THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Non-linear Canonical Methods in Strongly Correlated Electron Systems

Foundations and Examples

Matteo Bazzanella

GÖTEBORGS UNIVERSITET

Department of Physics
University of Gothenburg
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Matteo Bazzanella

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Department of Physics
University of Gothenburg
SE-412-96 Gothenburg, Sweden
Telephone: +46 (0)31-786 0000

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Abstract

In this thesis some new ideas to perform the analysis of Strongly Correlated Electronic Systems (SCES) are developed. In particular the use of non-linear canonical transformations is considered thoroughly. Using such transformations it is possible, in some circumstances, to simplify the quantum problem redefining the fermionic degrees of freedom used to describe the system. To understand and use effectively these non-linear transformations it is convenient to work in the Majorana fermion representation, i.e. to represent the quantum mechanical operators in terms of Majorana fermions. These objects can be imagined as algebraic constituents of the fermionic degrees of freedom. In a fermionic system, different equivalent sets of (emergent) Majorana fermions can be used to build the fermionic operators that characterize the system. The non-linear transformations can be seen as a way to mix these equivalent sets. Thanks to this insight, it becomes possible to characterize the full structure of the group of canonical transformations and to identify an advantageous framework, which allows their use in the study of a generic SCES system. To test these statements the Hubbard and the Kondo lattice models were intensively studied making use of non-linear canonical transformations, obtaining interesting results in both cases. For example, in the Hubbard model a free fermion mean-field description of the paramagnetic Mott insulator was identified, while in the Kondo lattice it was possible to describe already at mean-field level the spin-selective Kondo insulating phase, consistently (from a quantitative and qualitative point of view) with the known numerical results. Moreover the method elaborated for the study of the Hubbard model is suitable for a systematic generalization to other situations and shows great room for improvement. These results prove that, thanks to the redefinition of the degrees of freedom used in the analysis of the system, it becomes possible to obtain quite non-trivial results already at mean-field level, or to consider very involved (but meaningful) correlated quantum states via simple variational trial states. This will potentially permit a more judicious and profitable choice of the fundamental degrees of freedom, allowing for an improvement of the efficiency of the analytical and numerical techniques used in the analysis of many SCES systems.

Acknowledgments

This thesis is the summary of four years of work that I carried out at the University of Gothenburg. Of course such a work would have not been possible without the help of many other persons, who I want to mention. Great thanks go to my supervisor Dr. Johan Nilsson, who introduced me to this interesting topic and kept pushing me forward and listening to me, also when the ideas did not want to converge to anything meaningful. A special mention must go to Erik Eriksson, Hugo Strand and Prof. Mats Granath, who engaged me in many fruitful discussions and also helped me reviewing this Thesis. I want to acknowledge also all the other persons with whom I had the pleasure to have a continuos exchange of ideas, starting from the eldest members of our theoretical physics group: Prof. Stellan Östlund, Prof. Henrik Johannesson, Prof. Bernhard Mehlig, Prof. Bo Hellsing; and continuing with the other students (or ex-students) who met me here at the Department, in particular Kristian Gustavsson, Anders Ström, Marina Rafajlovic, Jonas Einarsson, Erik Werner and Anna-Karin Gustavsson. Ideas are the precious and delicious fruits of a tree with long and twisted roots. It's impossible to determine who or what promotes their growth. What's important is to keep watering the tree and its roots through critical thinking, exchange of ideas and mutual respect; so I thank everybody listed above, who have all done this with consideration and care.

I also want to thank my dear Abigail, who not only supported me daily, but also gave me an invaluable help proofreading the Thesis. As last acknowledgment, I must mention also the Department of Physics of University of Trento, where I obtained my undergraduate instruction and all the friends and relatives, who followed from home my work with high interest. In particular I thank my parents that with sacrifices supported my studies.

Matteo Bazzanella
Göteborg, 20/10/2014

List of papers

This thesis consists of an introductory text and the following papers:

Paper A:
Matteo Bazzanella and Johan Nilsson,
"Non-Linear methods in Strongly Correlated Electron Systems",
(in manuscript), arXiv:1405.5176.

Paper B:
Johan Nilsson and Matteo Bazzanella,
"Free fermion description of a paramagnetic Mott insulator",
(in manuscript), arXiv:1407.4310.

Paper C:
Matteo Bazzanella and Johan Nilsson,
"Ferromagnetism in the one-dimensional Kondo lattice: mean-field approach via Majorana fermion canonical transformation",
Phys. Rev. B **89**, 035121 (2014).

Paper D:
Johan Nilsson and Matteo Bazzanella,
"Majorana fermion description of the Kondo lattice: variational and path integral approach",
Phys. Rev. B **88**, 045112 (2013).

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Contents

Chapter 1

Preface

I first encountered the term "Majorana fermions" in 2010, at the beginning of this thesis project, at which time my attention was caught by the compelling name as well as the mysterious concepts behind it. The Majorana fermions discussed in condensed matter are indeed very unusual "quasiparticles": chargeless, uncountable, without a vacuum and not closely related to the original solution to the Dirac equation on real field, discovered by Ettore Majorana in the early Nineteens-thirties [1]. How can they be considered particles? Why are so many people interested in them? Can they somehow be useful? This thesis began when I, together with my supervisor Dr. Johan Nilsson, started to consider these issues; specifically, to pursue answers to the last question.

In recent years there has been increasing interest in the physics of Majorana fermions (Majoranas), or, to be more precise, in the physics of topological Majorana fermions[1] [3–5]. Their realization in real systems, their properties and their possible applications are still the subject of debate and they represent a truly interesting challenge being taken up by more and more physicists. The focus of this formidably innovative branch of research always lied outside my own greatest interests, though of course, like so many others, I was fascinated by the simplicity and the effectiveness of, for example, Kitaev's original paper [6]. Indeed what really caught my attention in that work, was not the possibility to build a fermionic mode with two spatially separated coherent components; instead my imagination was captured by the fact that the electrons can be broken into two well defined parts in such a formally elegant way, and that these half fermions can then be reassembled, like the pieces of a puzzle, to represent the Hamiltonian with fermionic operators that suit it nicely, exploiting its physical properties in a straightforward way. This feeling immediately forced me to focus on one single question: "Can this simple way to represent the original fermions of a model in terms of Majoranas bring some new insight in the study of strongly correlated electron systems?".

Strongly Correlated Electron Systems (SCES) have been the focus of research of a large part of the condensed matter community for the last thirty years. These systems represent such a challenge that even their rigorous def-

[1] Sometimes also indicated with by the name "Majorana zero modes" and others. See discussion in Chapter 2 and Ref. [2].

inition is controversial. Keeping a broad view, one could include in this class all the systems where the effect of correlations[2] between the electrons is more important than those due to their delocalization.[3] In this sense Mott insulators, cuprates, heavy electron compounds, quantum dots, spin systems, and many others can be considered as strongly correlated. These systems are often studied using model Hamiltonians, appositely designed to capture their main physical properties [7]. The most well-known model is certainly the Hubbard model [8], the extreme simplicity of which is contrasted by the conceptual and formal challenges posed by its analysis. The study of these model Hamiltonians relies on traditional analytical tools that have roots (in most cases) in the idea of the Landau-Fermi liquid and in perturbative analysis [9–11]. By definition, such ideas are inadequate in the SCES context: indeed the special role played by the kinetic terms, which implies the idea of free (bare) electrons and is also an expression of their delocalization, is not natural to the physics of the SCES. Therefore it is not a surprise if these techniques face major problems when the effect of correlations between electrons challenges their delocalization.

The only known universally feasible way to tackle a SCES systems relies on numerical studies. In the last decades numerical methods have blossomed thanks to the huge improvement of the available digital technologies, and these methods have been heavily applied in the study of many model Hamiltonians. Of course the results obtained numerically are a major leap forward towards the solution of many open questions, however they do not necessarily represent the ultimate tool. In fact, although capable of treating the interactions in a less approximate way, they descend from the same interpretations, ideas and paradigms used by the analytical approach. On the one hand the systems can be solved and the properties computed, but on the other hand it is not clear if the physical picture provided is the simplest and most rational. Moreover, in many model systems even numerical studies have not been successful in obtaining reliable solutions (for example in the case of the cuprates). Therefore a shift in the paradigms that we use to study the different Hamiltonians could have potential benefits for both analytical and numerical techniques.

An important lesson can be learnt from the few situations where analytical techniques proved themselves invaluable, providing exact solutions to involved quantum interacting problems. The analysis of the one dimensional Luttinger liquid [12] can be used as example, which has been solved making use of bosonization and Bethe Ansatz. Another example is given by the high (infinite) interacting limit of the Hubbard model, which can be tackled via unitary transformations. The techniques used in these two examples are not universal, in the sense that they are effective only in very specific situations, but the lesson that they teach is instead a fundamental one: the weakness of the concept of the electron. The bosonized solution of the Luttinger liquid is very representative in this sense, since it highlights the separation of the electrons into two different quantum modes, i.e. the holon (charge) and the spinon (spin) modes [12–14]. In

[2] With the term correlation I here mean the sensitivity of an electron mode to the disposition of the other electrons, i.e., on the global configuration of the system. The latter can substantially affect the dynamics and the properties of the electron quantum mode itself, also causing its "destruction", or in other words, making it not a good degree of freedom for the description of the physics of the system, i.e. a degree of freedom too far from the eigenstates of the system.

[3] Delocalization here means the tendency of the electron mode to spread its wavefunction over different lattice sites. In some sense it represents the tendency of the electron to "exist" as a good quantum mode in the system, as a convenient way to describe the physics of the system.

the Luttinger model these modes have the right to be considered fundamental. The general lesson that can be derived is that although electrons (the fundamental particles of charge $-1e$, total squared spin $3\hbar^2/4$ and mass approximately 0.5 MeV) are inside any solid state system, the modes that describe correctly the physics, e.g. the ground state and the excitations, at the energy scale typical of condensed matter studies (≈ 1 eV and less), cannot always be thought of as (dressed) electrons, because the dynamics and properties (quantum numbers) of the electron do not fit the physics of the system. This non-fundamental nature of the electron[4] is quite general, so in some circumstances it is expected that other degrees of freedom must be used to describe and understand the physics of a system. These are not mere theoretical speculation, but facts verified experimentally: for example it has been observed that the electron splits (under specific conditions) into three constituent quasiparticles named holon, spinon and orbiton [15–20]. With these lessons in mind, one cannot be surprised by conjectures about the existence of Majorana fermions. If the electrons, or better the electronic modes, cannot be seen as fundamental (universal) bricks, then it cannot be wrong either to split them into halves, as long as some caution is taken. Also this is not a mere mathematical speculation, since effects due to Majorana modes (may) have already been observed in experiments [21].

The main feature of SCES is probably the inadequateness of the original electron modes, which correspond to the electron operators used to represent the model Hamiltonian. This is not surprising, since the presence of high correlations between the electrons must imply a strong suppression of their coherent delocalization. So it seems natural that a method designed to deal with these complicated systems must not necessarily rely on the original electronic degrees of freedom. This consideration has a straightforward consequence: *because the study of a SCES Hamiltonian is nothing more than a difficult quantum problem, because this quantum problem is (typically) assigned in terms of quantum coordinates that do not have any special status, and because the representation in terms of these quantum coordinates proved itself not convenient, then there exists no reason to keep using the original coordinates*; as in any difficult physics problem, the first step towards the solution should be the choice of an adequate coordinate set: a set chosen on the basis of its conveniency, which permits the simplification of the problem, for example by exploiting symmetries, or by making the implementation of numerical methods less cumbersome. To go from one set of coordinates to another, an appropriate group of coordinate transformations must be defined. In quantum mechanics such a group must be able to change the basis states of the Hilbert space, preserving the matrix elements between them. Therefore it is natural to consider the group of unitary transformations. Such a group embraces a great variety of transformations and it has been often used in quantum mechanics. Unitary transformations are used widely in condensed matter, in particular in the analysis of high coupling limits of some model Hamiltonians, for example in the study of the (periodic) Anderson or Hubbard models [7]. In these circumstances the use of properly defined unitary transformations allows one to map the original Hamiltonians onto the Kondo (lattice) model Hamiltonian and the Heisenberg Hamiltonian respectively [22, 23]. In practice, the unitary transformations are used to write

[4]From now on the term "electron" will mean the dressed electron quantum mode of the Fermi-Landau liquid theory, or Landau quasiparticles.

down the effective Hamiltonian governing the low energy sectors of the original systems, in terms of appropriate low energy coordinates, i.e. spin degrees of freedom in both cases. The unitary transformations of the previous examples are therefore non-canonical: in fact the original set of coordinates comprises only fermionic operators, while the new set is composed also of spin operators. The commutation relations between the operators (quantum coordinates) used to represent the Hamiltonian are not preserved by the transformation.

An interesting subset of the unitary transformations group consists of the group of canonical transformations, which maps an initial set of fermionic operators into another set of fermionic operators. To work in terms of fermions only, rather than spins, is an advantage from a practical point of view. Indeed the powerful tool of the Wick theorem makes the use of fermions much easier [11]. It would therefore seem appropriate to understand this class of coordinate transformations and to find ways to manage them easily.

In recent decades, not so much has been written about the general properties of this group, in particular in the context of condensed matter physics. Moreover very few (non-trivial) examples of applications can be found in the literature (see for example Refs. [24–26]). This is due to the fact that this transformation group can be thought of as comprising two parts: the (trivial) subgroup of linear transformations and the set of non-linear ones. The first class includes all the many transformations, used throughout quantum mechanics, which mix linearly $2n$ fermionic operators (n of creation and n of annihilation) to obtain again $2n$ well defined fermionic operators; examples are is the Bogoliubov-Valatin transformation, the spin rotation around an axis, and the simple operation that allows for the diagonalization of tight-binding Hamiltonians. The second set instead is composed of all those transformations that take the original $2n$ fermionic operators and all their $2^{2n-1}-2n$ non-trivial odd products and mixes them properly in order to obtain again a set of well defined $2n$ fermionic operators. This class of non-linear canonical transformations can potentially be a powerful tool in the study of SCES systems. Indeed these transformations permit one to define new sets of fermionic modes that, in terms of the original ones, are correlated with each other. The new vacuum of this new set may, for example, be a correlated state of the original fermions. Since the new coordinates are "correlated" coordinates, it may happen that the choice of an appropriate transformation defines a set of fermions that are able to capture the correlations of the Hamiltonian and therefore able to simplify it.

The main aim of this thesis is to explain in detail the concepts introduced in the previous paragraphs, which so far may only seem very abstract to the reader. It is important to emphasize already at this point that the connection between the mathematical abstraction of the non-linear canonical transformations and the physics of a fermionic system becomes *straightforward* in terms of Majorana fermions. Representing the operators in terms of Majoranas immediately shows the rationale behind the non-linear canonical transformations. Indeed the Majorana representation proves the necessity of an analysis based on the full group of canonical transformations. Moreover, since the non-linear canonical transformations can be incorporated within any analytic or numerical scheme typically applied to SCES systems, another aim of this thesis is to show some ways to do this in an effective way. Indeed the Majoranas also provide an extremely easy way to represent and handle all these transformations; such a simplification allows the implementation of different strategies for the study of

SCES. Some of these strategies will be discussed in considerable detail in this thesis. With this in mind it is advisable to start the presentation of the results, concluding this short preface. This thesis has been written with the hope that it may be considered as a guide for the reader who is new to these topics. The results are not analyzed, but only introduced briefly, within the main text. In fact all the results have been already presented in the appended papers A, B, C and D. As the reader can see these works are quite lengthy and detailed. Moreover the authors kept a very pedagogical style in all of them, reducing the need for extra comments. What can be found in the main text of this thesis are therefore introductions that give the background necessary to understand the papers and the results. In this sense the text is meant to be self-complete and readable by any condensed matter physicists. It is implicit that a reader who is already familiar with the concepts contained in the introductory chapters (topological Majorana fermions, Hubbard model and Mott insulators, Kondo lattice) may confidently skip them.

In Part I, the results of paper A are introduced, together with the concept of the Majorana fermion. A brief summary of the ongoing discussion about topological Majorana fermions is also provided, together with an introduction to the concepts of non-linear canonical transformations. Paper A provides the theoretical and mathematical background on the relation between Majorana fermions and non-linear transformations.

In Part II the contents of paper B are explained. This paper used the framework developed in paper A to analyze the Hubbard model. In particular the high U, Mott insulating limit of the Hubbard model is studied. Therefore a very short introduction to this phase is provided.

In Part III the last two papers, C and D, are reviewed. In those works the analysis of the 1d Kondo lattice was performed in two different ways. Moreover in the second part of paper D the formalism of Majorana fermions was brought into Feynman path integral form. Since to understand these results one needs to have a good knowledge of the physics of the 1d Kondo lattice and since an updated review on this model is missing in the literature, a lengthy presentation of the model is provided.

It must be mentioned that half of the results (papers C and D) contained in this thesis have already been presented in my own Licentiate Thesis [27]. As is the tradition in Sweden, and in agreement with the policies of the University of Gothenburg, I will use again part of the material presented in that publication. In particular the chapters 2, 6, 7 and 8 and the appendices B and C have been taken from [27] with minor modifications; sections 2.2 and 3.2 have been substantially changed with respect to the original version.

Part I

Foundations

Chapter 2

Majorana fermions

Ettore Majorana published his celebrated work about a symmetric theory for the electron and the positron in 1937 [1]. The paper explored the possibility of obtaining solutions to the Dirac equation on the *real* field. As known, the Dirac equation [28, 29] describes the dynamics of quantum fields on the Minkowski space-time manifold. Naively speaking the (excited) modes of these fields represent particles; perturbations of these fields propagate according to the Dirac equation, and this propagation can be interpreted as the "motion" of the particles. The dynamics is not in conflict with relativity (contrarily to non-relativistic quantum mechanics, governed by the Schrödinger equation), because the combined effect of two fields applied at space-like distance is zero (the two fields commute), although the signal can propagate also at non-physical "speeds".

Dirac found a very elegant way to use these fields to describe spin-1/2 particles.[1] Such a fermionic field has to obey the equation

$$(i\partial_\mu \gamma^\mu - m)\,\Psi(x) = 0, \tag{2.1}$$

with the four matrices γ_μ that close to Clifford algebra $\{\gamma_\mu, \gamma_\nu\} = 2\eta_{\mu\nu}$, and $\eta_{\mu\nu}$ is the Minkowsky metric. Dirac discovered a set of matrices on the complex field that fulfilled the requirement. The solution $\Psi(x)$ of the equation is therefore given by a complex field. Summarizing, since complex fields are associated with charged particles,[2] the solution of the equation and its complex conjugate can be interpreted as the particle and the antiparticle.[3]

Majorana understood that the solution found by Dirac was not the only one possible. In fact (2.1) can be written using a different set of matrices on the real field, implying the existence of *real* solutions to the Dirac equation. This means

[1] In this manuscript the convention $\hbar = 1$ is used, if not stated otherwise.

[2] The relation between the complex/real character of the field and the existence/in-existence of a charge was already known. In fact the Klein-Gordon equation (that can describe spin-0 particles) for both the real and complex cases had been resolved years earlier. It had been noticed that in the case of complex solutions the requirement of local gauge invariance (invariance of the field upon the change in the phase), implied the appearance of other fields in the equation that could be interpreted as electromagnetic-like fields (gauge fields). The interaction with a electromagnetic field assumes the existence of a charge, so the complex character of the quantum fields implies the fact that the related particle is charged.

[3] This is not completely exact, but being irrelevant for the discussion I will not discuss the subtleties here. I recommend the reader to explore the vast literature, starting from Ref. [28, 29].

that the Dirac equation can describe also *chargeless* spin-1/2 particles, i.e. particles that are their own antiparticle. Particle with such features where named "Majorana fermions" in his honor. The search for Majorana particles is not yet concluded and it is still not clear if they represent interesting mathematical constructions, never realized in nature, or actual particles, like the neutrino, or the (still unobserved) photino [2, 30]. Fortunately the existence of fundamental particles that are Majorana fermions will not affect the condensed matter community: in fact Majorana fermions can be realized in condensed matter systems, although with some alteration of the original concept.

In condensed matter systems the wildest dreams of theoretical high-energy physicists can be made real. Recently many "mathematical artifacts" defined in theoretical high-energy physics contexts, describing exotic particles, have been observed in solid state systems. Examples are the massless Dirac(-Weyl) fermions in planar graphene [31], or the magnetic monopole that can be induced in topological insulators [32]. Of course these modes are not fundamental particles, but collective configurations of an entire system; however they are described by equations similar to those of their high energy partners and therefore obey (under specific circumstances) to similar physics.

Recently also the possibility to realize "Majorana fermions" has been considered, although the term has been heavily abused. In condensed matter this term is not associated with particles that behave according to the Dirac equation, nor to any quantum state, or excitation mode. Instead "Majorana fermion" is colloquially used to describe an object that carries *half* of the properties of an electronic degree of freedom. The operators that represent these objects must be hermitian, thus *if they could be thought of* as creation/annihilation operators, they would be associated with particles that are their own antiparticle. This latter property implies the (inadequate [2]) name. Condensed matter Majorana fermions are formally obtained making a symmetric linear combination of the creation and annihilation (hole annihilation and creation) operators of the same fermion and this may give the wrong idea of the definition of a new fermionic particle, which is not the case since no vacuum state exists for the operators defined in this way, so it is impossible to associate any quantum level to them. However it is very convenient to imagine them as actual particles that can be localized in space and manipulated. It must be mentioned that there also exists excitations and actual quantum states in condensed matter systems that behave as Majorana particles, whose dynamic is described by the Dirac(-Majorana) equation [33, 34]. However, those are not the kind of Majorana fermions that will concern us in this thesis.

