{E_a(x',t), U_j(x,t)\} = \sum_{i=1}^{3}\left(\{E_{a,i}(x',t), U_j(x,t)\} + \{E_{a,-i}(x',t), U_j(x,t)\}\right)$$

then

$$\{E_a(x',t), U_j(x,t)\} = -ig\left(\delta_{xx'}T_aU_i(x,t) - \delta_{x',x+e_i}U_i(x,t)T_a\right) \tag{6.55}$$
$$\{E_a(x',t), U_j^+(x,t)\} = ig\left(\delta_{xx'}U_i^+(x,t)T_a - \delta_{x',x+e_i}T_aU_i^+(x,t)\right) \tag{6.56}$$

The quantization procedure consist in the replacement observable→operators acting on a Hilbert space and $\{,\} \to -i[,]$, therefore at the Eq.(6.55) and Eq.(6.56) correspond the following commutation rules:

$$\begin{aligned}[E_a(x',t), U_j(x,t)] &= -g\left(\delta_{xx'}T_aU_i(x,t) - \delta_{x',x+e_i}U_i(x,t)T_a\right)\\ [E_a(x',t), U_j^+(x,t)] &= g\left(\delta_{xx'}U_i^+(x,t)T_a - \delta_{x',x+e_i}T_aU_i^+(x,t)\right)\end{aligned} \tag{6.57}$$

whereas at the fundamental Poisson Brakets Eq.(6.41) correspond the commutators

$$\begin{aligned}[(U_a(x,t))_{ij}, (\dot{U}_b^+(x',t))_{kl}] &= ig^2\delta_{ij}\delta_{xx'}\delta_{il}\delta_{kj}\\ [(U_i^+(x,t))_{ij}, (\dot{U}_j(x',t))_{kl}] &= ig^2\delta_{ij}\delta_{xx'}\delta_{il}\delta_{kj}\end{aligned} \tag{6.58}$$

In a quantum theory the charges are the generators of the generalized rotations belonging to the Gauge group. Indeed let $\psi(x)$ the classic matter field, if we perform the transformation $\psi(x) \to \psi'(x) = e^{-ig\theta_a(x)T_a}\psi(x)$ then, in a quantum theory, there is an unitary operator F such that

- for any state $|\alpha>$ we have $|\alpha> \to |\alpha'> = F|\alpha>$
- $<\alpha|\psi(x)|\alpha> \to$
  $\to <\alpha'|\psi(x)|\alpha'> = <\alpha|F^+\psi(x)F|\alpha> = e^{-ig\theta_a(x)T_a} <\alpha|\psi(x)|\alpha>$

where one can write $F = e^{-i\sum_{x\in\Lambda}\theta_a(x)Q_a(x)}$. Then, for an infinitesimal transformation, we have $F^+\psi(x)F = (\hat{I} - ig\theta_a(x)T_a)\psi(x)$ with $F = \hat{I} - ig\sum_{x\in\Lambda}\theta_a(x)Q_a(x)$ then the following commutation rules holds:

$$[Q_a(x'), \psi(x)] = -\delta_{x'x}T_a\psi(x)$$

$$[Q_a(x'), \psi^+(x)] = \delta_{x'x}\psi^+(x) \tag{6.59}$$

the charge operator is $Q_a(x) = \psi^+(x)T_a\psi(y)$. If we consider the Gauge field $U(x,y)$ and $F = e^{-ig\sum_{x\in\Lambda}\theta_a(x)G_a(x)}$ one has:

$$F^+U(x,y)F = e^{-ig\theta_a(x)T_a}U(x,y)e^{ig\theta_a(y)T_a}$$

from which one has the following commutation rules:

$$\begin{aligned}[G_a(x'), U(x,y)] &= -\left(\delta_{x',x}T_aU(x,y) - \delta_{x',y}U(x,y)T_a\right)\\ [G_a(x'), U^+(x,y)] &= \delta_{x',x}U^+(x,y)T_a - \delta_{x',y}T_aU^+(x,y)\end{aligned} \tag{6.60}$$

Now by Eq.(6.60) and Eq.(6.57) we can identify $G_a(x)$ with $gE_a(x)$, furthermore hold the commatation rules:

$$[E_{a,i}(x), E_{b,j}(x')] = if_{abc}E_{c,i}(x)\delta_{ij}\delta_{xx'}. \tag{6.61}$$

Indeed we have

$$[E_{a,i}(x), E_{b,j}(x')] = \frac{i}{g}\mathrm{Tr}([E_{a,i}(x), \dot{U}_j^+(x',t)]T_bU_j(x',t) + \dot{U}_j^+(x',t)T_b[E_{a,i}(x), U_j(x',t)] -$$

$$-[E_{a,i}(x), U_j^+(x',t)]T_b\dot{U}_j(x',t) - U_j^+(x',t)T_b[E_{a,i}(x), \dot{U}_j(x',t)]) =$$

$$= i\delta_{ij}\delta_{xx'}\mathrm{Tr}\left(\dot{U}_j^+(x',t)[T_a,T_b]U_j(x',t) - U_j^+(x',t)[T_a,T_b]\dot{U}_j(x',t)\right) =$$

$$= if_{abc}i\mathrm{Tr}\left(\dot{U}_j^+(x',t)T_cU_j(x',t) - U_j^+(x',t)T_c\dot{U}_j(x',t)\right).$$

If one consider the SU(2) Group the operators then $E_{a,i}(x)$ are the components of an angular momentum, hence taking $|(x,i)n,p>$ the eigenvectors of $E_{z,i}(x)$ and $\sum_{a=1}^3 E_{a,i}^2(x) = E^2(x,i)$ one has

$$E^2(x,i)|(x,i)n,p> = n(n+1)|(x,i)n,p> \tag{6.62}$$

$$E_{z,i}(x)|(x,i)n,p> = p|(x,i)n,p> \tag{6.63}$$

In conclusion the complete (Gauge fields + matter) generators of the Gauge transformations are

$$\begin{aligned}J_a(x) &= \sum_{i=-3}^{3} E_{ai}(x) + \psi^+(x)T_a\psi(x)\\ &\text{with } [J_a(x), J_b(x')] = if_{abc}J_c(x)\delta_{xx'}\end{aligned} \tag{6.64}$$

whereas the physical states are a subspace of the Hilbert space, indeed if $\mathcal{H}$ is the Hilbert space, then the space of physical states is $\mathcal{H}_{phys} \subset \mathcal{H}$ defined as

$$\mathcal{H}_{phys} = \{|\alpha> \in \mathcal{H} \;\; | \left(E_a(x) + Q_a(x)\right)|\alpha> = 0\}$$

the constraint $(E_a(x) + Q_a(x))|\alpha> = (\sum_{i=-3}^3 E_{a,i}(x) + Q_a(x))|\alpha> = 0$ is the Gauss law.

6.2.1 The Hubbard Model with Spin-Orbit interaction.

After having considered the main results for the lattice gauge theory in the preceding section, let us now discuss how they can be applied to the Hubbard model in the presence of SOIs.

Now we conside the non-degenerate Hubbard model with Rashba and Dresselhauss Spin-Orbit coupling, hence defining the spinor $\psi(x) = \begin{pmatrix} c_\uparrow(x) \\ c_\downarrow(x) \end{pmatrix}$, where c_σ is the annihilation operator at site $x \in \Lambda \subset \mathbb{Z}^d$ for an electron with spin σ, then the Hubbard Hamiltonian may be written as

$$H = \sum_{x,y\in\Lambda} t(x-y)\psi^+(x)\psi(y) + U\sum_{x\in\Lambda} n_\uparrow(x)n_\downarrow(x), \tag{6.65}$$

where $n_\sigma(x) = c^+_\sigma(x)c_\sigma(x)$ is the particle number operator with spin σ. This Hamiltonian is rotationally invariant in the spin space, i. e. $[H, S^a] = 0$, where $S^a = \sum_{x\in\Lambda} S^a(x)$ with

$$S^+(x) = c^+_\uparrow(x)c_\downarrow(x) \quad S^-(x) = c^+_\downarrow(x)c_\uparrow(x),$$

$$S^z(x) = \frac{1}{2}(n_\uparrow(x) - n_\downarrow(x)). \tag{6.66}$$

The operators defined by Eq. (6.66) are the SU(2) group generators, and their commutation rules are:

$$[S^+, S^-] = 2S^z \quad [S^z, S^\pm] = \pm S^\pm. \tag{6.67}$$

According to Mermin-Wagner theorem, a spontaneous magnetic order is absent in the Hubbard model. [97] This result has been obtained adding to this Hamiltonian of SU(2) symmetry-breaking term, and applying the Bogoliubov inequality. We notice that the SU(2) symmetry exhibited by the Hubbard model is a global one. To get a SU(2) local gauge symmetry for this model, we may implement the lattice gauge theory previously introduced. In this way the Hubbard Hamiltonian can be written as

$$H = \sum_{x,y\in\Lambda} t(x-y)\psi^+(x)U(x,y)\psi(y) + U\sum_{x\in\Lambda} n_\uparrow(x)n_\downarrow(x) + \\ + H_{gauge}, \tag{6.68}$$

where $U(x,y)$ is a lattice gauge field and H_{gauge} is the free gauge field Hamiltonian.

Introducing the following field operators

$$J^a = \sum_{x\in\Lambda} J^a(x) = \sum_{x\in\Lambda}(\sum_l E^{la}(x) + S^a(x)),$$

i. e. the transformation generators of the local SU(2) group, the Hamiltonian Eq. (6.68) is invariant under the considered group, that is $[J^a(x), H] = 0$. This result can be easily verified using Eqs.(6.59)-(6.60), that for SU(2) group are

$$[J^a, U(x,y)] = -[\frac{\sigma^a}{2}, U(x,y)], \tag{6.69}$$

$$[J^a(x), U(x,y)] = \frac{\sigma^a}{2} U(x,y),$$

$$[J^a(y), U(x,y)] = -U(x,y)\frac{\sigma^a}{2}, \tag{6.70}$$

and

$$[J^a, \psi(x)] = -\frac{\sigma^a}{2}\psi(x) \quad [J^a, \psi^+(x)] = \psi^+(x)\frac{\sigma^a}{2}, \tag{6.71}$$

where σ^i are the Pauli matrices.

The Spin-Orbit coupling can be introduced by the potenetials defined in Eq.(6.29), therefore we introduce SOI in Eq. (6.65) by using the SU(2) lattice gauge theory previously outlined. To this end, we define for our case the link gauge fields as

$$\begin{aligned} U_1(x) &= e^{-i\frac{e}{2\hbar c}\sigma^a A^{1a}(x)} = e^{ig(\beta\sigma^1+\alpha\sigma^2)} = \\ &= \lambda_1 \mathbb{1} + i\lambda_2(\cos\phi\sigma^1 + i\sin\phi\sigma^2) \\ &= \begin{pmatrix} \lambda_1 & \lambda_2 e^{-i(\phi-\frac{\pi}{2})} \\ -\lambda_2 e^{i(\phi-\frac{\pi}{2})} & \lambda_1 \end{pmatrix}, \\ U_2(x) &= e^{-i\frac{e}{2\hbar c}\sigma^a A^{2a}(x)} = e^{-ig(\alpha\sigma^1+\beta\sigma^2)} = \\ &= \lambda_1 \mathbb{1} - i\lambda_2(\sin\phi\sigma^1 + i\cos\phi\sigma^2) = \\ &= \begin{pmatrix} \lambda_1 & -\lambda_2 e^{i\phi} \\ \lambda_2 e^{-i\phi} & \lambda_1 \end{pmatrix}, \\ U_3(x) &= \mathbb{1}, \end{aligned} \tag{6.72}$$

with $g = \frac{m}{\hbar^2}$

$$\lambda_1 = \cos(g\sqrt{\alpha^2+\beta^2}), \quad \lambda_2 = \sin(g\sqrt{\alpha^2+\beta^2}),$$

and $\tan\phi = \frac{\alpha}{\beta}$.
We notice that the link gauge fields verify the following commutation rules:

$$[A^1(x), A^2(x')] = 2i(\alpha^2-\beta^2)\sigma^3,$$

$$[U_1(x), U_2(x')] = 2i(\lambda_2)^2(\cos^2\phi - \sin^2\phi)\sigma^3. \tag{6.73}$$

It is worth stressing that when the coupling constants α and β are equal, the symmetry group becomes an abelian $U(1)$ group. Furthermore, within the definition reported in Eq. (6.29), the gauge fields $U_l(x)$ are independent on the choice of the lattice site. This means that, if the pair of lattice sites (x, y) in

the hopping term of the Hamiltonian Eq. (6.68) are not nearest-neighbor sites, then $U(x,y)$ depends on sites x and y only. But this is not the general case and $U(x,y)$ may depend on the link sequence connecting the x site to the y site. Therefore, if $\Gamma = (x, x_1, ..., x_{n-1}, y)$ is a path on the lattice, then $U_\Gamma(x,y) = U_{i_1}(x)U_{i_2}(x_1)...U_{i_n}(x_{n-1})$ where i_k is the direction on the lattice connecting x_{k-1} and x_k of the path Γ. We point out that it is possible to obtain the general form of $U(x,y)$ by imposing the time reversal symmetry of the Hamiltonian in Eq. (6.68). The time reversal operator is given by

$$T = \prod_{x\in\Lambda} e^{-i\pi S^y(x)} K,$$

where K is the complex conjugation. By imposing $T^+HT = H$ one obtains

$$U(x,y) = \begin{pmatrix} g(x,y) & j(x,y) \\ -j^*(x,y) & g^*(x,y) \end{pmatrix}. \tag{6.74}$$

Here, the functions $g(x,y)$ and $j(x,y)$ are connected to the electronic jump from x to y with spin conservation and spin flip, respectively. These functions depend obviously on the electronic path followed in the jump.
Assuming the local SU(2) gauge symmetry on the lattice, the interaction is contained in the path ordered of the gauge field on the lattice $U(x,y)$, so that the group SU(2) algebra can be used when we apply the Bogoliubov inequality to get the upper bound on the order parameter.

It is important to observe that the spin-orbit coupling breaks explicitly the SU(2) spin symmetry, and therefore we cannot say anything on the spontaneous magnetization. Nevertheless, we will show that within our approach, if Rashba and Dresselhaus coupling constants are equal, then the Hubbard Hamiltonian in Eq. (6.68) exhibits a $U(1)$ rotational symmetry in spin space and the SU(2) can be restored by a gauge transformation in the spin space. This conclusion will be used to prove that if hopping matrix $t(x-y) \backsim O(\frac{1}{|x-y|^2})$ then the magnetic ordering is absent in $d = 2$, for any finite temperature, in agreement with Mermin-Wagner theorem. In $d = 1$, it is always possible to restore the SU(2) symmetry in spin space by a gauge transformation, and therefore the magnetic order is equally absent. On the other hand, the η pairing superconductivity is vanishing for any value assumed by α and β, because the U(1) symmetry in pseudospin space is not broken at all. To better clarify these points we consider separately the study of the magnetic order in the $d = 2$ and the $d = 1$ cases, and then the η pairing long-range.