Majorana fermion solutions appeared in solid state physics long ago [35], and since then they returned sporadically in a few works and in particular they have been used often to study spin systems [36–38]. However they have often been considered suspicious and seen more as artifacts or mathematical tools, than as real objects. There was a sea-change in perspective a few years ago, with the popularization of the concept of topological order in condensed matter systems.[4] The idea that not just the symmetry of the lattices, but also the

[4]The literature is very rich in reviews from which the interested reader can begin their research [39–41]; however I suggest that the best introduction to the subject maybe obtained by reading Ref. [42] which is based on a differential geometry approach. I will not discuss the concept of topological order or topological classification, the knowledge of which is not necessary for understanding the content of this thesis.

global properties of the Hamiltonian can be important, focused the attention of the community on some non-trivial effects that can be realized in "topological compounds". Although the original idea of topological order originated in the context of quantum Hall effect [43] and fractional quantum Hall effect [44–46], nowadays the so called "topological insulators" are the most discussed systems in which topological properties of matter are studied. In these systems the concept of topological order is quite unaffected by the nature of the compound, which can be either a band insulator or a superconductor. This is due to the fact that the topological properties rely on the existence of a gap in the spectrum and what is important is its structure, not its origin. It must be stressed that most of the literature on topological insulators deals with non-interacting systems. The interactions partially affect the results (for example the classification scheme [47, 48]), but not the main properties of the systems (see discussion in Ref. [42]). Because of this reason the systems considered have been mostly non-interacting, where with this term I mean that their Hamiltonians contain only quadratic fermion operators or constants, therefore they are straightforward to diagonalize.[5]

The study of the topological properties of matter followed two (very similar) directions: the characterization of the *topological insulators* and of the *topological superconductors*. Interestingly it was soon understood that the topological non-triviality of a system could cause the appearance of some exotic collective fermionic modes in the spectrum of the system; such fermionic modes are characterized by the compelling property of having no antiparticle counterparts.[6] Because of these properties they were named "Majorana fermions" initially, but now it is more common to refer to them as "Majorana modes". In both contexts the important ingredients for the appearance of these elusive Majorana modes are the simultaneous presence of *superconductivity* and *topological (non-trivial) order* in the system. In the Sec. 2.1 a brief introduction to this new and exciting topic is given, in order to convince the reader that these Majorana modes are not unphysical and that they could really be important in the future. In fact the results provided in the appended papers do not use the Majorana fermions in the fashion presented in Sec. 2.1. Of course some concepts are shared, so it is appropriate to be familiar with the known results, but the angle from which I would like the reader to view the Majoranas is completely different.

2.1 Topological Majorana fermions

Looking for a way to realize a condensed matter equivalent of the Majorana fermions, it is natural to start from a superconducting system [49, 50]. In fact the main property of the Majorana fermions is that they are their own antiparticle and therefore charge neutral. In normal band insulator systems, the only ingredients available are the excitation modes of the system, i.e., single or collective configurations of electrons and holes,[7] so it is in no way possible to

[5] In the context of superconducting systems I refer to the Bogoliubov-deGennes Hamiltonian, hence the reader should not be shocked if I consider the superconducting systems as *non-interacting*.

[6] This could seem an absurd. However in the next section it will be shown how the apparent confusion is due to a loophole in the formalism of creation and annihilation operators, which gets "confused" by the existence of a doubly degenerate ground state.

[7] Electrons and holes, and their collective configurations, are properly defined quantum states *only* after a definition of a reference vacuum, typically the non-interacting ground state. The reader's

build anything that resembles a Majorana fermion. In fact there exists quite a difference between adding (or exciting) an electron mode or an hole mode in the system, because the number of electrons (the electric charge) is a good quantum number. Quantum mechanics allows to count the number of electrons in normal insulating systems: it is therefore impossible to create a state where such number is uncertain.

The only way to bypass this difficulty is to work in a system where the number of the electrons is undetermined: the superconductors.[8] Indeed in a superconductor the notion of electron charge loses completely its meaning, because of the BCS condensate of Cooper pairs. To add an electron on top of the condensate or to remove one (i.e. to add a hole), makes no difference for the system, because in both cases the effect is to create an incomplete Cooper pair. Hence the superconducting condensate must play a fundamental role in the search of a solid-state analogous of the Majorana fermions. This is also the same idea behind the mechanism of Andreev reflection [51].

A prototypical system that can host objects with similar properties to the Majorana fermions has been elaborated[9] by Kitaev in 2001 [6]. He considered the Hamiltonian for a fully spin-polarized, one dimensional, p-wave superconductor (known now as the *Kitaev chain*) and solved the problem for different values of the parameters. The Kitaev chain Hamiltonian reads:

$$H_{kc} = -t \sum_{i=0}^{N-1} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + \Delta \sum_{i=0}^{N-1} \left(c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i \right) - \mu \sum_{i=0}^{N} c_i^\dagger c_i, \quad (2.2)$$

where it has been chosen to put $\Delta = \Delta^*$ and only one spin electron species is involved. This Hamiltonian can be written using different operators γ_i, according to the formal relation

$$\begin{aligned} c_i &= \tfrac{\gamma_{1,i} - i\gamma_{2,i}}{\sqrt{2}}, \\ c_i^\dagger &= \tfrac{\gamma_{1,i} + i\gamma_{2,i}}{\sqrt{2}}, \end{aligned} \quad (2.3)$$

$$iff \quad \gamma_{\alpha,i} = \gamma_{\alpha,i}^\dagger \quad \text{and} \quad \{\gamma_{\alpha,i}, \gamma_{\beta,j}\} = \delta_{ij}\delta_{\alpha,\beta}.$$

Because of the Hermitian character of the γ-operators, that cancels the difference between creation and annihilation of these (supposed) γ-particles, they were named *Majorana fermion operators*. At this point the reader new to this field could be confused, if this is the case I suggest to look at the these Majoranas as algebraic structures; later the physical meaning of the idea will become more clear.

attention is directed to the fact that the concept of the hole is meaningful only if there exists a Fermi volume from which the electrons can be removed.

[8] The electron number operator $\hat{N}$ is in fact the conjugate variable to the phase operator $\hat{\phi}$, so it is affected by quantum uncertainty.

[9] The first theoretical prediction of Majorana modes in condensed matter appeared in the literature of the superconductors [52]. Indeed Majorana modes can be localized in the center of Abrikosov vortices induced by an external magnetic field into a type-II superconductor. However this example would bring us far from the aims of this section.

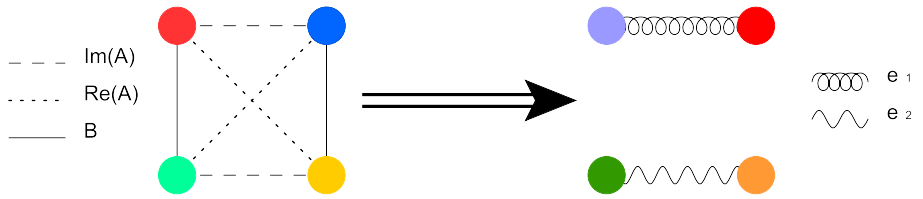


Figure 2.1: *Cartoon of process of fermion building. The Hamiltonian $Ac^\dagger f + Bc^\dagger c^\dagger + Bf^\dagger f^\dagger + h.c.$ generates interactions among all the Majoranas. The most suited Majoranas (fermions) to represent the Hamiltonian are found by the diagonalization procedure.*

Using the definitions (2.3), equation (2.2) reads:

$$\begin{aligned} H_{kc} =& it\sum_{i=0}^{N-1}(\gamma_{1,i}\gamma_{2,i+1} - \gamma_{2,i}\gamma_{1,i+1}) + i\Delta\sum_{i=0}^{N-1}(\gamma_{1,i}\gamma_{2,i+1} + \gamma_{2,i}\gamma_{1,i+1}) + \\ &- \mu\sum_{i=0}^{N}\left(\frac{1}{2} - i\gamma_{1,i}\gamma_{2,i}\right). \end{aligned} \tag{2.4}$$

Let us choose $\mu = 0$ and $\Delta = t$.

$$H_{kc} = i2t\sum_{i=0}^{N-1}\gamma_{1,i}\gamma_{2,i+1}. \tag{2.5}$$

One could now define a set of new fermionic operators $a_i = (\gamma_{2,i+1} - i\gamma_{1,i})/\sqrt{2}$, so that

$$H_{kc} = t\sum_{i=0}^{N-1}\left(a_i^\dagger a_i - \frac{1}{2}\right).$$

The ground state of this Hamiltonian is found very easily: no a-fermion is allowed in the ground state. However the careful reader should have noticed that two Majorana fermions escaped from the process of formation of the a-fermions. In fact the Majoranas $\gamma_{2,0}$ and $\gamma_{1,N}$, are not present in (2.5), i.e., they are unpaired. They can be used in the formation of a new fermion $a_0 = (\gamma_{1,N} - i\gamma_{2,0})/\sqrt{2}$ and the fermionic Hamiltonian would then look like

$$H_{kc} = t\sum_{i=1}^{N}\left(a_i^\dagger a_i - \frac{1}{2}\right) + 0\cdot a_0^\dagger a_0. \tag{2.6}$$

This means that the ground state of the Kitaev chain (for this choice of parameters) is doubly degenerate, because the energy with or without the *fermion* a_0 is exactly the same. The two degenerate states can be indicated on the base of their parity $|0\rangle$ (no a_0 fermion, i.e. even number of electrons) and $|1\rangle$ (one a_0 fermion, i.e. odd number of electrons).

The fermion state a_0 is quite peculiar: in fact it is delocalized on the two extremes of the wire, because the two Majoranas that compose it come from the electrons in $i = 1$ and $i = N$. It is convenient to think of the system in terms of Majoranas: each electron is formed by the coherent superposition of two Majoranas, that are in this sense *half of the electron degree of freedom*. These half-electrons interact according to the Hamiltonian, that determines which fermions

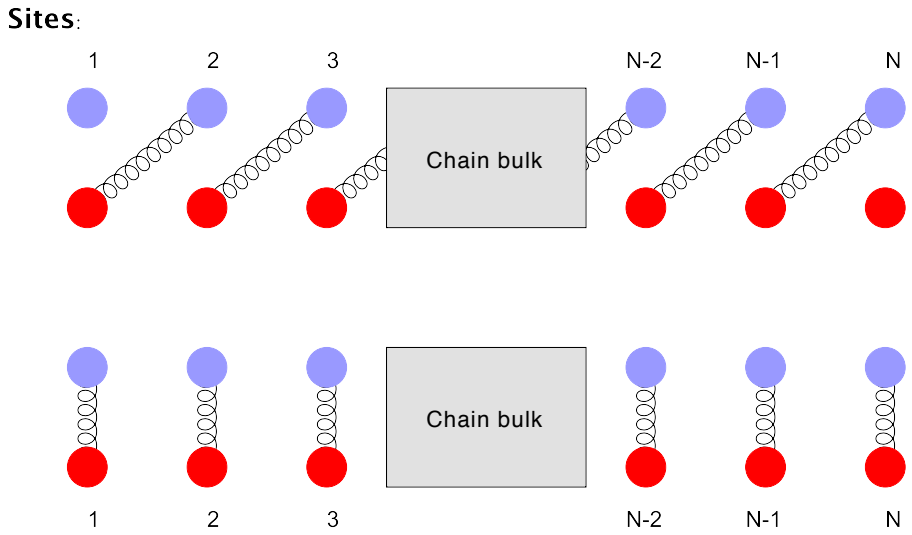


Figure 2.2: *Cartoon of the Kitaev chain for the simplest choices of the parameters: $t = \Delta$, $\mu = 0$ on the top; $\Delta = t = 0$ on the bottom. The red and blue spots represent the two Majorana fermions on a single site, belonging to the electron state. The springs represent the fermionic states that the Hamiltonian defines. As can be seen, in the topological phase (top) the two extrema Majoranas (of two different colors) remain unpaired, so they form a_0. The same does not happen in the topologically trivial case (bottom).*

is better to "build" using the available Majoranas, in order to optimize the energy. This process is sketched in the cartoon of Fig. 2.1. For the Hamiltonian in Eq. (2.5) the best fermions are the $N-1$ delocalized on two neighboring states, plus the a_0 fermion formed with the two decoupled half electrons at the ends of the wire, as shown in Fig. 2.2.

It should now be clear to the reader that it is absolutely *wrong to speak and think about Majorana states*. In fact only Majoranas combined in pairs can generate a quantum state. A single Majorana does not live in any quantum state and as a matter of fact it is *meaningless* to try to count them, or also fill such Majorana states, because $\gamma^2 = 1/2$. The confusion that the Majoranas can generate, comes form the fact that the Majorana operators are not really creation or annihilation operators. As a matter of fact the Fock space of the system does not contain any "Majorana vacuum", as a reformulation of the equations (2.3) shows:

$$\gamma_1 = \frac{c + c^\dagger}{\sqrt{2}}, \tag{2.7}$$

$$\gamma_2 = i\frac{c - c^\dagger}{\sqrt{2}}. \tag{2.8}$$

Written in the occupation number basis these operators are represented by the Pauli matrices, that have no kernel, ergo they cannot return a zero if applied to any state of the Fock space. *So the vacuum of the Majoranas does not exist and therefore the Majoranas are no particles.* The only measurable property of the system is not the occupation of the (non-sense) Majorana state, but the

occupation number of the fermionic state (a_0) built using the two Majoranas that are localized at the boundaries of the chain. This zero energy *fermionic* state is the *zero mode* or *Majorana mode*.

I must warn the reader that I have not been completely consistent with the literature in the use of the term "Majorana mode". In many (but not all) of the available works the latter term indicates the two Majorana components of the zero energy fermion. In my opinion it is non-sense to use the word "mode" for something that is not a quantum state, so I decided to use that term to indicate the real (physical) quantum mode, i.e. the zero energy fermionic excitation a_0. The two half-electron components will be indicated with the term "Majoranas" or "Majorana fermions".

One could then wonder why to these (*algebraic*) *objects* is given almost the status of actual quantum states. The fact is that it is *extremely convenient* to think and refer to the two localized (Majorana) parts of the non-local fermionic zero mode as actual particles. They can be moved around, interact with other local "half-fermions", interact with the leads of an external material, delocalize, etc... the formalism and the understanding of the physics is very much simplified considering these object as actual particles that live in the system and that bound together in order to form a fermion.

For example one can consider what happens if the parameters of the Kitaev model are not chosen as in (2.5). In that case there exist two possibilities: either no Majorana modes are present (so the ground state is not double degenerate), or the two Majoranas that compose the zero energy Majorana mode are delocalized on more sites. This also means that they can overlap, breaking the degeneracy between the $|0\rangle$ and the $|1\rangle$ states. The energy splitting depends upon the overlap, therefore it tends to zero in the limit of an infinitely long system, independently upon the choice of parameters. It is quite easy to imagine it as a normal quantum process where two degenerate overlapping quantum states combine and split, although the two separate halves of the fermion are not quantum states at all. Moreover the most important reason to consider the Majoranas as real objects is that they can be used to build and manipulate qubits, as will be discussed in section 2.1.2.

In the previous section we anticipated the two ingredients needed to obtain Majorana fermions: superconductivity and topology. So far the discussion focused on the superconducting properties, hence it is now time to illustrate the subtle role played by topology, which has been hidden in the previous description of the Kitaev chain. As said, the parameters must be chosen carefully in order to generate the Majorana mode. In particular it has to happen [6,53] that

$$|2t| > |\mu|, \quad \text{and} \quad \Delta \neq 0. \tag{2.9}$$

The reason for this condition must be searched in the bulk properties of the system. In fact the systems is a topological non-trivial state, for such values of the parameters [39–42]. In practice this means that the global properties of the Hamiltonian of the system are different with respect to the case $|2t| < |\mu|$. Even if both the phases (the topologically trivial and the topologically non-trivial) are gapped, the structure of the gap is different, because the Hamiltonians have two different structures and there exist no way to adiabatically connect them, without closing the gap. This means that if in a system we artificially induce a change in the structure of the Hamiltonian (in the example of the

Kitaev chain one could have a jump in the chemical potential, so that in one region of the space $|2t| > |\mu|$, while in the other $|2t| < |\mu|$), then between the two topologically gapped bulk regions there must exist a point (or a line or a surface) where the gap closes. This causes the appearance of zero modes (gapless excitations), highly localized close to these "transition zones". These regions, that form a sort of boundary of the topological non-trivial system, are called *topological defects* [54]. As an example the boundaries of any system (if the system is topologically non-trivial) are topological defects, but other cases exist as well. Hence it is possible to roughly understand why the topological non-triviality of the bulk and superconductivity are needed to have Majorana fermions. From the first property the mode gets the strongly localized and zero-energy characteristic, while from the second one, it gets the charge neutrality, i.e. the parity degeneracy of the two ground states $|0\rangle$ and $|1\rangle$. When a non-trivial topological region is created in a p-wave superconductor, the unpaired Majoranas sticks to the topological defects [40, 41, 54, 55]; the Majorana mode is the state that is left behind in the process of creation of the topological non-trivial phase, with the opening and closing of the gap [5, 56].

Although interesting, the topological properties of matter and how they are related to the presence of Majorana modes is largely irrelevant for the present study, therefore I will skip this discussion. Instead I will briefly introduce some realistic setups for systems that can support Majorana fermions. Moreover I will show why they are relevant for quantum computation. Before the end of this section it is appropriate to cite the experimental work by Mourik and collaborators [21], who were able to see in their experiment traces of something that could be a Majorana mode.

2.1.1 Convenient realizations: examples

So far the superconductors mentioned were always of the p-wave kind. This is because in the p-wave superconductors one of the two spin species can (in principle) be suppressed with a magnetic field, so that the final system is described as effectively spinless. One could object that nothing changes even if both the spin species are present. That is true, but it would imply that an even number of Majoranas is localized on both edges, allowing interactions to define two local fermionic modes, spoiling the non-local character.

The practical realization of a system like the Kitaev chain or its 2d counterpart, the chiral p-wave superconductor, is unfortunately a great challenge. Therefore physicists identified different systems where Majorana modes could appear. Two setups [5, 41, 56] received a lot of attention: the first based on 3d topological insulators [33, 57] and the second on 1d semiconducting nanowires with strong spin orbit coupling [58, 59].

Topological insulator based setups

There are two problems in the practical realization of the Kitaev chain: the presence of the p-wave superconductor and the fact that (superconducting) long range order is assumed in a system that is strictly one-dimensional. To overcome these difficulties the best thing to do is to remove both these ingredients from the equation, passing from 1d to 2d systems, and from p-wave to s-wave superconductivity. At first glance this could seem an impossible task but in

2008 Fu and Kane understood [60] how to realize Majorana fermions in a system with the previous characteristics. The key of the success goes under the name of "proximity effect". Such phenomena occurs when a superconductor is put in contact with a normal material. The Cooper pairs are then allowed to tunnel from the condensate into the metal (or vice-versa one could think that the electrons can tunnel into the condensate and back), inducing an effective pairing term into the Hamiltonian.

Fu and Kane [60] realized that if the proximity effect is used on the surface of a 3d strong topological insulator, then the (Dirac-like) gapless electrons on the surface of the topological insulator obey the Hamiltonian as a chiral p-wave superconductor. In practice it is possible to obtain p-wave pairing, without any real p-wave superconductor. Very well localized Majorana fermions appear upon inducing vortices in this effective p-wave superconductor [41].

It must be mentioned that on these kind of structures, also propagating Majorana fermions can be built. In fact the superconductor can be deposited on the 2d surface, leaving some space to form a junction [60], or beside a magnetic insulator [33]. In this way it becomes possible to study also how the propagating Majoranas create interference patterns between electrons and hole states that are injected into these junctions [5, 33, 57]. Similar setups can also be built using 2d topological insulators, by depositing, close to one boundary of the 2d system, magnetic insulators that sandwich the superconductor. This system also localizes two Majorana fermions on the interface between the magnetic insulators and the superconductor [61] causing interesting effects, such as crossed Andreev effects or electron teleportation [62]. Therefore these kind of setups are well suited for the detection of the Majorana modes.

Semiconducting nanowire setups

In 2010 two similar works [58, 59] demonstrated how it is possible to recreate a system that obeys to Kitaev Hamiltonian using three very simple ingredients: a (quasi-) 1 dimensional semiconducting nanowire with strong spin-orbit interaction, an s-wave superconductor and a strong magnetic field. Defining the electron creation operator in the wire as

$$\Psi^\dagger(k_x) = \left(\Psi^\dagger_\uparrow(k_x), \Psi^\dagger_\downarrow(k_x)\right),$$

the Hamiltonian for such a system looks like (see the reviews Ref. [4, 56] for details and further references)

$$\begin{aligned} H &= \int dk_x \Psi^\dagger(k_x) H_{wire}(k_x) \Psi(k_x), \qquad (2.10)\\ H_{wire}(k_x) &= \frac{k_x^2}{2m} - \mu + \alpha_0 k_x \sigma_y + \frac{1}{2} g\mu_B B \sigma_z = \\ &= \begin{bmatrix} \frac{k_x^2}{2m} - \mu + \frac{1}{2} g\mu_B B & -i\alpha_0 k_x \\ i\alpha_0 k_x & \frac{k_x^2}{2m} - \mu - \frac{1}{2} g\mu_B B \end{bmatrix}, \end{aligned}$$

where the spectrum of the wire has been approximated as parabolic, α_0 gives the (Rashba[10]) spin-orbit coupling ($E_\perp$ is the effective electric field felt by the

[10]The Rashba effect [63] is due, in 2d heterostructures, to the breaking of inversion symmetry of the confining potentials, needed to confine the electrons into the effective lower dimensional motion.

electron), g is the Landé factor and μ_B the Bohr magneton. To this Hamiltonian the superconducting pairing induced by the proximity effect must be added. The setup is shown in Fig. 2.3.