Magnetic order in two dimensional lattice with $\alpha = \pm\beta$: Here, we show that in the special case when Rashba and Dresselhaus SOI become equal in intensity, the magnetic order is excluded in two-dimensional lattices. When Rashba and Dresselhaus coupling constants are such that $\alpha = \pm\beta$, the link gauge fields, Eqs. (6.72), are:

$$U_1(x) = U_1 = \lambda_1 \mathbb{1} + i\frac{\lambda_2}{\sqrt{2}}(\pm\sigma^1 + \sigma^2),$$

$$U_2(x) = U_2 = \lambda_1 \mathbb{1} - i\frac{\lambda_2}{\sqrt{2}}(\sigma^1 \pm \sigma^2). \tag{6.75}$$

They are commuting operators $[U_1, U_2] = 0$, as it can be deduced looking at Eq. (6.73). Thus, the symmetry group is the $U(1)$ abelian group of rotations around a given direction. This statement implies that the ordering of the link gauge fields is not important and we can write the hopping term in the Hamiltonian in Eq. (6.65) as follows

$$\begin{aligned}
&\sum_{x,y\in\Lambda} t(x-y)\psi^+(x)U(x,y)\psi(y) = \\
&= \sum_{x,y\in\Lambda} t(x-y)\psi^+(x)U_1(x)U_1(x+e_1)* \\
&*...*U_1(x+le_1)U_2(x+le_1)U_2(x+le_1+e_2)...U_1(x+le_1+me_2)* \\
&*\psi(x+le_1+me_2),
\end{aligned} \tag{6.76}$$

where $y = x + le_1 + me_2$, e_1 and e_2 being the unit vectors on the $\hat{x}_1$ and $\hat{x}_2$ axis of the two dimensional lattice, respectively and l and m are integers. Moreover, we can also write

$$U(x,y) = U_1^{y_1-x_1}U_2^{y_2-x_2} = e^{ig'(l-m)\vec{n}_\pm\cdot\vec{\sigma}}, \tag{6.77}$$

with $g' = g\sqrt{\alpha^2+\beta^2}$ and $\vec{n}_\pm = \frac{1}{\sqrt{2}}(1,\pm1,0)$, where the sign + (-) holds if $\alpha = \beta$ ($\alpha = -\beta$). It is easy to verify that if $\alpha = \beta$ then the Hamiltonian in Eq. (6.65) is rotationally invariant around the $\vec{n}_+ = \frac{1}{\sqrt{2}}(1,1,0)$ axis, that is $[\vec{n}\cdot\vec{S}, H] = 0$ where $\vec{S}$ is the total spin. This is also easily observable in the Hamiltonian (6.30), whereas if $\alpha = -\beta$ the symmetry is around the $\vec{n}_- = \frac{1}{\sqrt{2}}(1,-1,0)$ axis. After straightforward algebra, the gauge interaction can be written as

$$U(x,y) = e^{-ig'\theta_\mp(x)\vec{n}_\pm\cdot\vec{\sigma}}e^{ig'\theta_\mp(y)\vec{n}_\pm\cdot\vec{\sigma}}, \tag{6.78}$$

where $\theta_\pm(x) = \sqrt{2}\vec{n}_\pm\cdot\vec{x}$.
Defining a gauge transformation F as

$$F = \prod_{x\in\Lambda} e^{ig'\theta_\mp(x)\vec{n}_\pm\cdot\vec{S}(x)},$$

we find that the Hubbard Hamiltonian with spin orbit coupling is globally SU(2) invariant in the spin space:

$$F^+\psi^+(x)U(x,y)\psi(y)F = \psi^+(x)\psi(y). \tag{6.79}$$

If we consider the average value of the spin projection along $\hat{x}_3$ axis, we can write

$$< S^3(x) >= \mathrm{Tr}(e^{-\beta H}S^3(x)) = \mathrm{Tr}(F^+e^{-\beta H}FF^+S^3(x)F) =$$

$$= \mathrm{Tr}(e^{-\beta F^+ HF}\vec{\rho}\cdot\vec{S}(x)),$$

where $\rho_i = R_{i3}(e_3)_i$ and R is a rotation matrix of $\theta_\mp(x)$ around $\vec{n}_\pm$ axis. The Hamiltonian is now SU(2) invariant, and then by the global gauge transformation $O = e^{-ig'\theta_\mp(x)\vec{n}_\pm\cdot\vec{S}}$ we get

$$< S^3(x) >=< S^3(x) >',$$

where $< >'$ is the average value of the $S^3(x)$ in the transformed Hamiltonian.

Since for the Hubbard model without spin orbit coupling the spontaneous magnetization is absent,[97] introducing the magnetic order parameter as

$$m_h(Q,\Lambda) = \frac{1}{|\Lambda|}\sum_{x\in\Lambda} e^{iQ\cdot x} < S^3(x) >= \frac{1}{|\Lambda|} < S^3(Q) >',$$

we trivially deduce

$$\lim_{h\to 0}\lim_{|\Lambda|\to\infty} m_h(Q,|\Lambda|) = 0.$$

Magnetic order in one dimensional lattice: We consider the Hubbard model on a chain of lattice sites with a constant lattice a assumed for simplicity equal to 1. Therefore, the crystal lattice is $\Lambda \subset \mathbb{Z}$, and the Hubbard Hamiltonian is

$$H = \sum_{l=1}^{|\Lambda|}\sum_{j=1}^{|\Lambda|-l} t(j)\psi^+(l)\psi(l+j) + U\sum_{l=1}^{|\Lambda|} n_\uparrow(l)n_\downarrow(l).$$

In one spatial dimension, we have one link direction, so that the lattice may be seen as a sequence of links. Also, it can be considered as U(1) subgroup of SU(2) where we have one gauge field associated with the link $(l, l+1)$, that is, the group is abelian and its elements are:

$$U_1(x) = e^{-i\frac{e}{\hbar c}\sigma^a A^{1a}} = \lambda_1 \mathbb{1} + i\lambda_2(\cos\phi\sigma^1 + \sin\phi\sigma^2).$$

To introduce the spin-orbit coupling we perform the replacement

$$\psi^+(l)\psi(l+j) \to \psi^+(l)U_1(l)U_1(l+1)...U_1(l+j-1)\psi(l+j) =$$

$$= \psi^+(l)U(l,l+j)\psi(l+j).$$

Since the gauge fields are independent on the site, we write

$$U(l,l+j) = e^{ig'j\vec{n}\cdot\vec{\sigma}}, \tag{6.80}$$

with $g' = g\sqrt{\alpha^2+\beta^2}$ and $\vec{n} = (\cos\phi, \sin\phi, 0)$.

Summarizing, the Hubbard Hamiltonian is rotationally invariant around the vector $\vec{n}$. Indeed if $\vec{S} = \sum_{l=1}^{|\Lambda|}\vec{S}(l)$ denotes the total spin operator, then we have

$[\vec{S}\cdot\vec{n}, H] = 0$. Furthermore, Eq. (6.80) is very similar to Eq. (6.77), so that we may define the unitary operator $F = \prod_{l=1}^{|\Lambda|} e^{ig' l\vec{n}\cdot\vec{S}(l)}$. Therefore, we can write

$$F^+\psi^+(l)U(l,l+j)\psi(l+j)F = \psi^+(l)\psi(l+j),$$

that is, the transformed Hamiltonian is the Hubbard model without the spin-obit interaction. Therefore, using the argument previously outlined for the two-dimensional lattice, we can conclude that the spontaneous magnetization is absent for any α and β values, also in the 1D case.

η pairing long-range order in one and two dimensional lattices: The η pairing long-range order is connected to the spontaneous symmetry breaking of the $U(1)$ invariance around the third axis in the pseudospin space of the Hamiltonian. [99] The Hubbard Hamiltonian exhibits this symmetry and the introduction of the spin orbit interaction does not modify this property. If we define the pseudospin operators as

$$\eta^-(x) = c_\uparrow(x)c_\downarrow(x) \quad \eta^+(x) = c_\downarrow^+(x)c_\uparrow^+(x),$$

$$\eta^3(x) = \frac{1}{2}(n_\uparrow(x) + n_\downarrow(x) - 1),$$

then $[\eta^3, H] = 0$. Here,

$$\eta^3 = \sum_{x\in\Lambda}\frac{1}{2}(n_\uparrow(x) + n_\downarrow(x) - 1).$$

From the commutators

$$[\eta^3, U_1] = [\eta^3, U_2] = 0,$$
$$[\eta^3, \psi(x)] = -\psi(x) \quad [\eta^3, \psi^+(x)] = \psi^+(x), \tag{6.81}$$

it is easy to prove that

$$[\eta^3, \psi^+(x)U(x,y)\psi(y)] = 0.$$

The absence of long-range η pairing in the Hubbard model without spin-orbit coupling has been widely studied. [98] Here, following the same approach, we extend this result to the Hubbard Hamiltonian with SOI. To this end, we introduce the symmetry breaking external field λ in the Hamiltonian as follows

$$H \to H - \lambda(\eta^+(Q) + \eta^-(-Q)),$$

and we define the η pairing order parameter as

$$\Delta(Q) = \lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\sum_{x\in\Lambda} e^{-iQ\cdot x} < \eta^+(x) >=$$

$$= \lim_{|\Lambda|\to\infty}\frac{< \eta^+(Q) >}{|\Lambda|}.$$

To show that long-range η pairing is absent in this model we have to show that

$$\lim_{\lambda \to 0} \Delta_\lambda = 0.$$

So, in the Bogoliubov inequality

$$| < [A, B] > |^2 \leqslant \frac{1}{2k_B T} < [A, A^+]_+ >< [B^+, [B, H]] >, \tag{6.82}$$

we define the operators A and B as

$$A(q) = \eta^+(q + Q) \quad B(q) = \eta^3(-q).$$

Then, from the commutator

$$[B, \psi^+(x)U(x, y)\psi(y)] = (e^{iq\cdot x} - e^{iq\cdot y})\psi^+(x)U(x, y)\psi(y),$$

we get the average value of the double commutator as

$$< [B^+, [B, H]] >=$$

$$= 2 \sum_{x,y \in \Lambda} t(x - y)(1 - \cos(q\cdot (x - y)))*$$

$$* < \psi^+(x)U(x, y)\psi(y) > -\lambda(< \eta^+(Q) > + < \eta^-(-Q) >).$$

Now, if one defines the scalar product by $(A, B) =< A^+ B >$, then by Schwartz inequality one gets

$$< \psi^+(x)U(x, y)\psi(y) ><\leqslant 2,$$

so that

$$| < [B^+, [B, H]] > | \leqslant |\Lambda|(\frac{2q^2}{\rho} + \lambda\Delta(Q, \Lambda)). \tag{6.83}$$

Since $< [A, B] >= |\Lambda|\Delta(Q, \Lambda)$ and

$$\sum_q < [A, A^+]_+ ><\leqslant |\Lambda|^2,$$

by using the Bogoliubov inequality Eq. (6.82) the proof is accomplished. Indeed, we get

$$|\Delta(Q)|^2 \int \frac{d^d q}{(2\pi)^d} \frac{1}{q^2 + \lambda \frac{\rho}{2}\Delta(Q)} \leqslant \frac{2}{\rho k_B T},$$

Thus, by solving the integral we find out that, when $\lambda \to 0$, $\Delta(Q) \to 0$ for d=1, 2, at finite temperature. This implies that the Hubbard model with SOI does not exhibit the η pairing long-range order.

In conclusion we presented an extension of the Mermin-Wagner theorem for the Hubbard model in the presence of SOI, and showed that spontaneous

magnetic order is ruled out in two dimensions, at finite temperature, if the Rashba (α) and the Dresselhaus (β) spin-orbit interactions are such that $\alpha = \pm\beta$. On the contrary, in one-dimension the magnetic order can be excluded, regardless of the values assumed by the spin-orbit coupling constants. We notice that, when Q=0 in $m(Q)$ the ferromagnetic order is forbidden, while choosing Q in such a way that $\exp(iQR_i) = \pm 1$ when R_i connects sites in the same sublattice and different sublattices, respectively, we argue that also the antiferromagnetic order is forbidden. We also proved the absence of long-range η pairing, at finite temperatures, in one- and two-dimensions, independently on α and β interaction parameters. As stated for the magnetic order, looking at the η-pairing order parameter $\Delta(Q)$, we may infer that for $Q = 0$ the s-wave pairing can be excluded, for $Q = \pm\pi$ we exclude the η-pairing, and finally for $Q \neq \{0, \pm\pi\}$ we rule out the existence of generalized η-pairing order with momentum Q.

For copleteness, we note that the Mermin-Wagner theorem follows from the fact that in low-dimensional cases, a diverging number of infinitesimally low-lying excitations is created at any finite temperature, and thus the assumption of a non vanishing order parameter is not self-consistent. This consideration, as well as the rigorous proof, does not apply at T=0, implying that the ground-state may be ordered. For instance, two-dimensional ferro(anti)magnetism is possible at zero temperature: quantum fluctuations oppose but do not prevent the appearance of a two-dimensional magnetically ordered phase. In contrast, for one-dimensional systems quantum fluctuations become so strong that they usually prevent even ground state ordering. Indeed, it is known that the ground-state of the one-dimensional Hubbard model is a non magnetic singlet at any band filling and for any value of Coulomb interaction U. More generally, if the energy spectrum has a gap, it can be shown that the model under investigation does not exhibit long range order, and interestingly, this energy gap plays the role of the temperature in conventional Bogoliubov inequality[46, 40, 47, 73].

Capitolo 7

Conclusions.

We studied the phase transitions in some model of Strongly Correlated System using the Bogoliubov's inequality and the Infrared bounds method, in particular we considered the d-band Hubbard Hamiltonian as theoretical model of the TMO materials. Therefore we defined the Nemetic order parameter as the expectation value of the Quadrupole momentum and in the first step (chapter four) we considered a degenerate multiorbital (d-bands) Hubbard model in the presence of the spin-orbit interaction (SOI) and using the Bogoliubov's inequality we excluded the existence of the nematic order in low dimensional cases at finite temperature of the adopted Hamiltonian specifing, furthermore, the conditions of validity of the our conclusions. We did also an extension to generic k-rank tensorial order parameters and we showed as the Bogoliubov inequality can be used in this cases.

For completeness, we note that the Mermin-Wagner theorem does not apply at T=0, implying that the ground-state may be ordered. Indeed, two-dimensional ferro(anti)magnetism is possible at zero temperature since quantum fluctuations oppose but do not prevent the appearance of a two-dimensional magnetically ordered phase. On the other hand, for one-dimensional systems quantum fluctuations become so strong that they usually prevent even ground state ordering. For instance, the ground-state of the one-dimensional Hubbard model is a non magnetic singlet at any band filling and for any value of Coulomb interaction U. On a more general ground, it can be rigorously shown that if the energy spectrum has a gap then the model under investigation does not exhibit long range order, and interestingly, this energy gap plays the role of the temperature in conventional Bogoliubov inequality[46, 40, 47, 73].

In the following step (chapter five), using the reflection positivity method, we showed that this model at half-filling supports a staggered nematic order if repulsive or attractive on-site inter-orbital and intra-orbital interactions and off-site repulsive inter-orbital interaction are introduced. In more explicit term we obtained that in two and three dimensions the order may exist at least in the Ground state, and we get the condition for its existence. The conclusion is that the the anisotropic off-site interorbital repulsion play an important role

in the formation of the staggered orbital long range order. The Mermin and Wagner arguments are not possible in this case because the rotational symmetry is explicitely broken therefore we can not exclude the order at finite temperature.

The 2D systems have an important role in the modern Condensed Matter Physics, in particular the 2D semiconductors systems with spin orbit interaction are important in spintronic. Therefore we investigated a specific model, namely the single-band Hubbard model, in presence of SOIs, and we rigorously showed that the existence of long-range orders may be ruled out also when SOIs are present and the Bogoliubov inequality method is applied. Since SOIs break the spin symmetry of the model, we first introduced SOIs in the model by imposing local SU(2) gauge symmetry on the lattice, then we re-wrote SOIs in such a way that they are included in the path ordered of the gauge field on the lattice. In this way, the SU(2) invariance is restored allowing the use of the Bogoliubov inequality and the derivation of upper bounds for order parameters. In the Pauli-Schroedinger Lagrangian density the spin orbit terms can be introduced also as a $SU(2)$ Gauge theory[84] where the Yang and Mills fields can be written in terms of the electric and the magnetic fields, this description is useful in the introduction of the covariantly conserved spin current. At this stage, it is worth mentioning that local symmetries, such as the local gauge symmetry, cannot be broken spontaneously, indeed, the Elitzur's theorem [88] states that a local gauge symmetry cannot be broken spontaneously, that is, the expectation value of any gauge non-invariant local observable (order parameter) must vanish. This result means that the spontaneous breaking of the gauge invariance can only occur when the local symmetry is explicitly broken by gauge fixing. Hence, first one chooses a gauge and in this gauge the remaining global gauge symmetry is spontaneously broken, as it happens for instance in the Anderson-Higgs mechanism [89]. We also mention that for two-dimensional systems, if the residual symmetry is continuous, after the gauge fixing, at finite temperatures the associated order parameter must vanish according to the Mermin-Wagner theorem. Nevertheless, when a discrete symmetry is considered then the ordered phase can still exist. In the chapter six, after an introduction of these concepts and a review of the Hamiltonian lattice gauge theory, we studied the non degenerate Hubbard model with Rashba (α) and Dresselhauss (β) spin orbit interaction obtaining that:

- In a two dimensional system if $\alpha = \pm\beta$ the magnetic order is absent whereas the superconductivity (η-pairing) is absent always at finite temperature.
- In a one dimensional system the magnetic order and the η-pairing superconductivity are absents always at finite temperature.