The Hamiltonian (2.10) is easily diagonalized, with eigenvalues and eigenvectors:

$$E_\pm = \frac{k_x^2}{2m} - \mu \pm \sqrt{\tilde{B}^2 + \alpha_0^2 k_x^2}, \qquad \Psi = \mathcal{N} \begin{pmatrix} -i\tilde{B} \pm \sqrt{\tilde{B}^2 + \alpha_0^2 k_x^2} \\ \alpha_0 k_x \end{pmatrix}, \quad (2.11)$$

where $\tilde{B} = g\mu_B B$ and $\mathcal{N}$ the normalization factor. The spin-orbit effect splits the two degenerate spin bands into two distinct parabolas, where the electrons have polarization axes that depend upon $k_x, \tilde{B}$ and α_0; the result is plotted in Fig. 2.4a.

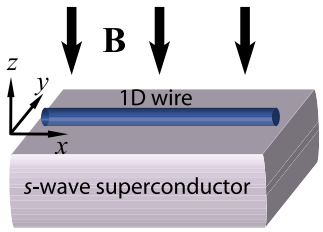


Figure 2.3: *The set up of the nanowire based proposal. This figure is taken from [56]. ©IOP Publishing. Reproduced with permission of IOP Publishing. All rights reserved.*

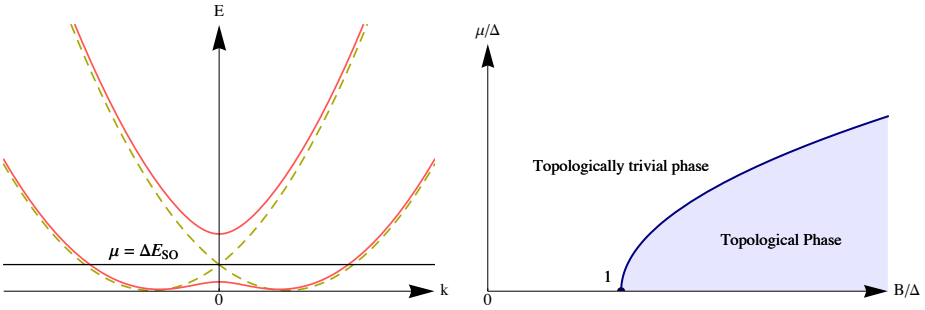
The role of the magnetic field B is to open a gap between the two bands, removing the degeneracy at the point $k_x = 0$. Moreover it also enforces the polarization in the two bands, so that if $\tilde{B}$ becomes large, then the electrons inside a single band have (approximately) all the same k-independent polarization. One can indicate the two spinless species as Ψ_- and Ψ_+ (the minus stands for the species in the lowest energy band). Therefore if the chemical potential is set in such a way that the Fermi surface is inside the $k_x = 0$ gap, then the low energy fermionic excitations are effectively spin-less. The superconducting s-wave pairing, induced by proximity effect, can now be considered inserting the term

$$H_{prox} = \int dk_x \Delta \left[\Psi_\uparrow(-k_x)\Psi_\downarrow(k_x) + \Psi_\downarrow^\dagger(k_x)\Psi_\uparrow^\dagger(-k_x) \right]. \quad (2.12)$$

This term is written in terms of the original polarization directions $\uparrow, \downarrow$ and must be expressed now in terms of the new fields Ψ_- and Ψ_+. The result of this operation is [56]:

$$H_{prox} = \int dk_x \frac{\Delta_p(k_x)}{2} \left[\Psi_+(-k_x)\Psi_+(k_x) + \Psi_-(-k_x)\Psi_-(k_x) + h.c. \right] + \\ + \Delta_s(k_x) \left[\Psi_-(-k_x)\Psi_+(k_x) + \Psi_+^\dagger(k_x)\Psi_-^\dagger(-k_x) \right], \quad (2.13)$$

This breaking of the symmetry can be modeled by an (typically unknown ab-initio) electric field *perpendicular* to the 2d nanowire. The electrons moving on the 2d submanifold, will not feel the direct effect of this electric field (of course, because it is a 3d effect), but instead its repercussion. It is well known that a charged particle moving in a static electric field will feel (in its at-rest reference frame) the presence of a magnetic field $\vec{B} = (\vec{v} \times \vec{E}_\perp)/c^2$, due to the Lorentz transformation of the fields, from the lab to the particle reference system. This magnetic field couples to the spin of the electron via the usual form: $g\mu_B \vec{B} \cdot \vec{\sigma}/2$. So typically the Rashba term is written as $g\mu_B(\vec{v}\times\vec{E}_\perp)\cdot\vec{\sigma}/2c^2$ in 2d systems, but since $|E_\perp|$ is unknown, all the parameters are summarized in the Rashba spin-orbit coupling α_0, in such a way that one gets $\alpha_0(k_y\sigma_x - k_x\sigma_y)$. In one dimension things change a bit, because it is not possible to understand the direction of $\vec{E}_\perp$. Anyway it is perpendicular to the wire, so this is enough to obtain the effective interaction used in the equation (2.10).



(a) *Effect of the Rahsba interaction;* **(b)** *Topological phase diagram.*

Figure 2.4: *(a) the effect of the spin-orbit without (dashed yellow) and with (continuous red) the magnetic field, from formula (2.11). The chemical potential has been chosen in order to cancel the gain in energy due to the spin-orbit coupling (ΔE_{SO}). (b) Sketch of the topological phase diagram; the boundary is located at the closing of the gap (the plot is symmetric for $\mu, B \to -\mu, -B$).*

with

$$\Delta_p(k_x) = \frac{\alpha_0 k_x \Delta}{\sqrt{\alpha_0^2 k_x^2 + \tilde{B}^2}}, \quad \Delta_s(k_x) = \frac{\tilde{B}\Delta}{\sqrt{\alpha_0^2 k_x^2 + \tilde{B}^2}}. \tag{2.14}$$

Therefore a p-wave intra-band paring appears in the Hamiltonian. The route towards a realization of the Kitaev chain model is therefore established. One can now add these terms to the (diagonalized) Hamiltonian (2.10) and diagonalize it via Bogoliubov-Valatin tranformation.

The pairing Δ and $\tilde{B}$ do not collaborate to open the gap. In fact at $|\tilde{B}| = \sqrt{\Delta^2 + \mu^2}$ the gap closes, separating the two topologically different phases $|\tilde{B}| > \sqrt{\Delta^2 + \mu^2}$ and $|\tilde{B}| < \sqrt{\Delta^2 + \mu^2}$. Considering that Hamiltonians of the same classes can be adiabatically transformed into each other without closing the gap, it is enough to check the topological properties of one single Hamiltonian of the two sectors to determine the topological properties of the entire phase [3]. One expects to find the topological behavior in the limit $|\tilde{B}| > \sqrt{\Delta^2 + \mu^2}$, because in that regime the electrons of the lower band are almost all spin down polarized, as shown previously, and because at $B = \Delta = 0$ the Hamiltonian is evidently trivial. At lowest order (i.e. considering the upper band empty [3] and neglecting the terms in the Hamiltonian that couple them, but nothing really changes if the matrix is diagonalized exactly [4]) one obtains the effective Hamiltonian

$$\begin{aligned} H &= \int dk_x \Psi_-^\dagger(k_x) \left[\frac{k_x^2}{2m} - \mu_{eff} \right] \Psi(k_x)_- + \\ &\quad + \frac{\Delta_{eff}(k_x)}{2} \left[\Psi_-^\dagger(k_x) k_x \Psi_-^\dagger(-k_x) + h.c. \right], \end{aligned} \tag{2.15}$$

with $\mu_{eff} = \mu + g\mu_B|B|$ and $\Delta_{eff} \approx \alpha_0\Delta/g\mu_B|B|$. This is the continuous version of the Kitaev chain Hamiltonian (2.2), with the chemical potential that sits on the bottom of the conduction band (giving the parabolic approximation of the dispersion law), therefore the system is in a topological non trivial state according to equation (2.9). Schematically the topological phase diagram is draw in Fig. 2.4b. The phase boundary is given by the closing of the gap at $|\tilde{B}| =$

$\sqrt{\Delta^2 + \mu^2}$. According to the theory, Majoranas should show up in a system build in this way. The experiment performed by Mourik and collaborators [21], seems consistent with these predictions, although it is not clear if the signal recorded is really a final proof of the existence of Majorana modes.

Although successful, this setup is very fragile: in fact the simultaneous presence of superconductivity and a high magnetic field is problematic; moreover also the tuning of the chemical potential in the middle of the gap opens new challenges. One can try to solve the first problem using materials with high Landé factors (it is typically possible to obtain nanowires with $g > 50$). The second problem can instead be avoided and in particular I would like to point out an extremely clever proposal by Klinovaja and Loss [64], where the RKKY effect is used to induce the topological phase and automatically set the parameters in the correct regime.

2.1.2 Quantum computation and non-abelian statistics

The most important reason for the excitement caused by the realization of systems that can host Majorana fermions is due to their *possible technological applications*. In fact Majorana fermions could lead to promising results in the context of quantum computation. The Majorana zero mode can in fact host a qubit of information in the two states $|0\rangle$ and $|1\rangle = a_0^\dagger|0\rangle$. This qubit is extremely stable with respect to decoherence, exactly because the high delocalization of the a_0 fermion makes the decay of the state highly improbable: in fact the perturbation should act coherently on the both sides of the wire. Therefore the main effect that can cause an error (invert the qubit), is given by the overlap between the two Majoranas, that implies an hybridization (transition probability) between $|0\rangle$ and $|1\rangle$ (together with the parity degeneracy breaking).

The creation of a stable qubit is not the only reason that makes the Majoranas important in the quantum computation context. In fact, thanks to their algebraic properties they can be used to manipulate the qubits, allowing for the creation of logic ports. This fact has been known for quite a few years, since Ivanov [65] in 2001 proved that the Majoranas located in the vortices of a 2d p-wave chiral superconductor obey non-Abelian statistics. This can be understood deriving the effect on the Majoranas of a $U(1)$ phase transformation of the superconducting condensate [4, 65]. Since the Majoranas are described by

$$\gamma = \frac{\alpha\, c^\dagger + \alpha^*\, c}{\sqrt{2}}, \quad \text{with} \quad |\alpha| = 1, \tag{2.16}$$

and the effect of the $U(1)$ gauge transformation is $c \to e^{i\phi/2}c$, $c^\dagger \to e^{-i\phi/2}c^\dagger$, then it implies

$$\alpha \to \alpha\, e^{i\phi/2}. \tag{2.17}$$

The phase of the condensate increases by 2π going around a vortex core; however such a function must be single valued, so there must exist a branch cut where the phase experiences a jump of 2π. In presence of n vortices there will be n branch cuts that go from the vortex cores to infinity. The action of exchanging two vortices should not change the wavefunction of the ground state, except for a phase. Trying to perform such an exchange it is clear (Fig. 2.5) that *only one* of the Majoranas will be forced to cross the branch cut of the other vortex core.

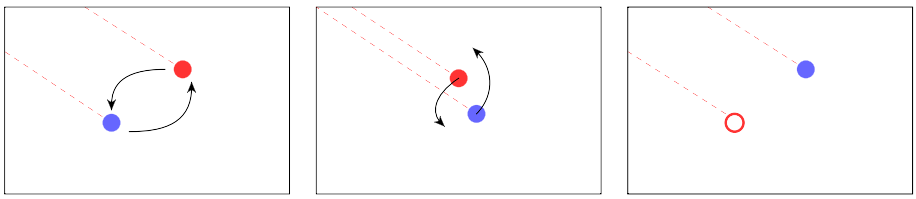


Figure 2.5: *Cartoon of the exchange process of two Majoranas trapped in two vortices. The dashed lines represent the branch cuts, while the empty circle represent the red Majorana with the extra π phase.*

This causes a difference in the phases gained by each Majorana performing this operation. So, besides a common phase factor, the Majorana that crossed the branch cut gains an extra $\exp(i\pi) = -1$ phase factor. Therefore the exchange of two vortices does create a (non-trivial) phase factor in the ground state(s), because:

$$\begin{aligned} \gamma_1 &\rightarrow \gamma_2 \\ \gamma_2 &\rightarrow -\gamma_1. \end{aligned} \tag{2.18}$$

Colloquially it is often said that this shows the non-Abelian statistics obeyed by the Majorana fermions. The group of all the exchange operations (modulo the common phase change, that is dropped) goes under the name of the *braid group* [65].

Now that the effect of the exchange of two Majoranas is understood, it is possible to formally elaborate these results. This permits on the one hand to discover some practical tools to deal with these braiding operations and on the other hand to disclose their physical meaning. The transformations (2.18) are realized by the operator $R_{12} = (1 + \gamma_1\gamma_2)/\sqrt{2}$, according to the definition:

$$\gamma_i \rightarrow R_{12}\gamma_i R_{12}^\dagger,$$

that can also be expressed as

$$R_{12} = \exp\left\{i\frac{\pi}{4}(-i\gamma_1\gamma_2)\right\}.$$

All of this is far from being new. In fact given the Clifford structure of the Majorana algebra[11] $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$, it is known [66–69] that R_{12} is the rotor operator associated to a $\pi/2$ rotation in the Euclidian space generated by the elements of the Clifford algebra (see appendix A for details), thought of as unit vectors.

It is important to note that $i\gamma_1\gamma_2$ is a proper hermitian operator, expressible in terms of $a_0^\dagger a_0$, with a_0 the usual fermion operator $a_0 = (\gamma_1 - i\gamma_2)/\sqrt{2}$. So it

[11] With respect to the previous definition, there is an extra factor of 2 here. Of course this makes no difference, if the normalizations of the fermion operators built with the Majoranas are properly renormalized. In most of the mathematical literature the extra factor of 2 appears, so that $\gamma^2 = 1$. This is also the case in part of the physics literature. However this definition generates an asymmetry in the equations when one goes form the Majorana to the fermion representation and vice versa. This can become annoying, so performing computations with the Majoranas it is preferable to choose the convention without the extra 2, hence $\gamma^2 = 1/2$. In the following the convention will be changed, depending upon which one is the most convenient in the specific circumstance.

is now possible to study its action on the degenerate ground states $|0\rangle$, $|1\rangle$, i.e. the *physical* effect of the Majorana exchange operation. Immediately one gets:

$$\begin{aligned} R_{12}|0\rangle =& \frac{1}{\sqrt{2}}\left[1+i\left(2a_0^\dagger a_0-1\right)\right]|0\rangle &= \frac{1}{\sqrt{2}}\left[1+i\right]|0\rangle, \\ R_{12}|1\rangle =& \frac{1}{\sqrt{2}}\left[1+i\left(2a_0^\dagger a_0-1\right)\right]|1\rangle &= \frac{1}{\sqrt{2}}\left[1-i\right]|1\rangle. \end{aligned} \tag{2.19}$$

Therefore the effect of exchanging the two vortices is that of creating two different phase factors on the two degenerate ground states. It is worth noting that $i\gamma_1\gamma_2$ can be represented as the Pauli matrix σ_z. The action of R_{12} on $|0\rangle$ and $|1\rangle$, i.e. on the eigenstates of σ_z with eigenvalues ± 1, is therefore easy to understand. It also becomes clear that the two states cannot be mixed in this way, so the case with just two Majoranas is not very useful.

The situation when four Majoranas are present is more interesting. This means that the ground state of the system is quadruple degenerate and that the braid group is much bigger, and generated by

$$-i\gamma_1\gamma_2,\ -i\gamma_3\gamma_4,\ -i\gamma_2\gamma_3,\ -i\gamma_1\gamma_2,\ -i\gamma_1\gamma_3,\ -i\gamma_2\gamma_4, \tag{2.20}$$

where the first two operators commute with each other and represent the parity of the a_0 and the similar a_1 fermion. With so many Majoranas and braiding operators many new operations become possible. For example

$$R_{23}|00\rangle = \exp\left\{i\frac{\pi}{4}(-i\gamma_2\gamma_3)\right\}|00\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + i|11\rangle\right). \tag{2.21}$$

Interestingly the latter is the superposition of states with the same parity (the same happens in the sector of odd parity: the two sectors cannot be mixed for obvious reasons[12]). This permits the use of $|00\rangle$ and $|11\rangle$ as two qubits, on which it is possible to operate. The non-Abelian nature of these braiding operators is evident looking at the form of the generators (2.20) and therefore the structure of the associated Lie group.

On this basis a scheme of topological quantum computation can be built. I recommend the interested reader to consult the literature [56, 70, 71], for more details; as this aspect is too much off topic it will not be developed any further in this thesis.

2.2 Majoranas in non-interacting systems

Although Majorana fermions appear in the papers A, B, C and D, they play a different role than the one just explained. In fact they are used as tools, in the fashion of the original work by Kitaev [6], but the actual realization of Majorana modes is completely irrelevant. Indeed the philosophy that lies behind the framework explained in paper A has very old roots, since it is based on ideas that go back at least fifty years, when in a famous paper by Freeman Dyson [72] the different ways to represent quantum mechanics were discussed. In that work it was pointed out that the choice of physicists, to represent quantum mechanics

[12] These operations commute with the total parity operator, which is proportional to $\gamma_1\gamma_2\gamma_3\gamma_4$, or $\left(a_0^\dagger a_0 - 1/2\right)\left(a_1^\dagger a_1 - 1/2\right)$ in fermionic notation.

only on the algebra of complex numbers, is based on a *prejudice* [72] and on no other fundamental reason. In many situations it is much more convenient to use the field of real numbers, instead of complex ones. Indeed, in some other cases, the algebra of quaternions can also prove itself useful. The Majorana fermions, as we are going to use them, realize a different representation of quantum mechanics: a *representation on the field of real numbers*. This representation is not less accurate nor less general than the standard (complex) one, which is given by the standard fermionic creation/annihilation operators. Indeed, thinking in these terms, it is possible to interpret the Majoranas as algebraic constituents of the fermions. These "bricks" can be glued together to build up any set of fermion operators that can span the entire Hilbert space if applied to a given special state (vacuum), which also depends upon how the Majoranas are combined together. What is more important however, is that these algebraic "bricks" can be chosen from different equivalent sets, much more general than the ones considered in the standard literature [4, 5, 56]. This allows the selection of a set of Majoranas (and therefore fermions) that can be more suited to describe a given SCES system. To understand these points, one has to study the algebraic structure of the Majorana fermions, which in fact are not a simple set of operators, but can be used to generate a Clifford algebra of operators. This is explained in paper A and introduced in the next chapter. In this section it is more important to explain, in the simple context of non-interacting systems, how one can combine the Majoranas to build customized fermions.

Equations (2.3) and the property $\gamma^\dagger = \gamma$ illustrate the algebraic nature of the Majorana fermions, which can be thought of as the two components of the complex fermion operator: its real and imaginary parts. Of course some gauge[13] freedom in how the Majoranas are joined together to form the fermion operators must exist. This does not mean that there exists any extra freedom in the physics described. In fact, after the introduction of the previous section, it should be clear that when we deal with Majoranas we are dealing with operators and not with quantum states, which instead are the physical objects. To understand both the theory and practice of the representation of quantum mechanics on the real field, we have to start from an analysis of the standard formalism of second quantization. Firstly I would like to remind the reader of the many assumptions that are hidden behind the creation and annihilation operators. Let us assume the existence of a two dimensional Hilbert space, spanned by two orthonormal vectors $|a\rangle$ and $|b\rangle$. We can define two operators $\hat{A}$ and $\hat{B}$ such that

$$\hat{A}|a\rangle = |b\rangle, \quad \hat{B}|a\rangle = 0, \quad \hat{A}|b\rangle = 0, \quad \hat{B}|b\rangle = |a\rangle. \tag{2.22}$$

These objects fulfill the properties of fermionic operators and in fact it is easy to prove that[14] $\{A, B\} = 1$, so it could be appropriate to use the standard creation/annihilation notation to represent them. This is not straightforward, because it assumes the identification of a vacuum state $|0\rangle$. Both $|a\rangle$ and $|b\rangle$ could be proper vacuum states. If one choses $|a\rangle = |0\rangle$ then $\hat{A} = c^\dagger$ and $\hat{B} = c$, vice versa if one choses $|b\rangle = |0\rangle$. The choice is *completely arbitrary*, and it is

[13] This word is not used in the wrong context: in fact the definition can change in time and space. This concept is clarified in paper D.

[14] It is also possible to see that they are hermitian conjugates, but this is not relevant for the discussion.

only our personal taste that makes us prefer one to the other, or to the other infinite possibilities: in fact it is also possible to make two orthonormal linear combinations of $|a\rangle$ and $|b\rangle$ and redefine two new operators with the same properties of $\hat{A}$ and $\hat{B}$ on this new basis set. Typically there exists some physical reason, that makes us prefer[15] one state to another as (reference) vacuum. In the most common cases it is possible to count the electrons (or better the electric charge) and so it is preferable to have a vacuum where the total electric charge is zero and the action of $c^\dagger$ represents the action of adding a charge unit. But the formalism does not forbid us to choose the fully charged state as vacuum and use a creation operator $h^\dagger(= c)$ that adds a positive charge (removes a negative one). Of course the two choices are related just by a $\mathbb{Z}_2$ transformation, which reflects the two possible *choices* for the vacuum, i.e. the two equivalent formalisms. These considerations seem trivial, but actually it is the misunderstanding of these simple rules that make superconductivity less intuitive: in fact in superconducting systems, where the charge is not conserved, the notion of vacuum gets "twisted" and the fermions change their original nature; indeed electrons and holes are substituted by Bogoliubov quasiparticles.