Capitolo 8

Appendices

8.1 Appendix A: Operator inequalities.

An operator on the Hilbert space $\mathcal{H}$, $O : \mathcal{H} \to \mathcal{H}$ is positive semidefinite if for each $|a>$ and $|b>$ one has $< a|O|b > \geq 0$. One can introduce a partial ordering indeed if A and B two operators then $A \geq B$ if $A - B$ is positive semidefinite.

If $f : I \to \mathbb{R}$ a function and O an Hermitian operator on Hilbert space $\mathcal{H}$ one defines a operator function $f(O)$ as:

$$f(O) = \sum_{\alpha} f(\lambda_\alpha)\hat{P}_\alpha$$

where $\{\lambda_\alpha\}$ are the eigenvalues of O and $\hat{P}_\alpha$ the projection operators on relative eigensubspaces.

For the function of operators one can defene the monotony and convexity concept as for real functions, hence:

- **Monotonicity:** Let A and B be two hermitian operators, a function $f : (0, \infty) \to \mathbb{R}$ is said to be operator monotone if for all $A \geq B$ then $f(A) \geq f(B)$
- **Convexity:** function $f : (0, \infty) \to \mathbb{R}$ is said to be operator convex if

$$f(tA + (1-t)B) \leq tf(A) + (1-t)f(B)$$

It is easy to prove the following lemma

Lemma: Let A be a positive defined and bounded selfadjoint operator, if p an integer then:

$$(\mathrm{Tr}A)^p \geq \mathrm{Tr}(A^p). \tag{8.1}$$

Theorem: If A and B are two operators with B selfadjoint and $||B||$ the its norm then one has:

$$\mathrm{Tr}(AB) \leq \mathrm{Tr}(A)||B||. \tag{8.2}$$

Proof: If B is selfadjoint then $\{|b>\}$ are its eigenvectors, hence

$$\mathrm{Tr}(AB) = \sum_b < b|AB|b >= \sum_b < b|A|b > \lambda_b,$$

but for each $|b>$ the eigenvalue $\lambda_b \leq ||B||$ from which the Eq.(8.2)

Peierls inequality: Let $O : \mathcal{H} \to \mathcal{H}$ be a Hermitian operator on Hilbert space $\mathcal{H}$ and f a convex function. if $\{|a>\}$ a basis in $\mathcal{H}$ then:

$$\sum_a f(< a|O|a >) \leq \mathrm{Tr} f(O)$$

Proof:

$$\mathrm{Tr} f(O) = \sum_a < a|\{\sum_\alpha f(\lambda_\alpha)\hat{P}_\alpha\}|a >= \sum_a < a|\{\sum_\alpha f(\lambda_\alpha)\hat{P}^2_\alpha\}|a >=$$

$$= \sum_a \{\sum_\alpha f(\lambda_\alpha)||\hat{P}_\alpha|a > ||^2\} \geq \sum_a f(\sum_\alpha \lambda_\alpha||\hat{P}_\alpha|a > ||^2) = \sum_a f(< a|O|a >)$$

where the inequality arises by Jensen inequality, indeed $\sum_\alpha ||\hat{P}_\alpha|a > ||^2 = 1$. There is equality if each $|\alpha >$ is an eigenvector of O. If $f(t) = e^t$ then

$$\sum_\alpha e^{<\alpha|O|\alpha>} \leq \mathrm{Tr}(e^O). \tag{8.3}$$

Theorem: If $A, B : \mathcal{H} \to \mathcal{H}$ are two bounded selfadjoint operators, then:

$$\mathrm{Tr}(e^{A+B}) \geq \mathrm{Tr}(e^A e^B). \tag{8.4}$$

Proof: Indeed by Trotter's formula and by Eq.(8.1) one write:

$$\mathrm{Tr}(e^{A+B}) = \lim_{n\to\infty} \mathrm{Tr}(e^{\frac{A}{n}} e^{\frac{B}{n}})^n \geq \lim_{n\to\infty} \mathrm{Tr}((e^{\frac{A}{n}})^n (e^{\frac{B}{n}})^n) = \mathrm{Tr}(e^A e^B)$$

Theorem: If $A, B : \mathcal{H} \to \mathcal{H}$ are two bounded selfadjoint operators, if they are positive semidefinite then:

$$\mathrm{Tr}(e^{A+B}) \geq \mathrm{Tr} e^A. \tag{8.5}$$

Proof: taking

$$\mathrm{Tr}(e^{A+B}) - \mathrm{Tr} e^A = \int_0^1 dt \frac{d}{dt} \mathrm{Tr}(e^{A+tB}) = \int_0^1 \mathrm{Tr}(e^{A+tB} B) \geq 0$$

this because $e^{A+tB}B$ is a positive semidefinite operator.

Klein inequality: Let $A, B : \mathcal{H} \to \mathcal{H}$ be two bounded selfadjoint operators and $f : (0, +\infty) \to \mathbb{R}$ then:

$$\mathrm{Tr}[f(A) - f(B) - (A - B)f'(B)] \geq 0. \tag{8.6}$$

Proof: Let $C = A - B$ so that for $0 \leq t \leq 1$, $B + tC = (1 - t)B + tA$. Defining $g(t) = Tr[f(B + tC)]$ then, by the Peierls inequality, it is easy to prove that $g(t)$ is a convex function, and so for all $0 \leq t \leq 1$ one has:

$$g(1) - g(0) \geq \frac{g(t) - g(0)}{t}$$

and in fact the right hand side is monotone decreasing in t. By taking the limit $t \to 0$ one proves the theorem.

Peierls Bogoliubov inequality 1: If $O : \mathcal{H} \to \mathcal{H}$ is an Hermitian operator then the function $f(O) = \ln(\mathrm{Tr}(e^O))$ is convex.
Proof: Let A and B be two Hermitian operators and taking $O(t) = tA + (1-t)B$ and $\{|\alpha >\}$ its eigenvectors fot t fixed then, using the Holder inequality with $p = \frac{1}{t}$ and $q = \frac{1}{1-t}$, one has:

$$Tr(e^{tA+(1-t)B}) = \sum_\alpha e^{<a|tA+(1-t)B|a>} = \sum_\alpha \{e^{t<a|A|a>} e^{(1-t)<a|B|a>}\} \leq$$

$$\leq (\sum_\alpha e^{<a|A|a>})^t (\sum_\alpha e^{<a|B|a>})^{1-t}.$$

By using the Peierls inequality one completes the proof.

Peierls Bogoliubov inequality 2: Let A and B be two bounded operators on the Hilbert space $\mathcal{H}$ then:

$$\ln(\frac{\mathrm{Tr}(e^{A+B})}{\mathrm{Tr}(e^A)}) \geq \frac{\mathrm{Tr}(Be^A)}{\mathrm{Tr}(e^A)}. \tag{8.7}$$

Proof: Indeed $f(t) = \ln \mathrm{Tr}(e^{A+tB})$ is a convex function then

$$f(t) - f(0) \geq t \frac{d}{dt} f(t)|_{t=0},$$

but

$$\frac{d}{dt} f(t) = \frac{1}{\mathrm{Tr}(e^{A+tB})} \mathrm{Tr}(Be^{A+tB})$$

hence by taking $t = 1$ the theorem is proved.