So the association of a quantum state to an operator $c^\dagger$, comes with a lot of assumptions, often forgotten and harmless, but which must be considered when the representation of the operators on the Hilbert space is changed, moving from the complex to the real field. In particular the first convention that one must fix is the choice of the phase of the Majoranas. In this chapter this (gauge) choice is done as follows:

$$c^\dagger = \frac{\gamma + i\mu}{\sqrt{2}}, \quad c = \frac{\gamma - i\mu}{\sqrt{2}}, \quad \gamma^2 = \mu^2 = \frac{1}{2}. \tag{2.23}$$

This means that, chosen as vacuum state $|0\rangle$ the kernel[16] of an operator c, the annihilation operator is decomposed on two Majoranas out-of-phase by a factor π, while the creation operator $c^\dagger$ is represented via two Majoranas in phase. The $\mathbb{Z}_2$ gauge choice mentioned previously is then given by the transformation that sends $\mu \to -\mu$. As can be seen, under this transformation, the operator c becomes (according to the previous definition, based on the phases of the Majoranas) a creation operator: $h^\dagger(= c)$, meaning that the reference vacuum has changed. It is important to stress again that there is *nothing physical* in all of this; however it is very important because in different situations a different gauge choice, or more generally a different choice of how the fermionic operators are represented, can simplify the problem a lot.

Given these conventions, it also becomes possible to represent the Majorana

[15] Readers familiar with the field of high-energy physics could be confused by these sentences. When QFT is used, a vacuum, which is by definition the state of minimal energy, is also defined (otherwise one speaks of false vacuum or metastable vacuum). Besides many practical and conceptual reasons [29], it is also difficult to imagine a different choice for the vacuum: naively speaking when QFT is used the vacuum is the surface of the Dirac sea; since the sea is unbounded below and above, it is difficult to imagine any other meaningful choice. In condensed matter the situation is different, because the theories have a *finite* number of degrees of freedom, i.e. the Hilbert space is typically finite dimensional. Therefore it is possible to choose a vacuum that is not the minimal energy state (ground state). In fact in the solid state the Fermi volume is *filled*, adding electrons to the vacuum; but it is the filled Fermi sphere, not the vacuum, that is the ground state of the theory.

[16] Please note that the kernel *must not be confused with the ground state*. The ground state is only the state in the Hilbert space with the lowest energy. So far we have not mentioned the Hamiltonian, which is an extra (important) structure, built on this formalism.

operators on the basis set $|0\rangle$, $|1\rangle = c^\dagger|0\rangle$. In fact starting from

$$c^\dagger \to \begin{bmatrix} \langle 0|c^\dagger|0\rangle & \langle 1|c^\dagger|0\rangle \\ \langle 0|c^\dagger|1\rangle & \langle 1|c^\dagger|1\rangle \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},$$

equation (2.23) gives

$$\gamma \to \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad \mu \to \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

Let us take a generic Hamiltonian and suppose that it is quadratic on a four dimensional Hilbert space spanned by $|0\rangle$, $g^\dagger|0\rangle$, $c^\dagger|0\rangle$, $g^\dagger c^\dagger|0\rangle$, where $g^\dagger = (\alpha + i\beta)/\sqrt{2}$. Then

$$H = \epsilon_1 c^\dagger c + \epsilon_2 g^\dagger g + \lambda g^\dagger c + \lambda^* c^\dagger g,$$

which is also

$$H = \left(c^\dagger, g^\dagger\right) \begin{bmatrix} \epsilon_1 & \lambda^* \\ \lambda & \epsilon_2 \end{bmatrix} \begin{pmatrix} c \\ g \end{pmatrix}. \tag{2.24}$$

This Hamiltonian is given in the standard fermionic representation (or complex representation). Using the previous definitions one can rewrite it in the Majorana representation (real representation):

$$\begin{aligned} H \;=\; & \epsilon_1 \frac{1}{2}(1 - i\gamma\mu + i\mu\gamma) + \epsilon_2 \frac{1}{2}(1 - i\alpha\beta + i\beta\alpha) + \\ & + \lambda_R \left(i\mu\alpha - i\mu\alpha + i\beta\gamma - i\gamma\beta\right) + i\lambda_I \left(\alpha\gamma - \gamma\alpha + \beta\mu - \mu\beta\right). \end{aligned} \tag{2.25}$$

where $\lambda = \lambda_R + i\lambda_I$. Putting aside a shift of the energy (whose role will become clear in the following) this Hamiltonian can be represented in a matrix form

$$H = i\left(\gamma, \mu, \alpha, \beta\right) \begin{bmatrix} 0 & -\frac{\epsilon_1}{2} & \lambda_I & -\lambda_R \\ \frac{\epsilon_1}{2} & 0 & \lambda_R & \lambda_I \\ -\lambda_I & -\lambda_R & 0 & -\frac{\epsilon_2}{2} \\ \lambda_R & -\lambda_I & \frac{\epsilon_2}{2} & 0 \end{bmatrix} \begin{pmatrix} \gamma \\ \mu \\ \alpha \\ \beta \end{pmatrix}. \tag{2.26}$$

Both (2.24) and (2.26) represent *the same* Hamiltonian. The first one is the standard complex representation, i.e. it is given by a matrix whose elements are complex numbers, the second is a real representation, which means that its elements take values on the field of real numbers.[17] The complex matrix (2.24) can be diagonalized making use of a properly chosen unitary transformation and one could argue that the same procedure should be followed for (2.26). The reader can immediately see that this not the correct route. In fact, although the eigenvalues could be found, the results would be meaningless, because the diagonalization procedure would produce linear complex combinations of the

[17] The imaginary unit in front of the Hamiltonian clearly does not invalidate this sentence, because it plays the role of a multiplicative prefactor. The imaginary unit is present because it is necessary to have hermitian self-adjoint operators in quantum mechanics, in order to represent physical observables. Clearly this goes beyond what was discussed by Dyson in Ref. [72], because in that paper only the representation of a generic group of transformations was discussed. In this case what matters is the representation of the generators of the group of transformations; clearly the two objects are still related as usual.

original Majoranas. The new objects created would not have (in general) Majorana character anymore, making the formalism not self-consistent. So (2.26) does not have to be diagonalized; instead one has to find a transformation that performs a block-diagonalization. To understand this, let us consider the case of $\lambda = 0$, i.e. when the complex Hamiltonian (2.24) is already diagonal. Then (2.26) looks like

$$H = i\begin{pmatrix}\gamma,\mu,\alpha,\beta\end{pmatrix}\begin{bmatrix}0 & -\frac{\epsilon_1}{2} & 0 & 0\\ \frac{\epsilon_1}{2} & 0 & 0 & 0\\ 0 & 0 & 0 & -\frac{\epsilon_2}{2}\\ 0 & 0 & \frac{\epsilon_2}{2} & 0\end{bmatrix}\begin{pmatrix}\gamma\\ \mu\\ \alpha\\ \beta\end{pmatrix}. \tag{2.27}$$

This is the form of the Majorana Hamiltonian equivalent to the diagonal form of the fermionic Hamiltonian without hybridization. The matrix form (2.27) is exactly of the same form of the one used by Kitaev [6] in the discussion of the polarized p-wave one dimensional superconductor of equation (2.2). The peculiarity pointed out by Kitaev in his work is that there exists a sort of "double spectrum" given by the two paired values ϵ, $-\epsilon$, a point on which we will return in a few paragraphs.

The question as to whether or not it is possible to obtain such block-diagonal form has been answered long ago and a discussion about it can be found in the paper [73] by Zumino, who proved that any $2n \times 2n$ skew-symmetric real square matrix can always be block-diagonalized making use of a real orthogonal transformation $O(2n)$. So to block-diagonalize (2.26) one has to use a $O(4)$ transformation. Actually, without loosing generality, one could focus the attention on the group $SO(4)$, if the eigenvalues ϵ_i are not restricted to real positive numbers. The interesting characteristic of this operation is that, as proved long ago [66–69], the group $SO(2n)$ acting on a set of $2n$-objects that closes under Euclidean Clifford algebra does not break the algebraic structure. In fact such elements can be thought of as unit orthogonal vectors in the $2n$-dimensional Euclidean space. This set of orthonormal unit vectors is sent into another by $SO(2n)$ and the algebraic structure does not change. As example of the generation of a new set of Majoranas, let us act with $SO(2)$ on the two Majoranas γ, μ:

$$\begin{pmatrix}\tilde{\gamma}\\ \tilde{\mu}\end{pmatrix} = \begin{bmatrix}\cos(\theta) & -\sin(\theta)\\ \sin(\theta) & \cos(\theta)\end{bmatrix}\begin{pmatrix}\gamma\\ \mu\end{pmatrix} = \begin{pmatrix}\cos(\theta)\gamma - \sin(\theta)\mu\\ \cos(\theta)\mu + \sin(\theta)\gamma\end{pmatrix}. \tag{2.28}$$

The reader can check that $\tilde{\gamma}^2 = \tilde{\mu}^2 = 1/2$ and $\{\tilde{\gamma}, \tilde{\mu}\} = 0$. Using the new $\tilde{\gamma}$ and $\tilde{\mu}$ to build the new fermion operator $\tilde{c}^\dagger$, one discovers that $\tilde{c}^\dagger = \exp(i\theta)c^\dagger$, so the $SO(2)$ matrix represents a complex phase transformation, but in a real space representation.[18]

The orthogonal transformation that block-diagonalizes the Hamiltonian (2.26) mixes the original Majoranas in a way that the new combinations form again a set of properly defined Majorana fermions. So the new set of Majoranas $\tilde{\gamma}, \tilde{\mu}, \tilde{\alpha}, \tilde{\beta}$ can be used to build well defined fermionic operators. At this point the role of the "double spectrum" ϵ, $-\epsilon$ becomes clear: indeed the couples of Majoranas must now be combined to produce fermionic operators and select the vacuum state, following a given gauge choice. This gauge choice is always

[18] I invite the reader to re-examine the equations (2.19) in the light of this new information.

twofold as we have seen, so depending upon the convention (2.23) one can have two formally opposite, but physically equivalent, results. The equivalence of the results is clear: for example let us consider (2.27) in the block diagonal form

$$H = \frac{\tilde{\epsilon}_1}{2}(i\tilde{\mu}\tilde{\gamma} - i\tilde{\gamma}\tilde{\mu}) + \frac{\tilde{\epsilon}_2}{2}(i\tilde{\alpha}\tilde{\beta} - i\tilde{\beta}\tilde{\alpha}). \tag{2.29}$$

Closing to a Clifford algebra, the new Majoranas can build proper fermion operators $\tilde{g}^\dagger = (\tilde{\gamma} + i\tilde{\mu})/\sqrt{2}$ and $\tilde{c}^\dagger = (\tilde{\alpha} + i\tilde{\beta})/\sqrt{2}$. The Hamiltonian then looks like

$$\begin{aligned} H &= \frac{\tilde{\epsilon}_1}{2}(\tilde{g}^\dagger\tilde{g} - \tilde{g}\tilde{g}^\dagger) + \frac{\tilde{\epsilon}_2}{2}(\tilde{c}^\dagger\tilde{c} - \tilde{c}\tilde{c}^\dagger), \\ &= \frac{\tilde{\epsilon}_1}{2}(2\tilde{g}^\dagger\tilde{g} - 1) + \frac{\tilde{\epsilon}_2}{2}(2\tilde{c}^\dagger\tilde{c} - 1). \end{aligned} \tag{2.30}$$

This final form clearly depends upon the previous selection of the gauge that fixes the form of the creation and annihilation operators, and the relation between the different choices is trivial. In this sense the Majorana representation works symmetrically with respect to the two possible and inequivalent definitions of the vacuum state. It is the gauge choice that one performs on the definition of the fermionic operators that generates a specific form of the Hamiltonian. The "double spectrum" cited by Kitaev is a mere feature of this fact: that the same physics can be described using many equivalent reference systems, i.e. many equivalent reference vacuums and sets of fermionic operators. This is why a constant term appeared in equation (2.25); that constant is supposed to be compensated by the zero point energy that was not explicitly written in (2.24). In principle the redundancy of the description should be present also in the original fermionic representation, where a quadratic term should always be written as

$$\frac{g^\dagger g - g g^\dagger}{2}, \tag{2.31}$$

reflecting the symmetry between the two possible choices of the vacuum. Picking a vacuum permits us to rewrite the previous term as $2g^\dagger g - 1$, so the redundancy is often not noted.

Concluding, the only difference between the two formalisms (standard and Majorana based) is then purely algorithmic: in the complex (fermion) representation the choice of the vacuum can be done at the beginning and the diagonalization procedure will keep track of it; in the real (Majorana) one, the diagonalization procedure automatically cancels any choice of the vacuum, which therefore must be made afterwards. This is why, in the Majorana fermion representation, the presence of superconducting terms is not problematic at all. Having clarified the meaning of choosing a set of Majoranas and described its use in building customized fermions, I will to move to more interesting situations, using these same ideas for the study of interacting correlated systems.

Chapter 3

Introduction to Paper A

3.1 Emergent Majoranas

Beside the details about the "double spectrum" and the block diagonalization procedure, the take home message of the previous Sec. 2.2 concerns the *flexibility* in the definition of the Majoranas. If proper transformations are chosen, one can start from a set of Majoranas and obtain a new set, with exactly the same properties. These Majoranas can then be combined to build fermionic operators. But this is not mandatory: for example one could be interested in building other degrees of freedom, such as spin operators. During recent decades this has been often reported [36, 37, 74, 75], mostly because the Majoranas offer a convenient alternative way to represent spin operators. In fact three Majoranas μ_1, μ_2, μ_3, can be combined to build the operators $S_k = -i\epsilon_{ijk}\mu_i\mu_j$ (with no summation on the repeated indices), which behave as spin operators, closing to a $su(2)$ Lie algebra. The choice of which operators are the most convenient to build depends *completely* on the type of Hamiltonian under consideration and on the strategy (analytical or numerical) that one is planning to use. The crucial point is that with the Majoranas it is possible to customize the quantum coordinates, tailoring them to a specific Hamiltonian.

So far nothing of what has been said is new. The real breakthrough comes from the understanding that, given a system with n fermionic modes, the set of $2n$ Majoranas that it generates is not the most general. There exists other inequivalent sets that can be used to build up different (correlated) fermionic degrees of freedom. The group of transformations that allows one to start from a specific $2n$ Majorana set and obtain another well defined set is not simply the linear group of transformations $SO(2n)$, but it is indeed much larger and includes also the group of non-linear canonical transformations. Since the Majoranas close to Clifford algebra (see appendix A), then given $2n$ Majoranas one can build the full algebra multiplying together the Majoranas in all the possible ways. So the full Clifford algebra contains the $2n$ original single Majoranas, the $\binom{2n}{2}$ bilinears, the $\binom{2n}{3}$ trilinears, and so on up to the single element that is built multiplying together all the Majoranas $\gamma_1 ... \gamma_{2n}$. One can now note that, for example, the term $2i\gamma_1\gamma_2\gamma_3$ resembles very much a Majorana, since it is hermitean and it squares to 1. Indeed this is true for all the objects built mul-

tiplying together an odd number of Majoranas: these objects form well defined *emergent Majorana* fermions[1] if properly multiplied by an imaginary unit (in order to make them hermitean) and by a normalization dependent numerical constant; fixing the normalization $\gamma^2 = 1$ this numerical constant is always 1, so we will stick to this normalization convention in this chapter. For example in the case of two fermionic modes (four dimensional Hilbert space) one has:

$$\begin{array}{ll} \text{original Majoranas} & \gamma_1, \quad \gamma_2, \quad \gamma_3, \quad \gamma_4, \\ \text{emergent Majoranas} & i\gamma_1\gamma_2\gamma_3, \quad i\gamma_1\gamma_2\gamma_4, \quad i\gamma_1\gamma_3\gamma_4, \quad i\gamma_2\gamma_3\gamma_4. \end{array} \tag{3.1}$$

In the formalism there is absolutely no reason behind the predilection of the single Majorana fermions on the composite (emergent) Majoranas, so the only discrimination can be done on the basis of the form of the Hamiltonian. *Therefore the emergent Majoranas have (in general) exactly the same dignity of the original ones and can be mixed with them and among each other.* Indeed the only constraint is that these composite Majoranas must be chosen and mixed properly, in order to create a new set of Majoranas that closes to Clifford algebra. In the context of the SCES this is a potentially powerful property, since the new set may *"suit the Hamiltonian better"*, representing the physics in a more transparent way.

In paper A it is shown that such group of transformations, which allows for this appropriate mixing of original and emergent Majoranas, is the group of canonical transformations. In particular it is the canonical linear group if the original Majoranas mix only among themselves, as in (2.28), and it is the more general non-linear canonical group if also the mixing with composite Majoranas is considered. Understanding these concepts makes it possible to grasp the fundamental rationale behind the non-linear canonical transformations. The very existence of this group relies on the equivalence of different Majoranas existing inside the Clifford algebra, i.e. on the possibility of identifying an infinite number of inequivalent $2n$ Majorana sets that can be used to build fermionic operators able to span the entire Hilbert space.

As mentioned previously one may not be interested in building fermionic operators. One could as well combine the Majoranas to obtain spin operators (non-canonical transformation) that form a well defined Lie algebra (for example $su(2)$). In this case instead of building an equivalent set of $2n$ Majorana fermions, the original Clifford algebra is broken in two: one part still gives rise to appropriate fermionic degrees of freedom, while the other part identifies spin operators. The idea of using non-canonical transformations is, of course, not original. As a matter of fact the Schrieffer-Wolff transformation is an example of non-canonical transformation [22, 77, 78]. This transformation connects the Periodic Anderson Model (PAM), where the Hilbert space is spanned by the application of fermionic operators on a single vacuum state, and to the Kondo Lattice (KL) model, where instead all the local states have two components: a fermion part, describing the conduction electrons, and a spin part, describing the quantum state of the impurity spins. In this thesis, also the Schrieffer-Wolff

[1] It is appropriate to warn the reader that the composite Majoranas mentioned previously (and in all our scientific production) are now becoming the subject of research to the rest of the condensed matter community. Following the recent works by Wilczek and Lee [2,76] these objects are more and more often called *emergent Majoranas*. Because of this the terms composite or emergent Majoranas will be considered interchangeable from now on and in the appended papers.

transformation is re-conceptualized and generalized in the light of our results, giving birth to the concept of hyperspin, introduced in paper A.

Of course choosing one approach over another, or the choice of one particular set of Majoranas over another, depends upon which representation "*suits the Hamiltonian more*". This is a quite relative concept, unless the Hamiltonian could be trivially diagonalized making use of the new degrees of freedom, which is typically not the case. In a more objective fashion, one could say that the choice of a representation depends on how convenient the form of the new Hamiltonian is, i.e. how much physics we can capture easily (at zeroth approximation) using one or the other representation. In the context of the SCES this is a very natural idea: a generic SCES Hamiltonian generates correlations between the dynamics of different fermionic modes; if one can choose a set of new fermionic modes, which incorporate parts of these correlations, i.e. whose free motion corresponds to the correlated motion of the original modes, then it is probable that the study of the Hamiltonian in terms of these new modes will be easier, since less approximations should be needed.

Although all these points are (thoroughly) explained in paper A, two examples will be provided also in this short introduction.

3.2 Examples

3.2.1 Canonical transformations

An example of a canonical non-linear transformation can be found in Ref. [24], where the symmetries of the half-filled Hubbard model and the entire group of its local (on-site) canonical transformations are studied. Here I will examine this example to illustrate the concepts introduced in the previous section.

The local Hilbert space of the Hubbard model is generated by the four states:

$$|0\rangle = |0_\uparrow\rangle \otimes |0_\downarrow\rangle, \tag{3.2}$$

$$|\uparrow\rangle = c_\uparrow^\dagger |0_\uparrow\rangle \otimes |0_\downarrow\rangle, \quad |\downarrow\rangle = c_\downarrow^\dagger |0_\downarrow\rangle \otimes |0_\uparrow\rangle \tag{3.3}$$

$$|\uparrow\downarrow\rangle = c_\uparrow^\dagger c_\downarrow^\dagger |0\rangle = |\uparrow\rangle \wedge |\downarrow\rangle, \tag{3.4}$$

where $c_\downarrow|0\rangle = c_\uparrow|0\rangle = 0$ and $\wedge$ is the antisymmteric tensor product. We define

$$c_\uparrow^\dagger = \frac{\gamma_1 + i\gamma_2}{2}, \quad c_\downarrow^\dagger = \frac{\gamma_3 + i\gamma_4}{2}, \quad \text{with} \quad \gamma_i^2 = 1. \tag{3.5}$$

The canonical transformation group of this space is $SU(2) \otimes SU(2) \otimes U(1) \otimes \mathbb{Z}_2$. The transformation groups that compose the tensor tensor product are:

- the usual operation of spin rotation, given by the group $SU(2)$:

$$\tilde{c}_\uparrow^\dagger = a c_\uparrow^\dagger + b c_\downarrow^\dagger, \quad \tilde{c}_\downarrow^\dagger = a^* c_\downarrow^\dagger - b^* c_\uparrow^\dagger, \tag{3.6}$$

  with $|a|^2 + |b|^2 = 1$, $a, b \in \mathbb{C}$, so

$$|\tilde{0}\rangle = |0\rangle,$$
$$|\tilde{\uparrow}\rangle = a|\uparrow\rangle + b|\downarrow\rangle, \quad |\tilde{\downarrow}\rangle = a^*|\downarrow\rangle - b^*|\uparrow\rangle$$
$$|\tilde{\uparrow}\tilde{\downarrow}\rangle = |\uparrow\downarrow\rangle.$$

The generators of these transformations are the spin operators:

$$S_k = -i\epsilon_{ijk}\gamma_i\gamma_j\frac{1+\gamma_1\gamma_2\gamma_3\gamma_4}{4}, \tag{3.7}$$

and evidently the transformation mixes linearly the original Majoranas to obtain the new set. Using to (3.6) it is easy to find:

$$\begin{aligned}\tilde{\gamma}_1 &= \mathrm{Re}(a)\gamma_1 + \mathrm{Re}(b)\gamma_3 - \mathrm{Im}(a)\gamma_2 - \mathrm{Im}(b)\gamma_4,\\ \tilde{\gamma}_2 &= \mathrm{Re}(a)\gamma_2 + \mathrm{Re}(b)\gamma_4 + \mathrm{Im}(a)\gamma_1 + \mathrm{Im}(b)\gamma_3,\\ &\text{etc...}\end{aligned} \tag{3.8}$$

- the $SU(2)$ pseudospin rotation operation:

$$\tilde{c}^\dagger_\uparrow = uc^\dagger_\uparrow - vc_\downarrow, \quad \tilde{c}^\dagger_\downarrow = uc^\dagger_\downarrow + vc_\uparrow, \tag{3.9}$$

with $|u|^2 + |v|^2 = 1$, $u, v \in \mathbb{C}$, therefore

$$\begin{gathered}|\tilde{0}\rangle = u|0\rangle + v|\uparrow\downarrow\rangle,\\ |\tilde{\uparrow}\rangle = |\uparrow\rangle, \quad |\tilde{\downarrow}\rangle = |\downarrow\rangle\\ |\tilde{\uparrow}\tilde{\downarrow}\rangle = u|\uparrow\downarrow\rangle - v|0\rangle;\end{gathered}$$

In this case the generators of this transformations are the pseudospin operators (see appendix C):

$$I_k = -i\epsilon_{ijk}\gamma_i\gamma_j\frac{1-\gamma_1\gamma_2\gamma_3\gamma_4}{4}. \tag{3.10}$$

Also in this case the transformation is linear. The new set of Majoranas is:

$$\begin{aligned}\tilde{\gamma}_1 &= \mathrm{Re}(u)\gamma_1 + \mathrm{Re}(v)\gamma_3 - \mathrm{Im}(u)\gamma_2 + \mathrm{Im}(v)\gamma_4,\\ \tilde{\gamma}_2 &= \mathrm{Im}(u)\gamma_1 + \mathrm{Re}(u)\gamma_2 + \mathrm{Im}(v)\gamma_3 - \mathrm{Re}(b)\gamma_4,\\ &\text{etc...}\end{aligned} \tag{3.11}$$

- the $\mathbb{Z}_2$ total parity transformation (building block of the Shiba transformation [79]):

$$\tilde{c}^\dagger_\uparrow = c^\dagger_\uparrow, \quad \tilde{c}^\dagger_\downarrow = c_\downarrow, \tag{3.12}$$

that means

$$\begin{gathered}|\tilde{0}\rangle = |\downarrow\rangle,\\ |\tilde{\uparrow}\rangle = |\uparrow\downarrow\rangle, \quad |\tilde{\downarrow}\rangle = |0\rangle\\ |\tilde{\uparrow}\tilde{\downarrow}\rangle = |\uparrow\rangle;\end{gathered}$$

the name of this transformation comes from the fact that the states with even and odd parity are exchanged by it. Since the local Hilbert space of the Hubbard model is very small, this is the only parity transformation that can be done. In higher dimensional spaces, more involved transformations of this kind can be defined. In terms of Majoranas this transformation does not change the set, since it can be reabsorbed into a gauge transformation of the definition of the fermionic creation/annihilation operators. Otherwise one can imagine that the sign in front of one Majorana gets inverted.

- the group $U(1)$, represented by the only non-linear component of the canonical transformation group:

$$\tilde{c}_\uparrow^\dagger = c_\uparrow^\dagger \left[1 + \left(e^{2i\chi} - 1\right) c_\downarrow c_\downarrow^\dagger\right], \quad \tilde{c}_\downarrow^\dagger = c_\downarrow^\dagger \left[1 + \left(e^{2i\chi} - 1\right) c_\uparrow c_\uparrow^\dagger\right]. \quad (3.13)$$

  In the particular case of the Hubbard model this transformation changes the phase in front of the double occupied state, with respect to the other three states of the Hilbert space. In fact

$$\begin{gathered} |\tilde{0}\rangle = |0\rangle, \\ |\tilde{\uparrow}\rangle = |\uparrow\rangle, \quad |\tilde{\downarrow}\rangle = |\downarrow\rangle \\ |\tilde{\uparrow}\tilde{\downarrow}\rangle = e^{-i2\chi}|\uparrow\downarrow\rangle. \end{gathered}$$

  Even if trivial in the appearance, such a phase shift brings physical consequences, as highlighted by studies of the correlated hopping Hubbard model [80–82]. The operator that represents the transformation and leads to the equations (3.13) is

$$R = \exp\left\{2i\chi\left(c_\uparrow^\dagger c_\uparrow - \frac{1}{2}\right)\left(c_\downarrow^\dagger c_\downarrow - \frac{1}{2}\right)\right\}; \quad (3.14)$$

  in fact one can check that $R^\dagger c_\sigma R = \tilde{c}_\sigma$, beside a $e^{i\chi}$ phase factor common to *both* the operators. This operation is done very conveniently in the Majorana representation where

$$R = \exp\left\{-i\frac{\chi}{2}\gamma_1\gamma_2\gamma_3\gamma_4\right\}, \quad \text{with} \quad \gamma_i^2 = 1. \quad (3.15)$$

  The generator of the transformation is the local parity operator, so the transformation can only mix states with the same parity. One can see that in terms of Majoranas the new set is given by $\tilde{\gamma}_i = R^\dagger \gamma_i R$:

$$\begin{aligned} \tilde{\gamma}_1 &= \cos(\chi)\gamma_1 - \sin(\chi) i\gamma_2\gamma_3\gamma_4, \\ \tilde{\gamma}_2 &= \cos(\chi)\gamma_2 + \sin(\chi) i\gamma_1\gamma_3\gamma_4, \\ \tilde{\gamma}_3 &= \cos(\chi)\gamma_3 - \sin(\chi) i\gamma_1\gamma_2\gamma_4, \\ \tilde{\gamma}_4 &= \cos(\chi)\gamma_4 + \sin(\chi) i\gamma_2\gamma_3\gamma_4, \end{aligned} \quad (3.16)$$

  The last formulas make evident that the non-linear canonical transformation $U(1)$ mixes (properly) the two sets of Majoranas in (3.1) γ_1, γ_2, γ_3, γ_4 and $i\gamma_1\gamma_2\gamma_3$, $i\gamma_1\gamma_2\gamma_4$, $i\gamma_1\gamma_3\gamma_4$, $i\gamma_2\gamma_3\gamma_4$, which is exactly the kind of operation explained in the previous section.

In higher dimensions (larger number of fermions) the group of canonical transformations becomes much more involved and many more non-linear transformations are allowed. Anyway it can be represented and handled very efficiently within the Majorana representation. It must be mentioned that this topic has been approached also in Ref. [26], but from a numerical perspective and in terms of normal fermion operators only.

3.2.2 Non-canonical transformations

The fact that three Majoranas multiplied together generate another Majorana, opens fascinating opportunities in the context of the interacting systems. Let us consider an interacting term of the form

$$-U\gamma_1\gamma_2\gamma_3\gamma_4, \tag{3.17}$$

that corresponds to the familiar fermionic interaction:

$$Uc_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow - \frac{U}{2}c_\uparrow^\dagger c_\uparrow - \frac{U}{2}c_\downarrow^\dagger c_\downarrow + \frac{U}{4} = U\left(c_\uparrow^\dagger c_\uparrow - \frac{1}{2}\right)\left(c_\downarrow^\dagger c_\downarrow - \frac{1}{2}\right),$$

i.e. the local interaction term of the half-filled Hubbard model.[2] This operator is invariant under the non-linear transformation (3.14). However it is not difficult to notice that if one thinks of $i\gamma_1\gamma_2\gamma_3$ as a single Majorana, introducing

$$\gamma_0 = i\gamma_1\gamma_2\gamma_3, \tag{3.18}$$

then the four fermion term (3.17) becomes a simple quadratic term $-i\frac{1}{2}\gamma_0\gamma_4$ and defining the fermionic operator $h_0 = (\gamma_4 - i\gamma_0)/2$, the expression (3.17) becomes

$$-U(h_0^\dagger h_0 - 1/2).$$

So the original interacting problem becomes effectively a non-interacting one.

Clearly this cannot be the entire story: in fact the original Hilbert space was four-dimensional, while the final one is only two-dimensional. Moreover it is clear that this operation is not contained into the canonical group introduced in the previous section and (therefore, as proved in paper A) the structure of the Clifford algebra is not preserved. The (3.18) performs a non-canonical unitary transformation of the quantum coordinates, that can easily be understood as a transformation that changes the way of *how the fermion operators are represented*. Typically the creation operator of a spinful fermion is represented (for example) as

$$c^\dagger = \begin{pmatrix} \frac{\gamma_1 + i\gamma_2}{2} \\ \\ \frac{\gamma_3 + i\gamma_4}{2} \end{pmatrix}, \tag{3.19}$$

however an equivalent way to represent it is [83]:

$$c^\dagger = \frac{1}{2}\begin{pmatrix} \Phi\sigma^+ \\ \\ \Phi\sigma_z + i\Psi \end{pmatrix}, \tag{3.20}$$

where Φ and Ψ are two Majorana fermions and σ are the Pauli matrices. Trying to relate the two representations, one gets:

$$\Phi = i\gamma_1\gamma_2\gamma_3, \qquad \Psi = \gamma_4 \tag{3.21}$$

$$\sigma_x = +i\gamma_2\gamma_3, \quad \sigma_y = +i\gamma_3\gamma_1, \quad \sigma_z = -i\gamma_1\gamma_2. \tag{3.22}$$

[2] Typically the term used is $U/2\left(c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow - 1\right)^2 = U\left(c_\uparrow^\dagger c_\uparrow - 1/2\right)\left(c_\downarrow^\dagger c_\downarrow - \frac{1}{2}\right) + U/4$, with the extra shift due to the usual zero point energy shift.

The fermion operator h_0 built previously (that from now on we will call "holon") is therefore obtained combining Φ and Ψ; besides the vacuum and single occupied state of this fermion, one has also the two possible eigenstates of the spin operator σ_z, that can be interpreted describing the internal degrees of freedom of $i\gamma_1\gamma_2\gamma_3$. In this representation the Hilbert space is not anymore generated by the application of the fermionic operators on a single vacuum state, but it is decomposed into two sectors:

$$\begin{aligned} \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\} &= \{|0_h\rangle, |1_h\rangle\} \otimes \{|\Uparrow\rangle, |\Downarrow\rangle\} \\ &= \{|0_h\rangle \otimes |\Downarrow\rangle, |1_h\rangle \otimes |\Uparrow\rangle, |1_h\rangle \otimes |\Downarrow\rangle, |0_h\rangle \otimes |\Uparrow\rangle\} \end{aligned} \tag{3.23}$$

A detailed analysis can be found in paper A an in Section II of paper C. The operators σ_i close to $su(2)$ Lie algebra, and operate on a Hilbert space that I will call $SU(2)$-sector or hyperspin sector of the Hilbert space. At first sight this transformation looks quite inconvenient and abstract. Analyzing it more carefully, it becomes evident that the transformation is actually very natural. Rewriting the shifted term (3.17) as $U(c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow - 1)^2/2 = U(1 - h_0^\dagger h_0)$, and looking at (3.23), it is evident that the states with $\langle h_0^\dagger h_0 \rangle = 1$ are the single fermion ones $|\uparrow\rangle$ and $|\downarrow\rangle$, while the $\langle h_0^\dagger h_0 \rangle = 0$ are $|0\rangle$ and $|\uparrow\downarrow\rangle$. As natural consequence, the $SU(2)$-sector is interpreted[3] as *spin sector* of the $|1_h\rangle$ state and *pseudospin sector* of the $|0_h\rangle$ state. This non-canonical transformation is therefore the reason behind the possibility to represent the spin operators in terms of Majorana fermions [74, 84]. In terms of Majoranas the non-canonical transformation breaks the Clifford algebra in two parts: one is related to the holonic sector of the Hilbert space and that contains γ_4, $\gamma_0 = i\gamma_1\gamma_2\gamma_3$ and their product; the other instead contains the three Majoranas γ_1, γ_2, γ_3 and their bilinears, and it is clearly connected with the hyperspin sector of the Hilbert space.

The analysis of any model can be performed also in this different non-purely fermionic representation of the quantum operators. In the case of the Hubbard model this was done in [25] and [83], and also the Heisenberg model is obtained in the high U limit of the Hubbard one via this transformation (plus a projection on the low energy sector) [23]. Clearly the change of representation generates advantages diagonalizing the interaction term, but it makes the structure of the hopping term much more complicated. In this representation the Hubbard model has two kind of degrees of freedom: *holons*, associated to the fermion h_0, and *(hyper-)spinons* given by the modes of the $SU(2)$ sector. The dynamics of these modes is correlated because of the hopping term. The most obvious advantages of this representation are evident in the limit of strong U. In that case, to a good approximation, the ground state has one h_0 fermion per site and the Hamiltonian becomes expressible in terms of the $SU(2)$ operators only; but on the $|1_h\rangle$ states the $SU(2)$ operators are interpreted as spin operators. Therefore one obtains the Heisenberg model, when it is seen as the low energy effective Hamitlonian of the high U half-filled Hubbard model. So (correctly) at infinite U, when the valence oscillations of the electrons are forbidden, the

[3] It is clear now why the choice for the phases of the Majoranas in the creation operators of the up and down electrons has been changed: if $c_\uparrow^\dagger = (\gamma_1 + i\gamma_2)/\sqrt{2}$, $c_\downarrow^\dagger = (\gamma_3 + i\gamma_4)/\sqrt{2}$ had been chosen, then the states with one holon would have corresponded to $|0\rangle$ and $|\uparrow\downarrow\rangle$, and consistently the states with no holon $|\uparrow\rangle$, $|\downarrow\rangle$. The final result would have been equivalent, but slightly more unnatural.

half-filled Hubbard Hamiltonian turns into a pure spin model [25, 83]. Anyway it is also possible to move away from the strong coupling limit, although the dynamics of the holons and the spinons get entangled, requiring non-trivial approximations.

The same kind of approach has been used in the description of the t-J model [85–88] and also the strong coupling analysis of the Kondo lattice [89], reviewed in the Sec. 6.3.1 shares the same concepts. Often the use of the non-linear non-canonical transformations permits an exact treatment of the interacting terms of the Hamiltonian, but it turns the hopping term into a complicated interaction term between the states of generalized-spin sector of the Hilbert space and the fermionic (holonic) ones.

This example was not particularly involved, since the number of local Majoranas was indeed very low. However it is clear that the situation changes when the number of fermionic modes increases. Using the Majorana fermion framework a study of this kind can be done for any number of fermions n, since it is straightforward to determine the set of hyperspin operators. All these concepts are developed in paper A, where it is also explained the close conceptual relation between this non-canonical approach and the idea of dynamical symmetries [90, 91]. Indeed the choice of the spin operators that one wants to use in the description of the system must rely on the specific case that is subject of analysis. The Majorana representation helps in identifying algebras that fulfill specific symmetry criteria, but the choice of such criteria (and so also the choice of how the Clifford algebra must be broken or reduced) depends upon the user of the framework. The best way to do it is, probably, the identification of the degenerate or quasi-degenerate subspaces of the local Hilbert space, that may be optimally described by spin operators; this way to proceed has indeed much in common with the analysis in nuclear and atomic physics based on the concepts of Spectrum Generating Algebra and Dynamical Symmetries.

3.3 Achievements of Paper A

This (long) paper is divided into two parts. In the first one we developed the foundations of the framework are developed in a mathematically complete way. In particular we:

- characterized the group structure of the general group of canonical transformations (which was only partially done in Ref. [24]);
- proved how the Clifford algebra generated by the Majorana fermions of a local Hilbert space can be modified to obtain a Lie algebra (providing a Majorana representation of the Lie generators that was previously unknown);
- showed how this Lie algebra can be restricted, in order to consider only the generators of the canonical (linear and non-linear) transformations, connecting in this way the Clifford algebra generated by Majorana fermions with the group of canonical transformations. This means that we connected the mathematical abstraction of the non-linear canonical transformations with the physics of the fermion modes, which represents a non-trivial conceptual achievement;

- provided a simple representation for the generators of the (non-)linear canonical transformations and for the unitary transformations that they generate; this result is important from a practical point of view, since it strongly simplifies (also computationally) the use of non-linear transformations;
- associated to all these mathematical concepts a physical understanding, in terms of composite (emergent) Majorana fermions.

In the second part instead we developed the idea of hyperspin. In particular:

- we defined the concept in a rigorous way;
- we showed how the Majorana fermion representation may be very useful in the implementation of a dynamical symmetry approach also to SCES systems.

Moreover we also provided a review of the main strategies that we have elaborated to apply in an effective way the non-linear transformation in the analysis of the SCES.

Part II

Application: the Hubbard model

Chapter 4

The Mott Insulator

4.1 Metals and Insulators

An introduction to the features of the Mott Insulating phase has no meaning without the definition of the terms *insulator* and *metal*.[1] Such a definition must mediate between the colloquial meaning and the mathematical rigor necessary in physics. In a naive way one could say that a material is metallic if it allows for the conduction of electric current, and an insulator otherwise. This definition is clearly too inaccurate, since everything can (in principle) conduct current if the difference in voltage between its two extremities is large enough, via dielectric breakdown. Thus, to give a more accurate definition, it is better to consider the conductive properties of a material in the presence of small external perturbation: a system is metallic if it conducts current for an infinitesimal applied external electric field. The use of the small field analysis, i.e. of the linear response approximation, makes this approach quite universal, since it is rooted in the concepts of the Boltzman equation [94]. Keeping a semiclassical point of view and without focusing on the details, the idea can be summarized as follows: in equilibrium, i.e. in absence of any external perturbation (electric field), the charge carriers are fully characterized by a given probability distribution function f_0, which depends on the degrees of freedom necessary to describe the configuration (state) of the system and upon the temperature. This equilibrium distribution is a stable fix point for the probability distribution function of the system, in the sense that any (small) deviation f_1 from the equilibrium f_0 is quickly suppressed by the dynamics of the system. For example, if we excite a few electrons in the system increasing their momentum, we modify the probability distribution function $f = f_0 + f_1$, but since the electrons scatter against the phonons and loose energy, we must expect that f relaxes to f_0 after a typical time τ. If the deviation from equilibrium f_1 is sustained by a steady external perturbation, then the system cannot relax back to equilibrium and the competition between the external force (in this case the external electric field E_i) and the internal restoring processes de-

[1] This brief introduction to the topic will necessarily follow the standard approaches, such as Refs. [7, 92, 93], since these are textbook notions and not so much more can be added to the discussion; however I decided not to entirely omit this discussion in order to keep the text fluent and self-contained.

termines the out of equilibrium form $f(E_i) = f_0 + f_1(E_i)$ of the probability distribution function, which in turns means that a steady current is flows inside the system [94]. Between the classical and the quantum case there are some technical differences, due mostly to the fact that in the quantum case one has to use a density matrix $\rho = \exp\{-\beta H\}/Z$ and not a probability distribution function, and due to the fact that the Hamiltonian picture of quantum mechanics assumes the conservation of energy and a unitary evolution in time, which must be "hidden under the carpet" in some circumstances (see for example discussion in Ref [95]). Beside these technicalities, and as long as one treats macroscopic systems, the basic concepts are the same. In both situations one can write the current j_i as $j_i = \sigma_{ij} E_j$, where σ_{ij} is the conductivity tensor. In the quantum mechanical case this relation is given by the Kubo formula, which can be derived[2] assuming a small perturbation of the Hamiltonian:

$$H_I = -\int dr A_a(r,t) \cdot \hat{j}_a^P(r,t), \tag{4.1}$$

where we decided to work in the Coulomb gauge $\vec{\nabla} \cdot \vec{A} = 0$ and the symbol $\hat{j}_a^P$ stresses the fact that the coupling involves the paramagnetic contribution to the electric current. In fact, keeping in mind the choice of the gauge and the fact that all the observables must be gauge invariant, one can understand that there are two different contributions to the current: a paramagnetic and a diamagnetic contribution. This is due to the enforcement of minimal coupling rules between the electrons and the electromagnetic field, which in the Schrödinger equation implies the substitution:

$$i\vec{\nabla} \to i\vec{\nabla} + e\vec{A}(\vec{x},t), \tag{4.2}$$

which determines the following formulas for the continuous current operator

$$\hat{j}(\vec{x}) = -\frac{ie}{2m^*}\hat{\Psi}^\dagger(x)\overleftrightarrow{\nabla}\hat{\Psi}(x) - \frac{e^2}{m^*}\vec{A}(\vec{x},t)\hat{\Psi}^\dagger(x)\hat{\Psi}(x). \tag{4.3}$$

So, evidently the response to a small external perturbation can be computed as the sum of two contributions: the paramagnetic and the diamagnetic part of the response. The latter is easily computed keeping only the part of the response that is linear in the external field:

$$j_a^D(r,t) = \langle \hat{j}_a^D(r,t)\rangle = -\frac{e^2}{m^*}\langle \hat{\Psi}^\dagger(x)\hat{\Psi}(x)\rho_0\rangle A_a(\vec{x},t) = -\frac{e^2 n}{m^*}A_a(\vec{x},t); \tag{4.4}$$

The former instead can be calculated using the linear response approximation:

$$\begin{aligned} j_a^P(r,t) = \langle \hat{j}_a^P(r,t)\rangle &\approx i\int_{-\infty}^{t} dt' \int dr' \langle \left[\hat{j}_a^P(r,t), \hat{j}_b^P(r',t')\right]\rangle A_b(r',t') \qquad (4.5)\\ &= i\int_{-\infty}^{t} dt' \int dr' \mathrm{Tr}\left(\left[\hat{j}_a^P(r,t), \hat{j}_b^P(r',t')\right]\hat{\rho}_0\right) A_b(r',t'), \end{aligned}$$

with the convention $\hbar = 1$; equivalently

$$j_a^P(r,t) = \int_{-\infty}^{+\infty} dt' \int dr' \tilde{\chi}_{ab}^{ret}(r,t,r',t') \cdot A_b(r',t'), \tag{4.6}$$

[2]Part of this derivation is taken from Refs. [93,96], although with some modifications, but many other text on electron transport theory deal with the Kubo formula and the computation of the conductivity. For example also Ref. [11] tackles the problem extensively.

where $\tilde{\chi}^{ret}_{ab}(r,t,r',t') = i\langle\left[\hat{j}^P_a(r,t),\hat{j}^P_b(r',t')\right]\rangle\theta(t-t')$ is the retarded current-current response function. Explicitly $\tilde{\chi}^{ret}_{ab}(\vec{q},\omega)$ is:

$$\tilde{\chi}^{ret}_{ab}(\vec{q},\omega) = i\int dr' \int_{-\infty}^{0} d\tau \mathrm{Tr}\left(\left[\hat{j}^P_a(0,0),\hat{j}^P_b(\vec{r'},\tau)\right]\rho_0\right) e^{-i\vec{q}\vec{r'}+i\omega\tau+\eta\tau}, \quad (4.7)$$

where $\eta \to 0$ is the usual infinitesimal regularization coefficient, needed to enforce the adiabatic switching on of the perturbation from $t' \to -\infty$.