8.2 Appendix B: Proprieties of the $U(n)$ and $SU(n)$ Group

The $M_U(n)$ is the set of the Unitary matrices, that is

$$M_U(n) = \{U \in M_{n\times n}(\mathbb{C}) \ \ |U^+U = \hat{1}\}$$

where $M_{n\times n}(\mathbb{C})$ is the set of the square complex matices of n order. On this set one can define a product between matrices. The pair $(M_U(n), \times)$ (with $\times$ we indicate symbolically the product of matrices) is the Group $U(n)$. If $U \in U(n)$ then $\det(U^+U) = 1$ hence $|\det U| = 1$. Therefore the Group of the matrices belonging $U(n)$ such that $\det(U) = 1$ is the $SU(n)$ Group. Let $U \in U(n)$ then $U = e^{iP}$ with P an Hermitean matrix, therefore it has $N = \frac{4n^2}{2} - 1 = n^2$ independents parameters, indeed one has $(2n)^2$ real parameters (this because there are n^2 complex parameters) but there are the constraint $p_{ij} = p^*_{ji}$ and the diagonal elements must be real. Hence one can defines the real o purely imaginary matrices T_a with $a = 0, ..., N = n^2 - 1$ (we take $T_0 = \hat{I}$) that they form a basis on the space of the Hermitean matrices of n order then: $P = \theta\hat{1} + \theta_i T_i$, hence if $U \in U(n)$ then $U = e^{i\theta\hat{I}+\theta_i T_i} = e^{i\theta}e^{i\theta_i T_i}$, whereas $U \in SU(n)$ then $U = e^{i\theta_i T_i}$. If one defines the inner product between matrices as $(A|B) = Tr(AB)$ then the basis element $\{T_i\}$ can be chosen orthogonal, that is

$$\mathrm{Tr}(T_iT_j) = n\delta_{ij}, \tag{8.8}$$

therefore any matrices Hermitean A is rewritten as

$$A = \alpha_0\hat{I} + \alpha_i T_i \tag{8.9}$$

with $\alpha_0 = \frac{1}{n}\mathrm{Tr}(A)$ and $\alpha_i = \frac{1}{n}\mathrm{Tr}(T_iA)$

Commutation rules for the generators: The commutator $[T_i, T_j]$ is an $n\times n$ matrix with elements real or imaginary, hence by Eq.(8.9) one has $[T_i, T_j] = \alpha_0\hat{I} + \lambda_{ijk}T_k$, but $\alpha_0 = \frac{1}{n}\mathrm{Tr}([T_i, T_j]) = 0$, whereas $\lambda_{ijk} = \frac{1}{n}\mathrm{Tr}(T_k[T_i, T_j])$. The quantities λ_{ijk} are completely antisymmrtryc under permutation of any pair of the indices and they can be chosen real, then $\lambda_{ijk} \to if_{ijk}$, indeed if

$$f_{ijk} = -i\frac{1}{n}\mathrm{Tr}([T_i, T_j]T_k)$$

then the complex conjugate is

$$f^*_{ijk} = i\frac{1}{n}\sum_a < a|[T_i, T_j]T_k|a >^* = i\frac{1}{n}\sum_a < a|T_k[T_j, T_i]|a >= -i\frac{1}{n}\sum_a < a|[T_i, T_j]T_k|a >= f_{ijk}$$

. Therefore the commutation rules of the generators T_i are:

$$[T_i, T_j] = if_{ijk}T_k, \tag{8.10}$$

and the constant f_{ijk} are called structure constant of the Group. By the same procedure one can obtain that

$$[T_i, T_j]_+ = 2\delta_{ij}\hat{I} + d_{ijk}T_k \tag{8.11}$$

where $d_{ijk} = \frac{1}{n}Tr([T_i, T_j]_+ T_k)$.

Fiertz Identity: By Eq.(8.9) one writes $A = \frac{1}{n}Tr(A)\hat{I} + \frac{1}{n}Tr(T_a A)T_a$ hence:

$$A_{ij} = \frac{1}{n}\delta_{ij}\delta_{kl}A_{lk} + \frac{1}{n}(T_a)_{ij}(T_a)_{kl}A_{lk}$$

but being $A_{ij} = A_{lk}\delta_{il}\delta_{jk}$ one has:

$$(T_a)_{ij}(T_a)_{kl} = n\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl} \tag{8.12}$$

Adjoint Representation: Let the generators $\{T_a\}_{a=1}^N$ of SU(n) Group, then it is possible choice the matrices T_a such that $(T_a)_{ij} = -if_{aij}$. This follows by Jacobi identity:

$$[[T_a, T_b], T_c] + [[T_c, T_a], T_b] + [[T_b, T_c], T_a] = 0$$

from which

$$f_{abj}[T_j, T_c] + f_{caj}[T_j, T_b] + f_{bcj}[T_j, T_a] = 0$$

therefore

$$f_{abl}f_{lck} + f_{caj}f_{jbk} + f_{bcj}f_{jak} = 0$$

then the commutation rules (8.10) correspondes to take $(T_a)_{ij} = -if_{aij}$

The Generators $\{T_a\}$ of the Group can be not all real matrices, indeed if the T_a are real for $a = 1, ..., N$ then doing the complex conjugate of the commutation rules $[T_a, T_b] = if_{abc}T_c$ one has $[T_a, T_b] = -if_{abc}T_c$, whereas they can be purely imaginary (Es. the Adjoint representation). If it is necessary to have generators with real representation then the following condition must be fulfilled: if $f_{abc} \neq 0$ then two generators must be real and one purely imaginary.

8.3 Appendix D: Foldy-Wouthuysen Transformation.

In order to obtain a non-relativistic approximation of the Dirac equation a systematic approach exist. Indeed the Foldy Wouthuysen transformation allows to decouple the small and large components of the Dirac wave function. Let $\Psi(x)$ be the Dirac wave function and if it fulfils the Dirac equation:

$$i\frac{\partial}{\partial t}\Psi = H\Psi$$

where H is the Dirac Hamiltonian, for the free case it is $H = -i\vec{\alpha}\cdot\vec{\nabla} + m\beta$. Then we consider the unitary transformation $\Psi = e^{-iS}\Psi'$ therefore the Dirac equation became:

$$i\frac{\partial}{\partial t}\Psi = ie^{-iS}\frac{\partial}{\partial t}\Psi' + (\frac{\partial}{\partial t}ie^{-iS})\Psi' = He^{-iS}\Psi'$$

from which one has:

$$i\frac{\partial}{\partial t}\Psi' = e^{iS}(H - i\frac{\partial}{\partial t})e^{-iS}\Psi'$$

with $H' = e^{iS}(H - i\frac{\partial}{\partial t})e^{-iS}$ the transformed Hamiltonian. The operator S is an opportune Hermitean operator and now we find it. Let us call odd the operators which couple large and small components (like α^i, γ^5,...), even those which do not (as $\hat{I}$, β,...). Now we want to study the non relativistic approximation at the order $\sim (\frac{v}{c})^2$ of a Dirac particle in an external electromagnetic field, then the Hamiltonian is

$$H = -i\vec{\alpha}\cdot(\vec{\nabla} - e\vec{A}) + m\beta + eA_0, \tag{8.13}$$

The actual dimensionless expansion parameters are the operators $(\hbar/mc)\vec{\nabla}$ and $(\hbar/mc^2)(\partial/\partial t)$ then in roughly terms $1/m$. Now we want to compute the non-relativistic correction at the order $\sim O(1/m^2)$, hence as the first step we compute the term

$$e^{iS}i\frac{\partial}{\partial t}e^{-iS} = e^{iS}\int_0^1 dx e^{-i(1-x)S}\dot{S}e^{-ixS} = \int_0^1 dx e^{ixS}\dot{S}e^{-ixS}. \tag{8.14}$$

Then, at the wanted order, the transformed Hamiltonian is:

$$H' = H - \dot{S} + i[S,H] - \frac{1}{2}[S,[S,H]] - \frac{i}{6}[S,[S,[S,H]]] +$$

$$+\frac{1}{24}[S,[S,[S,[S,H]]]] + ... - \frac{i}{2}[S,\dot{S}] + \frac{1}{6}[S,[S,\dot{S}]] + ... \tag{8.15}$$

The Hamiltonian Eq.(8.13) has the form $H = \beta m + \mathcal{E} + \mathcal{O}$ where
$\mathcal{O} = -i\vec{\alpha}\cdot(\vec{\nabla} - e\vec{A})$ is the odd term, whereas $\mathcal{E} = eA_0$ is the even term. In the expansion Eq.(8.15) we take $S = -i\frac{\beta\mathcal{O}}{2m}$, this operator is of the order $\sim O(1/m)$ (of the order $\sim O(v/c)$). Therefore we compute the following commutators:

$$\begin{aligned} [S,\mathcal{O}] &= -i\frac{\beta}{m}\mathcal{O}^2 \quad [S,\mathcal{O}^3] = -i\tfrac{\beta}{m}\mathcal{O}^4 \\ [S,\mathcal{O}^2] &= 0 \qquad [S,\mathcal{O}^4] = 0 \\ [S,\beta] &= \frac{i}{m}\mathcal{O} \qquad [\beta,\mathcal{O}] = 2\beta\mathcal{O} \qquad [S,\dot{S}] = \frac{i}{2m}[\mathcal{O},\dot{\mathcal{O}}]. \end{aligned} \tag{8.16}$$