Summing the two parts and performing a Fourier transform one gets:

$$j_a(\vec{q},\omega) = L_{ab}(\vec{q},\omega)\cdot A_b(\vec{q},\omega), \quad (4.8)$$

where $L_{ab}(\vec{q},\omega)$ is given by

$$L_{ab}(\vec{q},\omega) = \tilde{\chi}^{ret}_{ab}(\vec{q},\omega) - \frac{ne^2}{m}\delta_{ab}. \quad (4.9)$$

Formula (4.8) can be conveniently rewritten in terms of the applied electric field, using the (Coulomb gauge) relation $\vec{E}(\vec{x},t) = -\partial\vec{A}(\vec{x},t)/\partial t$:

$$j_a(\vec{q},\omega) = \frac{1}{i(\omega+i\eta)} L_{ab}(\vec{q},\omega)\cdot E_b(\vec{q},\omega). \quad (4.10)$$

Therefore the conductivity is given by:

$$\sigma_{ab}(\vec{q},\omega) = \frac{1}{i(\omega+i\eta)}\left\{\tilde{\chi}^{ret}_{ab}(\vec{q},\omega) - \frac{ne^2}{m}\delta_{ab}\right\}. \quad (4.11)$$

The difference between a metal and an insulator can now be defined exactly, computing the transverse DC conductivity at zero temperature:

$$\sigma^{DC}_{aa} = \lim_{T\to 0}\lim_{\omega\to 0}\lim_{\vec{q}\to 0}\sigma_{aa}(\vec{q},\omega). \quad (4.12)$$

If such a limit is zero, then the material is an insulator, otherwise it is a metal. It is worth stressing that it is the *limit* of the conductivity that determines the difference between a metal and an insulator. In fact the gauge invariance enforces the equality:[3]

$$\tilde{\chi}^{ret}_{aa}(\vec{q},0) - \frac{ne^2}{m} = 0, \quad \forall\vec{q}. \quad (4.13)$$

One therefore understands that it is the limit of $L_{ab}(\vec{q},\omega)$ and not its value at zero, which determines the metallic or insulating behavior. If $L_{ab}(\vec{q},\omega)$ is not

[3]Indeed a Gauge transformation acts as $\vec{A} \to \vec{A} + \vec{\nabla}\alpha$, $\phi \to \phi - \partial\alpha/\partial t$, where the gauge field is $\alpha(\vec{x},t)$. The current response to this gauge field must necessarily be zero, since the gauge transformation does not change the electric field. However Eq. (4.8) relates linearly the vector potential and the current via $L_{ab}(\vec{q},\omega)$, so it is evident that if the former is changed also the latter must change accordingly. In absence of external charges $\phi = 0$, so if one uses $\alpha(\vec{x},t) = \alpha(\vec{x})$, no new scalar potential is induced. This means that in Fourier space only the $\omega = 0$ component of $\vec{A}(\vec{q},\omega)$ is changed by the transformation and therefore this must imply a constraint on the value of $L_{ab}(\vec{q},0)$. At this point one could argue that this must be true for any value of $\vec{A}(\vec{q},\omega)$, so also for $\vec{A}(\vec{q},\omega) = 0$. In this case, given (4.8) and considered the arbitrariness of $\alpha(\vec{q})$, the only conclusion is that (4.13) holds. For a full mathematical demonstration of this (and other) gauge constraints, I suggest to read Ref. [96].

zero for $\omega \to 0$, then the conductivity (4.11) becomes infinity, which means it behaves as in a perfect conductor.[4] If instead $L_{ab}(\vec{q},\omega)$ goes (quickly enough) to zero, then the conductivity can also go to zero, as in an insulator.

Equivalently one could focus the attention on the behavior of $\tilde{\chi}^{ret}_{aa}(\vec{q},\omega)$, which is the object that must be computed carefully, depending on the current-current commutator. Since the quantum average $\langle\left[\hat{j}^P_a(t),\hat{j}^P_b(\tau)\right]\rangle_0$ can be performed in any basis, the momentum basis seems the natural choice, since (in a crystal) the crystalline momentum is a good quantum number. It is important to point out that the computation of the conductivity depends upon the calculation of a four fermion average, so it is clear that electric conduction is a many body phenomena, which cannot in general be described exactly in terms of single particle properties or quantities. In particular it is clear that the conduction of current concerns the coherent propagation of electron-hole pairs. Indeed, in order to generate non-zero current at vanishing fields, two things must necessarily happen [92]: there must be electron-hole excited states available at vanishing energy; such electron-hole pairs must be able to generate coherent macroscopic states, to be able to propagate through the entire system. Since it is particularly complicated to describe the coherent dynamics of an electron-hole pair, typically these two quasi-particles are considered as uncorrelated, so that it is enough to study the energy, the density and the properties of the single particle excitations, for both electrons and holes, to discover whether the system is or is not insulating. In particular one can determine if a gap Δ exists, i.e. if energy is required to add or remove an electron. If Δ is not zero for both electrons and holes the system is insulating. This approach has obvious limitations if the system is correlated, since the operation of adding and removing electrons seriously affects the eigenstates of the system and so also one-particle properties as, for example, the density of states.

As mentioned in the previous discussion, the conduction properties can distinguish between an insulator and a conductor only at zero temperature. This is due to the fact that temperature implies an incoherent occupation of conductive quantum states also in the insulators. So at $T \neq 0$ even a material classified as insulator can conduct. However the insulators can be identified by the temperature dependence of the conductivity. Indeed the conductivity tensor of an insulator must show a temperature activated behavior like:

$$\sigma_{ab}(0,0,T) \propto \exp\left\{-\frac{\Delta}{k_B T}\right\}, \tag{4.14}$$

for $k_B T$ of the order of Δ or smaller, where Δ is the typical energy scale of the insulator. In general such a value is given by the value of the gap at zero temperature, though some variations may occur [92].

The classification of the insulators into different classes is done on the basis of the origin of the gap Δ. The simplest classification comprises four different classes of insulators:

i. **Band insulators:** in this case the gap is due to the energy of the orbitals that give rise to the bands inside a material; if the electrons completely

[4] The reader can understand that the difference between a perfect metal and a superconductor cannot be defined only on the basis of the transverse conductivity. The difference is enclosed in the longitudinal behavior of the conductivity, which in a similar limit goes to zero in the case of a metal and is finite for a superconductor.

fill an integer number of bands, which means if the crystal has an even number of electrons per unit cell, then there are no zero-energy single-particle excitation states for the electrons and therefore the system is insulating.

ii. **Peierls and Stoner insulators:** in these insulators the gap is generated by a symmetry reduction, which results in the establishment of a band insulator [97, 98]. The symmetry breaking can involve the electron wave function only (Stoner insulators) as well as distortions of the lattice (Peierls insulators).

iii. **Anderson insulators:** in a system with lattice disorder the conduction gap is not between the ground state and the first available excited state, but between the ground state and the first excited state that is macroscopically extended over the entire system. Indeed the lattice disorder can coherently scatter back the electrons, which effectively become caged: so to create current one has to excite electrons with high energy, which are able to escape this process.

iv. **Mott insulators:** in this case the gap is created by the local (screened) interaction between the electrons, preventing them from moving freely in the system. These are the insulators that are considered in paper B.

4.2 Mott physics

4.2.1 A correlation driven insulator

As mentioned in the previous section, the insulating character of a system can be caused by the interactions between the electrons (or carriers in general), via a process that is strongly reminiscent if the Wigner crystallization of a 2d electron gas [99]. This idea developed by Mott [100] looks simple, but it hides important technical problems. To clarify the concept, let us consider a half-filled system. If no interaction is present the electrons are free to delocalize over the entire system, jumping from site to site and occupying them randomly, following only the restrictions enforced by the Pauli principle. In presence of a small interaction this picture of free propagating electrons must still be valid, at least for excitations infinitesimally close to the Fermi surface, since the Landau-Fermi liquid theory [9, 10] ensures the existence of a one-to-one correspondence between the low energy states lying close to (on) the Fermi surface of the interacting model and the eigenstates of the free model. However, if one imagines increasing the interaction more and more, the possibility of a breakdown of this picture must be considered, since the interaction prevents two electrons (even of different spins) from approaching each other. At some point every electron must necessarily find itself frozen in one position, because its motion gets stopped by the surrounding electrons that effectively generate an electrostatic trap. Given that the electrons get confined into their positions, it seems plausible that somewhere, between the non-interacting and the strongly interacting limit, the Landau-Fermi liquid picture can break down since one cannot speak anymore of propagating fermions (formally this can happen via a divergence of the electron's effective mass [10, 101–104]); thus the one-to-one correspondence

(adiabatic connection) and therefore the Fermi surface do not necessarily have to exist anymore.

The debate about the necessity of a Fermi-Liquid breakdown is still vivid, and I leave to the reader the burden of exploring it, since it is only marginally related to our work. Instead it is important to focus our attention on a less controversial point: the fact that in the high (infinite) interaction regime, the most natural degrees of freedom for the description of the system are no longer the electrons, as already pointed out by Mott [100]. Indeed assume that the interaction is so intense[5] that each electron gets stuck in one position (atomic limit), without the possibility to delocalize and propagate, then little of their original electronic nature is left. For example at the low energy scale the relevant degrees of freedom are spins, and the electrons (which generate the local momenta) enter in the description only as *virtual* high energy degrees of freedom, which are able to justify the spin-spin interaction via their virtual motion. In the case of a half-filled system in the atomic limit this seems quite natural and indeed *what characterizes a Mott insulator is the appearance of local moments [92,100].* Away from half-filling the scenario is more complicated, but still very similar. The electronic degrees of freedom are not good quantum coordinates and the one-to-one mapping of Landau-Fermi liquid does not hold anymore, since some excitations that exist in the interacting model do not have counterparts in the free model [105,106]. Clearly away from half-filling the system is not anymore an insulator, but rather it becomes a strongly correlated metal, where the current is in general transported by the correlated motion of doubly-occupied and unoccupied sites (or doublon-holon coherent states). Such a situation is analyzed in detail in Ref. [105,106], where it is also pointed out that the process of creation of these new degrees of freedom implies a full reorganization of the spectral distribution of the system, via a process known as spectral weight transfer. This redistribution of the spectral weight and the mixing of UV and IR energy scales proves that the electrons are no longer the proper degrees of freedom for the description of the system, but correlated doublon-holon states must emerge as fundamental particles. Such an emergence reminds us of the same mechanism that binds quarks into mesons at low energy scales. Although this discussion is very interesting, the present chapter will focus only on the half-filled case and therefore on the properties of the insulating phase.

Surprisingly all this complex physics is summarized very well in a simple model, due to Hubbard [8]:

$$H_H = -t \sum_{\langle i,j\rangle,\sigma} \left\{ c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. \right\} + U \sum_i c^\dagger_{i,\uparrow} c_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} + \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}, \quad (4.15)$$

where the choice $\mu = -U/2$ forces the half-filling of the system. The Hubbard model makes the appearance of local moments in the high-U limit evident. Indeed, in this limit, it is possible to map it exactly onto the Heisenberg model, via a unitary transformation [23,107]. For pedagogical purposes, it is convenient to show the main passages of this map. The first thing to do is to separate the kinetic term into three main processes: the hopping of the holes T_h, the hopping of the doublons T_d and the other type of hoppings T_{mix}. It must be pointed out that the first two processes do not change the total local parity of the states,

[5] Or alternatively that the hopping is zero.

while the last one does.

$$\begin{aligned} T_h &= -t \sum_{\langle i,j\rangle,\sigma} \left\{ (1-n_{i,-\sigma}) c^\dagger_{i,\sigma} c_{j,\sigma} (1-n_{j,-\sigma}) + h.c. \right\}, \\ T_d &= -t \sum_{\langle i,j\rangle,\sigma} \left\{ n_{i,-\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} n_{j,-\sigma} + h.c. \right\}, \\ T_{mix} &= -t \sum_{\langle i,j\rangle,\sigma} \left\{ n_{i,-\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} (1-n_{j,-\sigma}) + (1-n_{i,-\sigma}) c^\dagger_{i,\sigma} c_{j,\sigma} n_{j,-\sigma} + h.c \right\}. \end{aligned} \tag{4.16}$$

Since the third process implies an energy expense of order U, one expects its suppression at high coupling, so a unitary transformation $\exp(-iS)$ with $S = S^\dagger$ can be set up to make this term disappear, at least at first order in S:

$$H_{\text{eff}} = e^{iS} H e^{-iS} = H + i[S, H] + O(S^2). \tag{4.17}$$

Calling V the interacting term one has:

$$\begin{aligned} &H = T_d + T_h + T_{mix} + V, \\ &H_{\text{eff}} = T_d + T_h + T_{mix} + V + i[S, T_d + T_h + T_{mix} + V]. \end{aligned} \tag{4.18}$$

So, to make T_{mix} disappear, S must obey the following constraint:

$$\begin{aligned} &i[S, T_d + T_h + V] = -T_{mix}, \\ &iS(T_d + T_h + V) - i(T_d + T_h + V)S = -T_{mix}. \end{aligned} \tag{4.19}$$

Using the eigenstates and eigenvalues ϵ_i of $T_d + T_h + V$, one gets:

$$i \sum_{n,m} |n\rangle\langle n|S|m\rangle\langle m|\epsilon_m - i \sum_{n,m} \epsilon_n |n\rangle\langle n|S|m\rangle\langle m| = -T_{mix}, \tag{4.20}$$

which immediately implies

$$S = \sum_{n,m} |n\rangle \frac{\langle n|T_{mix}|m\rangle}{i(\epsilon_n - \epsilon_m)} \langle m|. \tag{4.21}$$

Of course the ϵ_i are unknown, but one has to keep in mind that T_{mix} is non-zero only if it connects a state from one parity sector to a state in another parity sector (i.e. with different numbers of doublons and holes), and that in the limit of infinite-U the parity sectors are very well separated in energy by the interaction; so evidently in this limit $\epsilon_n - \epsilon_m \approx \pm U$. In conclusion, substituting T_{mix} with (4.16) and keeping track of the parity of the states connected by the different operators in T_{mix}, one gets:

$$S = -i \frac{t}{U} \sum_{\langle i,j\rangle,\sigma} \left\{ n_{i,-\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} (1-n_{j,-\sigma}) - (1-n_{i,-\sigma}) c^\dagger_{i,\sigma} c_{j,\sigma} n_{j,-\sigma} - h.c. \right\},$$

which is hermitian as expected. The new effective Hamiltonian is now

$$H_{eff} = T_h + T_d + V + i[S, T_{mix}] + \mathcal{O}(S^2). \tag{4.22}$$

At the first order of t/U there are no operators that mix the two parity sectors, which can therefore be analyzed separately. Focusing on the sector with no doublons (low-energy sector) and dropping the higher order terms one gets:[6]

$$H_{\text{eff}} = T_h + 4\frac{t^2}{U}\sum_{\langle i,j\rangle}\left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}n_i n_j\right). \tag{4.23}$$

Moreover at half-filling $T_h = 0$, since there are no holes (given the fact that there are no doublons) and $\langle n_i n_j\rangle = 1$ exactly [23, 107]. What one finds is therefore that H_{eff} is the Hamiltonian of the spin-1/2 Heisenberg model.

The reader has certainly noticed the many assumptions that are needed to connect the Hubbard model with the Heisenberg model, i.e. to connect a model for electrons propagating on a lattice to a model describing interacting spins. Indeed this procedure shows very well that the Mott insulator is realized via the appearance of local moments, although how this happens in the intermediate-U region is still obscure. In fact the previous assumptions are justified only in the $U = \infty$ limit, since only in this limit the contribution of the doublon hopping and the higher order terms can be completely discarded.

The exact mechanism that leads to emergence of the Mott insulating phase via an increase of U is still not well determined (see Sec. 4.2.2), however there are no doubts about the fact that the increase of the correlations between the electrons must drive this process. When one speaks about correlations there is always quite a lot of confusion. Electrons are naturally correlated with each other, because of the Pauli principle. This effect is present also in the Fermi gas, where it produces the exchange-hole effect [93]: this is visible in the equal-spin electron-density correlation function $P_{\sigma,\sigma}(\vec{x},\vec{x}')$, which is related to the probability of finding an electron in $\vec{x}'$ given the presence of another electron with the same spin in $\vec{x}$,

$$P_{\sigma,\sigma}(\vec{x},\vec{x}') = \rho_0^2\left[1 - \left(3\frac{\sin x - x\cos x}{x^3}\right)^2\right], \tag{4.24}$$

with ρ_0 the density of the gas (assuming translational and spin rotation invariance) and $x = |k_F|\,|\vec{x} - \vec{x}'|$. Between electrons with different spin the correlation function is instead much simpler:

$$P_{\sigma,-\sigma}(\vec{x},\vec{x}') = \rho_0^2. \tag{4.25}$$

The exchange correlation explained above is a trivial part of the correlation that is not of interest in the present discussion. Of course it can lead in combination with Coulomb interaction to dramatically important effects (e.g. Hund's first rule, Stoner ferromagnetism, RKKY interaction), but exchange is not the kind of correlation that one has in mind speaking about Strongly Correlated Electron Systems. The correlations *beyond* exchange are responsible for the involved physics of these systems, and thus also of the Mott physics. The existence of extra correlations is evident in the Mott insulator, since clearly $P_{\sigma,-\sigma}(\vec{x},\vec{x}) \to 0$ in the infinite-U limit.

[6] To be precise, performing carefully the maths and paying attention to the role of the chemical potential, an energy shift $-U/4$ is also found, with respect to the non-interacting limit.

To understand where the formalism hides these correlations, it is convenient to analyze the structure of the density correlation function, which on the lattice reads [92]:

$$P_{\sigma,\sigma'}(i,j) = \langle \hat{n}_\sigma(i)\hat{n}_{\sigma'}(j)\rangle = \langle c^\dagger_\sigma(i)c^\dagger_{\sigma'}(j)c_{\sigma'}(j)c_\sigma(i)\rangle. \tag{4.26}$$

As stated previously, such a function is related to the probability of finding an electron in i with spin σ, given the presence of an electron with spin σ' in j. To compute (4.26) one has to perform the quantum average of the four fermion operator $c^\dagger_\sigma(i)c^\dagger_{\sigma'}(j)c_{\sigma'}(j)c_\sigma(i)$, which alternatively means that one has to determine the two-particle Green's function of the system. This task is trivial in the case of a non interacting system, since one can factorize (4.26) into the Hartree and Fock contributions[7], or alternatively break the Green's function into the sum of the direct and the exchange contributions. In both cases what guarantees the correctness of the result is always the Wick theorem:

$$P^0_{\sigma,\sigma'}(i,j) = \langle c^\dagger_\sigma(i)c_\sigma(i)\rangle\langle c^\dagger_{\sigma'}(j)c_{\sigma'}(j)\rangle - \langle c^\dagger_\sigma(i)c_{\sigma'}(j)\rangle\langle c^\dagger_{\sigma'}(j)c_\sigma(i)\rangle. \tag{4.27}$$

The first term (Hartree) generates the ρ_0^2 in both (4.24) and (4.25), while the second gives the correction in (4.24).

Evidently, if the system is interacting, the situation becomes much more complicated, since not all the correlation, but only the exchange is contained within the Hartree-Fock terms. Typically a support function called the *pair correlation function* is defined as

$$g_{\sigma,\sigma'}(i,j) = \langle c^\dagger_\sigma(i)c^\dagger_{\sigma'}(j)c_{\sigma'}(j)c_\sigma(i)\rangle - \langle c^\dagger_\sigma(i)c_\sigma(i)\rangle\langle c^\dagger_{\sigma'}(j)c_{\sigma'}(j)\rangle. \tag{4.28}$$

The non-trivial part of the correlations should more properly be described by

$$g(i,j)_{\sigma,\sigma'} + \langle c^\dagger_\sigma(i)c_{\sigma'}(j)\rangle\langle c^\dagger_{\sigma'}(j)c_\sigma(i)\rangle, \tag{4.29}$$

which contains the pure many-body correlated effects. If such a function is zero or very small, compared to the Hartree-Fock components, then the system is weakly correlated. If instead this component dominates, the system is strongly correlated.

It is clear that the computation of this quantity is crucial in the analysis of the Hubbard model, since the term $c^\dagger_\uparrow(i)c^\dagger_\downarrow(i)c_\downarrow(i)c_\uparrow(i)$ is the interaction term and its value on the ground state determines the interaction contribution to the energies of the eigenstates. Unfortunately the computation of $P_{\sigma,\sigma'}(i,i)$ is a formidable problem, which becomes very difficult to tackle at high-U, where perturbative techniques typically break down. A technique that clearly cannot take into account the strong correlation between the electrons is mean-field analysis. In the light of the previous discussion this can be understood very well, in fact the study of the Hubbard Hamiltonian via a mean-field decoupling[8] assumes the approximation of the interaction term as:

$$\langle c^\dagger_\uparrow(i)c^\dagger_\downarrow(i)c_\downarrow(i)c_\uparrow(i)\rangle \approx \langle c^\dagger_\downarrow(i)c_\downarrow(i)\rangle\langle c^\dagger_\uparrow(i)c_\uparrow(i)\rangle - \langle c^\dagger_\downarrow(i)c_\uparrow(i)\rangle\langle c^\dagger_\uparrow(i)c_\downarrow(i)\rangle,$$

[7] Here the anomalous contribution of the Cooper pairing is neglected, because not relevant for the present discussion.

[8] An introduction to mean-field decoupling schemes can be found in any condensed matter basic textbook. However an effective scheme for its implementation can be found in the appendix B of paper C.

where the four mean-fields that appear on the r.h.s. must be determined self-consistently or imposed on the base of symmetry arguments (see for example appendix B of paper C). By construction this approximation of the interacting term misses the contribution of the many-body correlations. Therefore a mean-field description cannot capture the physics of a Strongly Correlated Electron System, like the Mott insulator, since it completely neglects the correlations that drive the physics. This is in complete contrast with the case, for example, of Slater antiferromagnetic insulators, where instead the mean-field decoupling perfectly describes the stabilization of the order that causes the insulating behavior. In paper B, thanks to the results of paper A, we challenge this paradigm, since we show that using appropriate non-linear canonical transformations it is possible to set up a mean-field analysis that includes part of the electronic correlations. In this way we are able to give a description of the Mott insulating phase, via a free fermion (mean-field) representation.

4.2.2 Metal-Insulator transition

Previously it has been shown that a system described by the Hubbard Hamiltonian (4.15) must turn from a metal to an insulator increasing the value of the coupling U, via an increasing localization of the electrons. How this process takes place is still subject of intense research. Evidently at some critical U_c (at $T = 0$) the energy of the ground state characterized by delocalized (weakly correlated) electrons and connected adiabatically to the non-interacting ground state, must become higher than the energy of a state with localized (strongly correlated) electrons that is instead adiabatically connected with the ground state of the $U \to +\infty$ limit. Whether or not the transition between these two states is discontinuous or continuous at zero or finite temperature, or whether or not this transition preserves its properties in different circumstances (lattices, dimensions, etc...) is still the subject of debate (see for example [92,102,108–116]).

Since the Mott-insulating state is characterized by the appearance of local moments, remnants of the localized electrons, it is clear that in principle the ground-state could be highly degenerate, like the atomic limit one. The degeneracy is given by the fact that every local electron has a twofold spin degeneracy, which is an unavoidable feature, unless the Mott state orders magnetically. Indeed in many theoretical works on the Hubbard model an antiferromagnetic dome often appears on top of the region where the metal-insulator transition appears [92, 117, 118]. However the fact that these localized electrons develop some spin order, is completely irrelevant from the point of view of the Mott physics. The possible ordering is due to the fact that the Néel Temperature, which rules the establishment of the antiferromagnetic spin order that we consider as example, is quite high, so as soon as the local moments emerge they also order; actually the same thing happens in the the Slater metallic state at low coupling U, where the electrons coherently stabilize an antiferromagnetic order. These two states are sometimes called correlated and uncorrelated antiferromagnets, more details can be found in Ref. [118, 119]. For the purpose of this discussion the properties of the antiferromagnetic phase are irrelevant, so it will always be assumed that such a mechanism is suppressed by some kind of frustration (for example induced by the lattice or by next-to-nearest neighbor hopping).

The study of the $d = \infty$ limit is very convenient, since using a Bethe lattice[9] the results obtained using Dynamical Mean-Field Theory (DMFT [102]) become exact, in a sense that will be clarified in the next paragraphs. Even if this system is clearly unphysical and the final picture can be completely different in real situations (see for example Ref. [116]), the DMFT study of the Hubbard model phase diagram is paradigmatic in the context of general Metal-Insulator transitions. In the light of the effectiveness of this method on the Bethe lattice, it is convenient to summarize its findings concerning the Metal-insulator transition, in order to identify the processes and the quantities important to the establishment of a Mott state. Many details can be found in the original papers [102, 110, 120], however I prefer the insight given in Ref. [121], where the DMFT solutions are treated as they really are: fix points of a self-consistent algorithm.

The DMFT algorithm permits the analysis a quantum interacting system, mapping it onto a quantum impurity problem interacting with a bath. The algorithm is self-consistent and is based on a cyclic update of the local impurity Green's function, via the continuous calculation of its self-energy $\Sigma(\omega)$. Comprehensive reviews of the method can be found in Refs. [102, 122]), so it is enough to just mention the main steps of the algorithm. The DMFT algorithm is the logical (but technically involved) extension of standard Weiss single site mean-field method: the basic idea is in fact the same, i.e. the conceptual separation of the system into a single site embedded into the rest of the system. In this way the original problem gets mapped into the problem of an impurity interacting with an external bath, where the properties of the bath must be determined on the basis of the impurity's properties, which in turn depend on the mean-fields that the bath itself generates. One therefore understands that the entire process must be based on a self-consistency procedure. The difference between the standard Weiss mean-fields and the DMFT ones is that the first are static, while the second are dynamic, i.e. they allow time modulation and therefore a non-trivial spectral structure. In DMFT the procedure that permits the separation of the problem into bath and impurity is called *cavity construction* and it is easily understood if one considers the path integral representation of the partition function of the system $\mathcal{Z}$ in the grand-canonical ensemble, as in Ref. [122]. The partition function depends upon the system's action S, which can be separated into three parts:

$$S = S_{local}(c_0^*, c_0) + \Delta S(c_0^*, c_0, c_i^*, c_i) + S_{lattice}(c_i^*, c_i), \tag{4.30}$$

where S_{local} is the part of the action describing a single local site $i = 0$, $S_{lattice}$ describes the rest of the lattice with $i \neq 0$, and ΔS describes the hopping of the electrons from $i = 0$ to the rest of the lattice and vice-versa. In practice, ΔS determines the interaction between the local site and the rest of the system. Of course the c_j^*, c_j symbols represent the Grassmann variables, since the use of the action S assumes the path-integral representation. From this point the algorithm evolves in a very straightforward way: the degrees of freedom c_i^*, c_i are integrated out, so that computing the average of $\exp\{\Delta S(c_0^*, c_0, c_i^*, c_i)\}$ one generates an effective action that is only a function of c_0^*, c_0 and that therefore can be seen as the action of the bath on the local site $i = 0$. Predictably, the

[9] The term Bethe lattice in this thesis refers to the Bethe graph with infinite coordination number [11].

problem is the averaging of $\exp\{\Delta S(c_0^*, c_0, c_i^*, c_i)\}$, so it is in this passage that many approximations are hidden. Indeed it can be proved that in the $d \to \infty$ limit, only contributions to $\langle \exp\{\Delta S(c_0^*, c_0, c_i^*, c_i)\}\rangle$ that depend upon the single particle lattice Green's function are not suppressed by the high dimensionality of the system. This is due to the fact that, to be meaningful, the infinite limit must be performed with a simultaneous rescaling of the hopping term $t \to t^*/\sqrt{d}$. So in the high dimensional limit it becomes possible to have an (exact) closed expression for the effective action generated by the term $\langle \exp\{\Delta S(c_0^*, c_0, c_i^*, c_i)\}\rangle$, which depends only on the values of the hopping parameters between the local site $i = 0$ and the bath, and on the Green's function of the lattice itself. In practice this means that

$$S \to S_{local}(c_0^*, c_0) + \mathcal{W}(c_0^*, c_0), \tag{4.31}$$

where $\mathcal{W}(c_0^*, c_0)$ are the mean-fields (typically called hybridization functions) generated by $\langle \exp\{\Delta S(c_0^*, c_0, c_i^*, c_i)\}\rangle$ and they are quadratic in c_0^* and c_0. These fields may be thought of as generated by virtual excursions of the impurity electrons into the bath, so it is not surprising that dynamical effects appear. In conclusion, one can map the original action into an effective quantum impurity model, that can now be solved with some numerical technique (NRG, DMRG, QMC, etc...). For sake of clarity, the action of the impurity model (in imaginary time) is given by:

$$S_{IMP} = -\int\int_0^\beta d\tau_1 d\tau_2 \sum_\sigma c_\sigma^*(\tau_1)\left[\left(\frac{\partial}{\partial\tau_1} - \mu\right)\delta_{\tau_1\tau_2} + \mathcal{W}_\sigma(\tau_1 - \tau_2)\right] c_\sigma(\tau_2) + \\ + U\int_0^\beta d\tau c_\uparrow^*(\tau)c_\uparrow(\tau)c_\downarrow^*(\tau)c_\downarrow(\tau) \tag{4.32}$$

It is important to stress that the previous equation is exact only in infinite dimensions, since only in this limit the mean-fields appear so neatly in the action. Assuming that one can compute the interacting Green's function $\mathcal{G}_\sigma(\omega)$ of this impurity model (here the computational difficulties of DMFT are hidden), it is possible to set up a self-consistent procedure. In fact, the other non-trivial passage of the algorithm, i.e. the determination of the mean-fields $\mathcal{W}(c_0^*, c_0)$, is indeed not necessary to the development of the algorithm, since their knowledge can be inferred implicitly. In (4.32) one understand that defining the propagator in the case $U = 0$ (bath Green's function) as

$$\mathcal{G}_\sigma^{-1}(z) = z + \mu - \mathcal{W}_\sigma(z), \tag{4.33}$$

then the full local propagator of (4.32) is:

$$G_\sigma^{-1}(z) = z + \mu - \mathcal{W}_\sigma(z) - \Sigma_\sigma(z), \tag{4.34}$$
$$= \mathcal{G}_\sigma^{-1}(z) - \Sigma_\sigma(z), \tag{4.35}$$

where the algebra is typically carried out in Fourier transformed imaginary time, so the functions can be evaluated on the Matsubara frequencies $z = i\omega_n$. Therefore, setting up the self-consistency procedure in a convenient way, the computation of the dynamical mean-fields can be avoided:[10]

[10]The trivial spin index has been dropped in the following

i. define the local Green's function $G_0(z)$ (where 0 is the iteration number), i.e. define a starting guess for the lattice self-energy $\Sigma_0(z)$ and average the lattice Green's function over the momentum space $\vec{k}$:

$$\begin{aligned} G_0(z) &= \int \frac{d\vec{k}}{(2\pi)^d} \frac{1}{z - \epsilon(\vec{k}) + \mu - \Sigma_0(z)} \\ &= \int_{-\infty}^{+\infty} d\epsilon \frac{\rho(\epsilon)}{z - \epsilon + \mu - \Sigma_0(z)}, \end{aligned} \tag{4.36}$$

where $\epsilon(\vec{k})$ and $\rho(\epsilon)$ are the free dispersion and density of states respectively;

ii. use $G_0(\omega)$ and $\Sigma_0(\omega)$ to compute the Green's function $\mathcal{G}_0(\omega)$ that takes into account the effect of the bath, using the relation (4.34);

iii. use $\mathcal{G}_0(\omega)$ to find the new local Green's function $G_1(\omega)$, by solving (numerically) the interacting quantum impurity problem defined by the action (4.32);

iv. extract the new self-energy $\Sigma_1(\omega) = {G_0}^{-1}(\omega) - {G_1}^{-1}(\omega)$;

v. put $G_0(\omega) = G_1(\omega)$, $\Sigma_0(\omega) = \Sigma_1(\omega)$ and repeat from point (ii), until convergence of the self-energy.

The reader has probably noticed that the entire procedure uses only local propagators, which therefore are independent of $\vec{k}$. Since the method is based on a mapping between the original problem and a quantum impurity problem, this is not surprising. This $\vec{k}$ independence is actually the greatest liability in the DMFT, which by construction is not able to capture (non-trivial) non-local correlations. However, in the limit $d \to \infty$ this is not a problem at all, since it has been proved that the self-energy is independent of $\vec{k}$ in that limit [123]. Because of this independence, and because of the fact that the dynamical mean-fields appear only quadratically in the effective action for the impurity (4.32), the DMFT solutions are exact in the $d \to \infty$ limit.

So the DMFT (exactly as for normal mean-field theory) is a self-consistent procedure, and to solve the DMFT equations simply means to find a fix point for the DMFT algorithm. The fixed points can be found changing the starting point, i.e. changing the form of the local Green's function of point (i) above. If just one of them exists then the algorithm will converge to the fix point independently upon the initial choice of $G_0(\omega)$, or it will not converge at all. If n fix points exist for the same value of parameters, then the algorithm will approach one of the n fix points depending upon the initial condition (or again it may not converge, depending upon the situation). These considerations automatically determine the kind of processes that can be identified in the analysis of the phase diagram of a model Hamiltonian. Indeed everything depends upon the evolution of the fix points as function of some physical parameter, e.g. the strength of the many-body interaction. This evolution cannot be arbitrarily wild, since the fix points follow always a very simple rule: they either evolve adiabatically or appear and disappear via bifurcation processes.[11] Clearly with self-consistent

[11] The term bifurcation should be considered in its wider meaning, so indicating the separation of one fix point (or more) into two or more fix points.

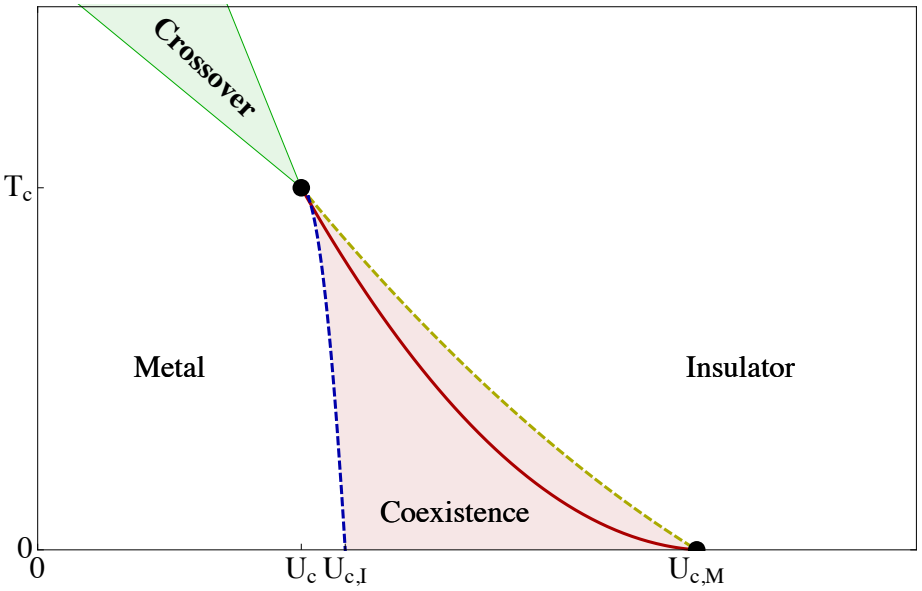


Figure 4.1: *Sketch of the infinite dimensional Hubbard model phase diagram, qualitatively similar to the one obtained by DMFT [102, 122]. The blue and yellow dashed lines represent the critical curves $U_{c,I}(T)$ and $U_{c,M}(T)$ respectively, and they form the boundaries of the coexistence region. This region disappears above T_c, where instead a crossover region appears and where the distinction between metal and insulator is not defined anymore. The two black dots indicate the two second order critical points [102].*

algorithms it is possible to find first and second (or higher) order transitions, and also crossovers. In the first case one should expect the coexistence of two solutions for a range of parameters around some critical value of the interaction at which the two solutions exchange their status of ground-state; clearly in this circumstance one has an abrupt change in the value of the order parameters (in the physical quantities) used to distinguish the two states. In the second circumstance instead, one must expect that a bifurcation of a the ground-state fixed point takes place at a specific critical interaction value; in such a situation one must expect a discontinuity of the derivative of the order parameters with respect to the parameters that are driving the transition. In the third case instead one expects no critical evolution of the fix point, which simply connects adiabatically the non-interacting solution with the infinite interacting one.

The DMFT phase diagram of the Hubbard model, in the case of the infinite dimensional Bethe lattice, is sketched in Fig. 4.1. The solution clearly shows a first order phase transition at $0 < T < T_c$, characterized by a hysteresis region between the interaction values $U_{c,I}(T)$ and $U_{c,M}(T)$, which represent the minimum and maxim interaction values for the existence of the Mott-insulating and the metallic solutions respectively. At $T = T_c$, $U_{c,I} = U_{c,M}$ and above this (second-order critical) point the phase transition turns into a smooth crossover.[12]

[12]The features of this transition are not at all unintresting and its understanding may hide the explanation to the non-trival physics of the psudogap in high Temperature superconductors. In particular the Widom line above T_c has been studied recently by many authors [124–126].

Inside the hysteresis region three DMFT solutions can be found [121]: two stable ones (Mott-insulating and metallic) and an "unstable" one.[13] The characterization of the full phase-diagram shows that the DMFT solutions form a continuous surface in the order parameter space T, U, D (where D is the double occupancy density), allowing therefore for the determination of a transition curve $U_c(T)$ via a Maxwell construction. In this picture the origin of the different critical curves and points becomes straightforward: the $U_{c,M}(T)$ curve is given by the merging (and mutual annihilation) of the stable metallic and unstable fix-points; the $U_{c,I}(T)$ is instead given by the merging of the insulating and unstable fix-points; the critical point U_c, T_c must evidently be of the second order, since decreasing the temperature from $T > T_c$ to $T < T_c$ the three fix-points appear as a pitchfork bifurcation of the only fix point that exists at $T > T_c$. At $T = 0$ one must necessarily have that $U_c(T) \to U_{c,M}(T)$, since the contribution of the (high) entropy of the Mott-insulating state to the free energy becomes less and less relevant for $T \to 0$ and eventually vanishes at $T = 0$, turning the transition into a second order one. This feature is anyway a characteristic of the $d = \infty$ Bethe lattice, since on different lattices and dimensions [128] the inclusion of space fluctuations of the self-energy [129,130] and the consequent establishment of correlations of the local spins keep $U_c(T)$ well separated from $U_{c,M}(T)$, for any $T < T_c$.

Beside the structure of the phase diagram, the DMFT solutions allow us to understand the role of two important quantities: the double occupancy density D and the quasi-particle weight Z. One could argue that the double occupancy parameter D is the most logical choice for the characterization of the Mott-insulating state [110,120,121], since has to expect a huge difference between its value in the metallic region (close to 1/4) and in the insulating region (close to zero). In the light of the particle-hole symmetry that exists at half-filling, the band parity parameter $P = -(2n_\uparrow - 1)(2n_\downarrow - 1)$ seems an even better indicator of the Mott-insulating feature of the quantum state. Indeed it is trivial to understand that in the non-interacting limit $\langle P \rangle = 0$, since the state must contain the same contribution from states with $\langle P \rangle = 1$ (single occupied) and states with $\langle P \rangle = -1$ (doubly occupied and unoccupied); accordingly in the atomic limit $\langle P \rangle = 1$. Clearly one expects these two values will only be slightly modified close to the corresponding limits, so a value of $\langle P \rangle$ very different from zero should be the signature of the predominance of the contribution of the singly occupied states contribution to the wave-function, i.e. the signature of Mott-insulating behavior. Therefore at the transition it is necessary to have a jump in the average value of P (and equivalently in D, as well proved by DMFT [102, 110, 121]). Although the previous considerations are correct, the value of D or P cannot be used rigidly as an order parameter, since their value at the transition (in the insulating side) is not exactly zero [102]; this is expected since the Mott-insulator at finite t must be characterized by virtual hopping processes. Therefore one can use D as an indication of the characteristics of the ground-state, but then the results must be interpreted carefully, since given the value of D or P of a solution one cannot say to which phase that solution belongs; in other words, one cannot understand if the solution considered is connected adiabatically to the non-interacting solution. This information is

[13] In this context unstable means that the energy of this solution is always higher than the other two, so this state is never an acceptable trial ground-state of the system. For details see Ref. [121, 127].

instead contained within the quasi-particle weight Z.