Then we have

$$[S,H] = i(\mathcal{O} - \frac{\beta}{m}\mathcal{O}^2 - \frac{\beta}{2m}[\mathcal{O},\mathcal{E}]) \tag{8.17}$$

$$[S,[S,H]] = \frac{\beta}{m}\mathcal{O}^2 + \frac{\mathcal{O}^3}{m^2} + \frac{1}{4m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]]$$
$$[S,[S,[S,H]]] = i(\frac{\mathcal{O}^3}{m^2} - \frac{\beta\mathcal{O}^4}{m^3} - \frac{\beta}{8m^3}[\mathcal{O},[\mathcal{O},[\mathcal{O},\mathcal{E}]]])$$
$$[S,[S,[S,[S,H]]]] = \frac{\beta\mathcal{O}^4}{m^3}$$

where we neglect all terms of the order $\sim O(1/m^4)$ ($\sim O((v/c)^4)$), furthermore

$$\dot{S} = -i\frac{\beta}{2m}\dot{\mathcal{O}} \tag{8.18}$$
$$[S,\dot{S}] = \frac{1}{4m^2}[\mathcal{O},\dot{\mathcal{O}}]$$
$$[S,[S,\dot{S}]] = -\frac{i\beta}{8m^3}[\mathcal{O},[\mathcal{O},\dot{\mathcal{O}}]]$$

Therefore by Eq.(8.15) the transformed Hamiltonian is:

$$H' = \beta m + \mathcal{E} - \frac{\beta}{48m^3}([\mathcal{O},[\mathcal{O},[\mathcal{O},\mathcal{E}]]] + i[\mathcal{O},[\mathcal{O},\dot{\mathcal{O}}]]) +$$

$$+\beta(\frac{\mathcal{O}^2}{2m} + \frac{1}{2m}[\mathcal{O},\mathcal{E}] - \frac{\mathcal{O}^4}{8m^3}) - \frac{\mathcal{O}^3}{3m^2} - \frac{1}{8m^2}([\mathcal{O},[\mathcal{O},\mathcal{E}]] + i[\mathcal{O},\dot{\mathcal{O}}]) + i\frac{\beta}{2m}\dot{\mathcal{O}}. \tag{8.19}$$

The equation (8.19) has the same form of the original Hamiltonian $H' = \beta m + \mathcal{E}' + \mathcal{O}'$ but now the odd term is an infinitesimal of higher order. Indeed

$$\mathcal{E}' = \mathcal{E} + \beta(\frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3}) - \frac{1}{8m^2}([\mathcal{O},[\mathcal{O},\mathcal{E}]] + i[\mathcal{O},\dot{\mathcal{O}}]) \tag{8.20}$$
$$\mathcal{O}' = -\frac{\mathcal{O}^3}{3m^2} + \frac{\beta}{2m}[\mathcal{O},\mathcal{E}] + i\frac{\beta}{2m}\dot{\mathcal{O}} - \frac{\beta}{48m^3}([\mathcal{O},[\mathcal{O},[\mathcal{O},\mathcal{E}]]] + i[\mathcal{O},[\mathcal{O},\dot{\mathcal{O}}]])$$

In order to delete $\mathcal{O}'$ is necessary another step and one defines $S' = -\frac{i\beta}{2m}\mathcal{O}' \sim O(1/m^2)$ and one compute the new Hamiltonian:

$$H'' = e^{iS'}(H' - i\frac{\partial}{\partial t})e^{-iS'} \approx$$

$$\approx H' + i[S',H'] - \frac{1}{2}[S',[S',H']] - \dot{S}' \tag{8.21}$$

then

$$[S',H'] = i\mathcal{O}' - i\frac{\beta}{2m}[\mathcal{O}',\mathcal{E}'] - i\frac{\beta}{m}\mathcal{O}'^2 \tag{8.22}$$
$$[S'[S',H'] = \frac{\beta}{m}\mathcal{O}'^2$$
$$\dot{S}' = -i\frac{\beta}{2m}\dot{\mathcal{O}}'$$

where we neglected all terms of the order $\sim O(\frac{1}{m^4})$ then the Eq.(8.21) can be rewritten as:

$$H'' = \beta m + \mathcal{E}' + \frac{\beta}{2m}[\mathcal{O}', \mathcal{E}'] + \frac{\beta}{2m}\mathcal{O}'^2 + i\frac{\beta}{2m}\dot{\mathcal{O}}' = \beta m + \mathcal{E}' + \mathcal{O}'' \tag{8.23}$$

It is necessary another step, hence one defines $S'' = -i\frac{\beta}{2m}\mathcal{O}'' \sim O(1/m^3)$ where

$$\mathcal{O}'' = \frac{\beta}{2m}[\mathcal{O}', \mathcal{E}'] + \frac{\beta}{2m}\mathcal{O}'^2 + i\frac{\beta}{2m}\dot{\mathcal{O}}'$$

then, at this order one has:

$$H''' = e^{iS''}(H'' - i\frac{\partial}{\partial t})e^{-iS''} = H'' + i[S'', H''] - i\dot{S}'' \tag{8.24}$$

then we compute

$$[S'', H''] = i\mathcal{O}'' - \frac{i}{2m}\beta[\mathcal{O}'', \mathcal{E}'] - \frac{i}{m}\beta\mathcal{O}''^2$$

but $\frac{i}{m}\beta\mathcal{O}''^2 \sim O(\frac{1}{m^5})$, $\frac{i}{2m}\beta[\mathcal{O}'', \mathcal{E}'] \sim O(\frac{1}{m^3})$ and $\dot{S}'' \sim O(\frac{1}{m^3})$, therefore, neglecting all terms $\sim O(1/m^4)$ one has

$$H''' = H'' - \mathcal{O}'' + \frac{1}{2m}\beta[\mathcal{O}'', \mathcal{E}'] - \frac{\beta}{2m}\dot{\mathcal{O}}'' = \beta m + \mathcal{E}' + \mathcal{O}''' \tag{8.25}$$

with

$$\mathcal{O}''' = \frac{\beta}{2m}[\mathcal{O}'', \mathcal{E}'] - \frac{\beta}{2m}\dot{\mathcal{O}}'' \tag{8.26}$$

therefore we define $S''' = -\frac{i\beta}{2m}\mathcal{O}'''$ obtaining

$$H^{(4)} = H''' + i[S''', H'''], \tag{8.27}$$

now computing the commutator we have that $[S''', H'''] \approx i\mathcal{O}''' + O(1/m^4)$ then $H^{(4)} = \beta m + \mathcal{E}' + O(1/m^4)$. After these considerations one can write the Eq.(8.24) as

$$H^{(4)} =$$
$$= \beta(m + \frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3}) + \mathcal{E} - \frac{1}{8m^2}([\mathcal{O}, [\mathcal{O}, \mathcal{E}]] + i[\mathcal{O}, \dot{\mathcal{O}}]) \tag{8.28}$$

then the Dirac equation with the transformed Hamiltonian correspondes to two independent equations for the big and small component of the Dirac spinor Ψ at the considered order. Now we must compute in explicit way the terms in Eq(8.28). Being $\mathcal{O} = -i\vec{\alpha}\cdot(\vec{\nabla} - ie\vec{A})$ and $\dot{\mathcal{O}} = -e\vec{\alpha}\cdot\dot{\vec{A}}$ we have:

$$i[\mathcal{O}, \dot{\mathcal{O}}] = -e\{\alpha^i\alpha^j\partial^i\dot{A}^j + [\alpha^i, \alpha^j]\dot{A}^j(\partial^i - ieA^i)\} \tag{8.29}$$

and, being $[\mathcal{O}, \mathcal{E}] = -ie\alpha^i\partial^i A^0$ one has:

$$[\mathcal{O}, [\mathcal{O}, \mathcal{E}]] = -e\{\alpha^i\alpha^j\partial^i\partial^j A^0 + [\alpha^i, \alpha^j]\partial^j A^0(\partial^i - ieA^i)\} = \tag{8.30}$$
$$= -e\nabla^2 A_0 + 2e\vec{\Sigma}\cdot(\vec{\nabla}A_0 \times (\vec{\nabla} - ie\vec{A})),$$

where $\Sigma^i = \begin{pmatrix} \sigma^i & 0 \\ 0 & \sigma^i \end{pmatrix}$. Furthermore $[\mathcal{O}, -e\nabla^2 A^0] = ie\nabla^2\vec{\alpha}\cdot\vec{\nabla}A^0$ therefore summing the Eq.(8.29) with Eq.(8.30) one has

$$[\mathcal{O},[\mathcal{O},\mathcal{E}]] + i[\mathcal{O},\dot{\mathcal{O}}] = e\{\alpha^i\alpha^j\partial^i E^j + [\alpha^i,\alpha^j]E^j(\partial^i - ieA^i)\} \tag{8.31}$$

where we used the identity $E^i = -(\partial^i A^0 + \dot{A}^i)$ with $\vec{E}$ the electric field. The Dirac spinor is $\Psi = \begin{pmatrix} \psi \\ \chi \end{pmatrix}$ hence if we consider only the upper component then the Eq.(8.31) can be rewritten as

$$[\mathcal{O},[\mathcal{O},\mathcal{E}]] + i[\mathcal{O},\dot{\mathcal{O}}] = e\vec{\nabla}\cdot\vec{E} - ie\vec{\sigma}\cdot\frac{\partial\vec{B}}{\partial t} - 2ie\vec{\sigma}\cdot(\vec{E}\times(\vec{\nabla} - ie\vec{A})). \tag{8.32}$$

On the other hand one has

$$\frac{\mathcal{O}^2}{2m} = -\frac{1}{2m}(\vec{\nabla} - ie\vec{A})^2 + \frac{e}{2m}\vec{\sigma}\cdot\vec{B} \tag{8.33}$$

where $\vec{B}$ is the magnetic field. Furthermore

$$\begin{aligned} -\frac{\mathcal{O}^4}{8m^3} &= -\frac{1}{2m}(\frac{1}{2m}(\vec{P} - e\vec{A})^2 + \frac{e}{2m}\vec{\sigma}\cdot\vec{B})^2 = \\ &= -\frac{1}{8m^3}((\vec{P} - e\vec{A})^4 + e^2(\vec{\sigma}\cdot\vec{B})^2 + e(\vec{P} - e\vec{A})^2(\vec{\sigma}\cdot\vec{B}) + \\ &\quad + e(\vec{\sigma}\cdot\vec{B})(\vec{P} - e\vec{A})^2) \end{aligned} \tag{8.34}$$

therefore the complete Dirac equation approximation is

$$\begin{aligned} i\frac{\partial\psi}{\partial t} = \{m + \frac{1}{2m}(\vec{P} - e\vec{A})^2 + eA^0 + \frac{e}{2m}\vec{\sigma}\cdot\vec{B} - \frac{e}{4m^2}\vec{\sigma}\cdot\vec{E}\times(\vec{P} - e\vec{A}) - \frac{ie}{8m^2}\vec{\sigma}\cdot(\vec{\nabla}\times\vec{E}) - \\ - \frac{e\vec{\nabla}\cdot\vec{E}}{8m^2} - \frac{e^2}{8m^2}\vec{B}^2 - \frac{1}{8m^3}((\vec{P} - e\vec{A})^4 + e(\vec{P} - e\vec{A})^2(\vec{\sigma}\cdot\vec{B}) + e(\vec{\sigma}\cdot\vec{B})(\vec{P} - e\vec{A})^2\}\psi. \end{aligned} \tag{8.35}$$

For time independent electric and magnetic fields with $\vec{B}$ uniform the equation, in the Coulomb gauge, becames

$$i\frac{\partial\psi}{\partial t} = \{m + \frac{1}{2m}\vec{P}^2 + eA^0 + \frac{e}{2m}(\vec{L} + 2\vec{S})\cdot\vec{B} - \frac{\vec{P}^4}{8m^3} - \frac{e\vec{\nabla}\cdot\vec{E}}{8m^2} + H_{so}\}\psi \tag{8.36}$$

where $\vec{L} = \vec{x}\times\vec{P}$ is the angular momentum of the particle, $\vec{S} = \frac{\vec{\sigma}}{2}$ and H_{so} the spin orbit interaction defined as $H_{so} = -\frac{e}{4m^2}\vec{\sigma}\cdot\vec{E}\times\vec{P}$. In a central electrostatic potential the spin orbit interaction has the following expression:

$$H_{so} = \frac{e}{2m^2 r}\frac{\partial A^0}{\partial r}\vec{S}\cdot\vec{L}$$

Now we know that $[P^i - eA^i, (\vec{\sigma} \times \vec{E})_i] = -i\partial^i(\vec{\sigma} \times \vec{E})_i$ then with reference to the Eq.(8.35) we rewrite the spin orbit term as follows:

$$H_{so} = -\frac{e}{4m^2}\vec{\sigma} \cdot (\vec{E} \times (\vec{P} - e\vec{A})) - \frac{ie}{8m^2}\vec{\sigma} \cdot (\vec{\nabla} \times \vec{E}) =$$

$$= -\frac{e}{4m^2}(\vec{\sigma} \times \vec{E}) \cdot (\vec{P} - e\vec{A}) + \frac{ie}{8m^2}\vec{\nabla} \cdot (\vec{\sigma} \times \vec{E}) =$$

$$= -\frac{e}{4m^2}(\vec{\sigma} \times \vec{E}) \cdot (\vec{P} - e\vec{A}) - \frac{e}{8m^2}[P^i - eA^i, (\vec{\sigma} \times \vec{E})_i] =$$

$$= -\frac{e}{8m^2}((\vec{\sigma} \times \vec{E}) \cdot (\vec{P} - e\vec{A}) + (\vec{P} - e\vec{A}) \cdot (\vec{\sigma} \times \vec{E})), \tag{8.37}$$

therefore the kinetic and spin orbit terms in Eq.(8.35) can be rewritten as

$$\frac{1}{2m}(\vec{P} - e\vec{A})^2 + H_{so} =$$

$$= \frac{1}{2m}(\vec{P} - e\vec{A} - \frac{e}{2m}\frac{\vec{\sigma}}{2} \times \vec{E})^2 - \frac{e^2}{32m^3}(\vec{\sigma} \times \vec{E})^2. \tag{8.38}$$

In order to cancel the rest energy m in the Eq.(8.35) one performs the phase transformation $\psi \to e^{-imt}\psi$, then the complete Hamiltonian is

$$H = \frac{1}{2m}(\vec{P} - e\vec{A} - \frac{e}{2m}\frac{\vec{\sigma}}{2} \times \vec{E})^2 + eA^0 + \frac{e}{2m}\vec{\sigma} \cdot \vec{B} -$$

$$-\frac{e^2}{8m^3}(\vec{B}^2 + (\frac{\vec{\sigma}}{2} \times \vec{E})^2) - \frac{1}{8m^3}((\vec{P} - e\vec{A})^4 + e(\vec{P} - e\vec{A})^2(\vec{\sigma} \cdot \vec{B}) + e(\vec{\sigma} \cdot \vec{B})(\vec{P} - e\vec{A})^2$$

then the complete equation is:

$$i\frac{\partial\psi}{\partial t} = \{\frac{1}{2m}(\vec{P} - e\vec{A} - \frac{e}{2m}\frac{\vec{\sigma}}{2} \times \vec{E})^2 + eA^0 + \frac{e}{2m}\vec{\sigma} \cdot \vec{B} + H_{GSB}\}\psi, \tag{8.39}$$

where

$$H_{GSB} = -\frac{e^2}{8m^3}(\vec{B}^2 + (\frac{\vec{\sigma}}{2} \times \vec{E})^2) - \frac{1}{8m^3}((\vec{P} - e\vec{A})^4 + e(\vec{P} - e\vec{A})^2(\vec{\sigma} \cdot \vec{B}) + e(\vec{\sigma} \cdot \vec{B})(\vec{P} - e\vec{A})^2)$$

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