The parameter Z appears naturally in the Green's function of an interacting system [28, 93]. Remembering that the Green's function of an electron system is

$$G_{\sigma,\sigma'}(t,i;t',j) = -i\langle \mathrm{T} c_{\sigma'}(j,t') c^{\dagger}_{\sigma}(i,t)\rangle, \tag{4.37}$$

and assuming time and space translational invariance indicating $\tau = t - t'$, $\vec{x} = i - j$, one can perform a Fourier transform. Hence the Green's functions can be written using the Källen-Lehmann spectral representation [11, 28]:

$$G(\vec{k},\omega) = \int_{-\infty}^{+\infty} d\tau d\vec{x}\, G(\tau,\vec{x}) e^{-i\omega t} e^{-i\vec{k}\cdot\vec{x}} = \sum_{\lambda} \frac{\left|M(\lambda,\vec{k})\right|^2}{\omega - (\epsilon_\lambda - i\delta_\epsilon)} \tag{4.38}$$

where the trivial spin indices have been omitted for sake of notation, as usual $\delta_\epsilon = \delta \mathrm{sgn}\epsilon$ and $\delta \to 0^+$, and λ labels all the eigenstates of the (interacting) system, so that

$$\begin{aligned} \left|M(\lambda,\vec{k})\right|^2 &= \langle 0|c_k|\lambda\rangle\langle\lambda|c^{\dagger}_k|0\rangle \quad \text{for} \quad \epsilon_\lambda > 0, \\ \left|M(\lambda,\vec{k})\right|^2 &= \langle 0|c^{\dagger}_k|\lambda\rangle\langle\lambda|c_k|0\rangle \quad \text{for} \quad \epsilon_\lambda < 0, \end{aligned}$$

where $|0\rangle$ is the ground state of the interacting system. A derivation and a complete discussion of the spectral representation can be found elsewhere [28, 93]. The only point that is important here to make is that $M(\lambda,\vec{k})$ depends upon $\langle\lambda|c^{\dagger}_k|0\rangle$ (and similarly $\langle\lambda|c_k|0\rangle$), which is the matrix element of the electron (hole) creation operator $c^{\dagger}_k$ between the exact ground state of the system and another exact eigenstate. So, in the case of a free system, $M(\lambda,\vec{k})$ must be zero unless $|\lambda\rangle = c^{\dagger}_k|0_{\mathrm{free}}\rangle$ (and similar for the holes); instead in the case of an interacting system the latter relation clearly does not have to be true. Of course the total particle weight is unchanged by the interaction, and in fact it can be proved that

$$\sum_{\lambda} \left|M(\lambda,\vec{k})\right|^2 = 1, \quad \forall\vec{k}, \tag{4.39}$$

as a direct consequence of the fermion anticommutation relations of creation and annihilation operators [11]. Only in the limit of a free system one has that $\left|M(\epsilon,\vec{k})\right|^2 \to \delta(\epsilon - \epsilon_k)$, so that (4.38) is easily rewritten in the standard representation as

$$G(\vec{k},\omega) \to \frac{1}{\omega - (\epsilon_k - i\delta_{\epsilon_k})}, \quad \forall k, \tag{4.40}$$

where $\epsilon_k = 0$ on the Fermi surface. The interactions blur the spectral function, spreading $\left|M(\epsilon,\vec{k})\right|^2$ on many eigenstates lambda at different energies, which means that the Green's function has a non-zero residue (cut-density) not only at the original free particle pole position $\omega = \epsilon_k$, but also at other values of ω. This means that the propagation of the electrons inside the many-body system

happens not only via the coherent propagation of a single particle, but also via incoherent many-particle processes. The quasi-particle weight Z_k quantifies how much (which portion) of the transport process still happens coherently, due to the single particle component.

Another way to understand this quantity is to consider the effect of the interactions on the creation/annihilation operators. Using the familiar concept of adiabatic evolution, assuming that the interaction in the Hamiltonian is slowly switched-on starting from $t \to -\infty$, it is possible to obtain new "dressed" creation/annihilation operators $a_k^\dagger, a_k$ from the original operators $c_k^\dagger, c_k$ [93], using the unitary transformation generated by the time ordered interaction operator. Reversing the relation one can in principle write:

$$c_k^\dagger = \sqrt{Z_k} a_k^\dagger + \sum_{k_1+k_3=k_2+k} A(k_1, k_2; k_3, k) a_{k_4}^\dagger a_{k_3}^\dagger a_{k_2} + ...$$

Therefore it is possible to conclude that the Green's function $G(\vec{k}, \omega)$ is indeed built up by the superposition of many quantum processes that fully specify the possible evolution of the excitation created in a given point at a given time. These processes include the coherent propagation of a single mode, its partial propagation followed by a decay, the propagation of incoherent many-particle modes, etc... Of course this propagation can happen only along the "resonating channels" of the system, i.e. via the eigenstates of the system. Therefore the Green's function of the system contains the full information about its eigenstates. In particular the spectral function at a given value of $\vec{k}$ and ω can be computed by

$$A(\vec{k}, \omega) = -\frac{1}{\pi} \mathrm{Im} G^{\mathrm{ret}}(\vec{k}, \omega) = \sum_\lambda \left| M(\epsilon, \vec{k}) \right|^2 \delta(\omega - \epsilon_\lambda), \tag{4.41}$$

which also means

$$A(\vec{k}, \omega) = Z_{\vec{k}}\, \delta(\omega - \tilde{\epsilon}_{\vec{k}}) + \sum_{\lambda \neq \vec{k}} \left| M(\epsilon, \vec{k}) \right|^2 \delta(\omega - \epsilon_\lambda). \tag{4.42}$$

The function $\tilde{\epsilon}_k$ can be different from the original ϵ_k, since the center of the quasiparticle peak can be shifted by the interactions (see footnote on the next page). The density of states $\rho(\omega)$ is trivially obtained making the integral $\int d\vec{k}\, \delta(\omega - \epsilon_k)$ over the Brillouin zone. The latter form of the spectral function exploits very efficiently the separation between the contribution of the coherent single particle state and the incoherent ones. However this distinction should be further refined, since the incoherent part contains both the contribution due to the propagation of highly incoherent multi-particle states, and the one that comes from the decay of the coherent single particle excitation into the particle hole continuum. The two parts have very different behaviors, since the former implies the development of a broad $A(\vec{k}, \omega)$ spread over the entire bandwidth, while the latter is responsible for a broadening of the peak around $\vec{k}, \tilde{\epsilon}_k$.

From the previous considerations one can conclude that Z_k gives the overlap between the original non-interacting fermionic states and the interacting ones. Therefore it is immediately clear that in a Landau-Fermi liquid one must have $Z_k \neq 0$ for each $|k|$ close (equal) to $|k_F|$, otherwise clearly the one-to-one

correspondence between the interacting and the non-interacting system breaks down [9,10,93,104], since a vanishing Z_k means that the exact interacting states are orthogonal to the original ones and therefore not adiabatically connected with them. The existence of a non-vanishing quasiparticle-weight at the Fermi surface is however not the only feature characterizing the Fermi liquid. In fact, beside the one-to-one correspondence between the quasi-particle states close to the Fermi surface and the free states, it must also happen that the quasi-particle states are "long-lived", i.e. characterized by an extremely small (vanishing) scattering time. The quasi-particles must be able to travel for a long time before being damped by (decay into) the electron-hole continuum around the Fermi surface. This, as mentioned, must correspond to the existence of a very narrow peak $A(\vec{k},\omega)$ for $|\vec{k}| = k_F$, around $\omega = \epsilon_F$, since a broadened peak should imply the overlap of the coherent electron state with scattering state very close in energy and therefore extremely efficient in the damping of the quasiparticle. To understand this point it is convenient to change the representation of the Green's function, passing from the spectral to the self-energy one [11]. In such a representation one has the advantage to be able to always think of (unstable) particles propagating in the system, rather than as a simultaneous superposition of coherent and incoherent contributions:

$$G(\vec{k},\omega) = \frac{1}{\omega - (\epsilon_k + \Sigma(\omega,\vec{k}) + i\delta_{\epsilon_k})}, \tag{4.43}$$

where we wrote down the formula for the standard Green's function, but equivalently one could write down all the other possible Green's functions (such as the retarded, etc...). This representation (given an appropriate self-energy Σ) produces the same results of spectral one. In particular, if one separates the real and imaginary part of the (retarded) self-energy: $\Sigma(\omega,\vec{k}) = \Sigma_R(\omega,\vec{k}) + i\Sigma_I(\omega,\vec{k})$, one can see that

$$A(\vec{k},\omega) = \frac{-\Sigma_I(\omega,\vec{k})}{\left[\omega - \epsilon_k + \Sigma_R(\omega,\vec{k})\right]^2 + {\Sigma_I}^2(\omega,\vec{k})}. \tag{4.44}$$

The imaginary part of the self-energy is inversely proportional to the typical time needed for the coherent electron to decay on the many particle continuum. If the dependence of $\Sigma(\omega,\vec{k})$ on ω is not too pronounced, then $A(\vec{k},\omega)$ looks like a Lorentzian centered[14] at $\tilde{\epsilon}_k = \epsilon_k - \Sigma_R(\tilde{\epsilon}_k,\vec{k})$ [10,11]. Clearly the smaller $\Sigma_I(\omega,\vec{k})$, the sharper the Lorentzian and therefore the more stable the particles have to be. Thinking in these terms, it becomes possible [93] to approximately

[14] As visible the equation for $\tilde{\epsilon}_k$ is a self-consistent one. The meaning of this relation and the role of the real part of the self-energy can be understood considering the spectral function at the Fermi surface: the (hyper-)surface in k-space (k_F) where the imaginary part of the self-energy is zero and that is put in correspondence to $\omega = 0$. This means that at $\omega = \tilde{\epsilon}_{k_F} = 0$ we expect to find the simple poles of the quasiparticles that live on the Fermi surface. The self-consistent relation becomes $0 = \epsilon_{k_F} - \Sigma_R(0,k_F)$. Remembering that ϵ_k is given by the free dispersion ξ_k as $\epsilon_k = \xi_k - \mu$, then $\Sigma_R(0,k_F) = \xi_{k_F} - \mu$. So the real part of the self-energy can be regarded as a correction to the chemical potential. Such a correction is necessary to fit the correct number of particles (states) inside the Fermi surface, fulfilling in this way the Luttinger theorem. In some cases it is easy to know what this correction to the chemical potential must be. For example in the Hubbard model at half filling $\mu = U/2$, if the model is written as in (4.15), which can be taken into account immediately writing the interaction term as $(c^\dagger_\uparrow c_\uparrow - 1/2)(c^\dagger_\downarrow c_\downarrow - 1/2)$.

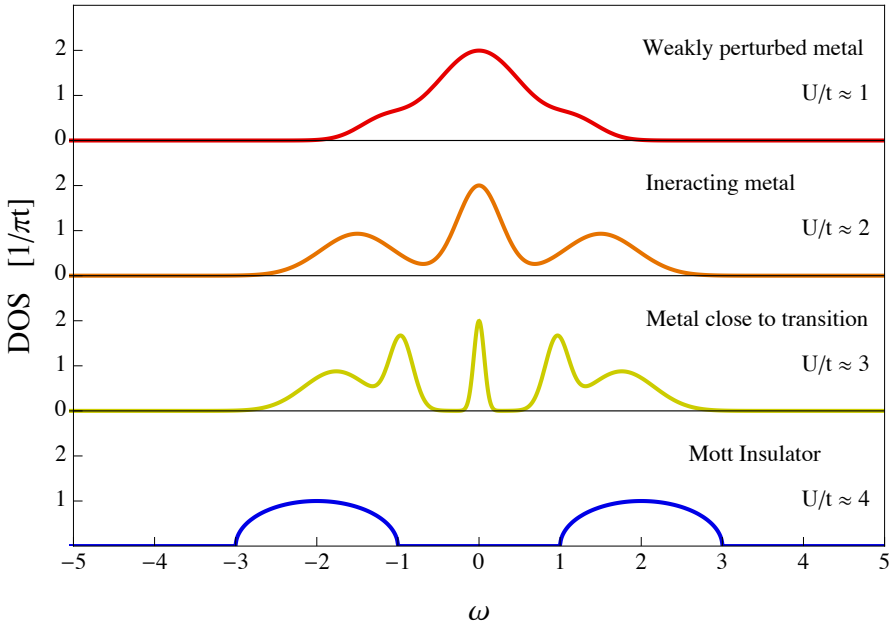


Figure 4.2: *Cartoon of the evolution of the DOS, as computed by DMFT on the Bethe lattice at $T = 0$. A figure with the exact DMFT result can be found in [102]. The main features that characterize the appearance of the Mott-Insulator are qualitatively reproduced. In particular the appearance of the peak in the middle of the preformed quasiparticle gap. This peak disappears at the Metal-Insulator transition, which happens slightly above $U_c(T = 0)/t \approx 3$. The development of the central peak is accompanied by the establishment of the two upper and lower Hubbard bands, which have a quite rich structure below $U_c(T = 0)$. In the figure such a structure is only sketched, marking the appearance of two neat lumps near the edges of the preformed-gap. Above U_c the Hubbard bands become more and more symmetric increasing U, approaching two semicircular DOS.*

separate the Green's function into the quasi-particle peak at energy $\tilde{\epsilon}_k$ and incoherent parts, in the spirit of (4.42):

$$G(\vec{k},\omega) = \frac{Z_k}{\omega - \tilde{\epsilon}_k - i\delta_{\tilde{\epsilon}} - iZ_k\Sigma_I(\vec{k},\tilde{\epsilon}_k)} + G_{inc}(\vec{k},\omega), \tag{4.45}$$

where, with respect to the approach that led to (4.42), one has

$$Z_k^{-1} = 1 - \partial_\omega \Sigma_R(\vec{k},\omega)\Big|_{\omega=\tilde{\epsilon}_k}, \tag{4.46}$$

moreover the life-time of the quasiparticles can be expressed as:

$$\tau^{-1} = -Z_k\Sigma_I(\vec{k},\tilde{\epsilon}_k). \tag{4.47}$$

As mentioned previously the parameter Z_k is important in the establishment of the Fermi-liquid properties of a system. Typically, in systems where the direction of the momentum is irrelevant as in the infinite dimensional Bethe lattice, it is convenient to integrate any formula with respect to $\vec{k}$, since any physical quantity can depend only upon ω. So one usually considers

$$Z = [1 - \partial_\omega \Sigma_R(\omega)]^{-1}\Big|_{\omega=\tilde{\epsilon}_k}. \tag{4.48}$$

The understanding of the role played by Z is crucial in the interpretation of the phase diagram of the Hubbard model. Indeed the DMFT solution, as well as the Gutzwiller one [101], demonstrate that in the infinite dimensional Bethe lattice the disappearance of the metallic solution takes place via a Gutzwiller-Brinkmann-Rice transition, i.e. via a reduction of Z that eventually becomes zero *on the Fermi surface* at a critical value of the coupling. This explains very well the evolution of the density of states $\rho(\omega)$ with U, sketched in Fig. 4.2. At small U the density of states is very close to the free one, which is determined only by the geometric factor related to ϵ_k. Increasing U the states at extremes of the band become less and less close to the original electronic states and the incoherent part builds up the precursors of the upper and lower Hubbard bands. At some point a peak becomes visible at the middle of a pre-formed gap (that is not as clean as for $T < T_c$), between the two Hubbard bands. This peak represents the only Fermi-Liquid-like part of the system, responsible for the conduction properties of the systems.[15] Increasing U the imaginary part of the self-energy increases (with the exception of $\Sigma_I(0)$, which keeps its zero value, as is normal in a Fermi liquid), but the quasi-particle weight Z decreases, making the peak sharper and sharper, although its height at $\omega = 0$ keeps constant at $\rho_0(0)$. At a critical value $U_{c,M}(T = 0) \approx 3\rho_0(0)$, the parameter Z goes to zero and therefore the entire construction (the Fermi liquid picture) breaks down, making the peak and the Fermi liquid disappear.

This is therefore the nature of the Metal-insulator transition in the infinite dimensional Bethe lattice. The transition happens via the destruction of the Fermi liquid, that survives into a (Kondo) peak in the middle of the insulating Mott gap, until the interaction becomes too strong. The spectral weight is pushed away from the Fermi surface by the interaction, and is accumulated at typical energy scales of order U. The eigenstates at these energies do not resemble free electrons and cannot be described as such. It is important to keep these concepts in mind, reading the introduction to paper B.

[15] Indeed inside the pre-formed gap at two energies $\pm\omega^*$, symmetrically placed around the peak, a change in the slope of $\Sigma(\omega)$ can be found [122], which means that a Fermi-Liquid description is valid only for $|\omega| < |\omega^*|$ [131].

Chapter 5

Introduction to Paper B

5.1 Enlarged Mean-Field Scheme

In paper B we focused our attention on the mean-field description of the Mott-Insulting phase, trying to understand if via the use of canonical non-linear transformations it is possible to take into account the correlations that cause the localization of the electrons and therefore the development of the Mott insulating phase. This idea can be traced back to the considerations written in paper A and Chapter 3, where we pointed out that with an appropriate transformation a multifermionic term can be (typically only partially) turned into a quadratic one. In order to do this for the case of the Hubbard model, one has to act smartly, since it is clear that the only local non-linear transformation that exists in the Hilbert space of the Hubbard model commutes with the interaction term. To tackle this problem, we considered a second auxiliary lattice site beside each physical site. On this extra site is a spin-full fermion, so every local auxiliary Hilbert space contains 4 states in total. These second sites are *not coupled* with the original ones, so the auxiliary fermions *cannot* jump from the auxiliary chain to the physical one; moreover we also assumed (for sake of convenience) that no hopping between different auxiliary sites occurs. Evidently this operation did not modify the quantum problem, in the sense that *any physical quantity* of the original fermions does not get modified by the addition of the auxiliary fermions. However the dimension of the local Hilbert space and therefore the *number of available non-linear transformations changes tremendously.*

Indicating with γ_1, γ_2, γ_3, γ_4 the Majorana fermions that correspond to the physical fermions c_σ, while using μ_1, μ_2, μ_3, μ_4 for the auxiliary Majorana fermions, the half-filled Hubbard model Hamiltonian can be represented as:[1]

$$H = \frac{it}{4} \sum_{\substack{a=1..4 \\ \langle i,j \rangle}} \gamma_a(i)\gamma_a(j) - \frac{U}{4} \sum_i \gamma_1(i)\gamma_2(i)\gamma_3(i)\gamma_4(i), \tag{5.1}$$

where the sum over nearest neighbors $\langle i, j \rangle$ is meant to count every combination once and not twice (so if $\gamma(x_n)\gamma(x_{n+1})$ is in the sum, then the term $\gamma(x_{n+1})\gamma(x_n)$

[1] We also used a convenient gauge choice for the fermionic operators. For details see paper B.

is absent). Evidently the μ_i do not appear, since we assumed no dynamics for them. In this eight-Majorana local system there is a huge number of non-linear transformations, since the canonical group is $SU(4) \otimes SU(4) \otimes U(1) \otimes \mathbb{Z}_2$ and it is therefore necessary to understand which transformations are more promising, from an operative point of view. Since our aim is to apply a mean-field decomposition scheme on the non-linearly transformed Hamiltonian, it seems a good idea to use only transformations that leave the symmetries manifest. At half-filling the Hubbard model is characterized by $SO(4)$ and time-reversal symmetry, so one has to look for generators of non-linear transformations that preserve these symmetries. To obtain only the transformations that preserve $SO(4)$ one has to impose the commutation of the generator of the transformation with the generators of $SO(4)$, which in our case are:

$$Q_{ab} = i\gamma_a\gamma_b + i\mu_a\mu_b \quad a > b,$$

where the local site index has been dropped. This task is conveniently performed using a computer and special packages able to deal with Clifford algebras [132], so that the computer can determine the appropriate combination of non-linear generators. The resulting operators S_α must then be processed to check which ones preserve the time-reversal invariance Θ, i.e.

$$\Theta S_\alpha \Theta^{-1} = -S_\alpha, \tag{5.2}$$

with Θ that acts as explained in equation (4) of paper B.

This procedure shows that there are only two available non-linear transformations:

$$S_1 = -\left(\sum_{a=1..4} \gamma_a\mu_a\right)\gamma_1\gamma_2\gamma_3\gamma_4, \quad S_2 = -\left(\sum_{a=1..4} \gamma_a\mu_a\right)\mu_1\mu_2\mu_3\mu_4. \tag{5.3}$$

Consequently, the canonical transformations that we can consider are parametrized by two angles θ_1, θ_2:

$$V = \exp\left(i\frac{\theta_1}{2}S_1 + i\frac{\theta_2}{2}S_2\right); \tag{5.4}$$

the reader can check that $[S_1, S_2] = 0$ and that all the four terms that form S_1 (S_2) commute with each other. This *enormously simplifies* the calculation, allowing one to rewrite the transformation V as the multiplication of eight combinations of sines, cosines and non-linear generators:

$$V = \prod_{j=1..4}\left(\cos\frac{\theta_1}{2} + iS_{1,j}\sin\frac{\theta_1}{2}\right)\prod_{j=1..4}\left(\cos\frac{\theta_2}{2} + iS_{2,j}\sin\frac{\theta_2}{2}\right), \tag{5.5}$$

with $S_{1,j}$ ($S_{2,j}$) the *j-th* of the four components of S_1 (S_2), introduced in (5.3). The transformation (5.5) can be used on the Majoranas (and in general on any operator) that appear in (5.1).

The complete formulas for the transformed Majoranas and the transformed interaction term can be found in the paper. However it is appropriate to point out that using the transformation V one can partially diagonalize the interaction term, since:

$$V\gamma_1\gamma_2\gamma_3\gamma_4V^\dagger = -\frac{\sin(4\theta_1 + 4\theta_2) + 2\sin(2\theta_1 - 2\theta_2)}{8}\left(\sum_{a=1..4} i\gamma_a\mu_a\right) + \ldots \tag{5.6}$$

which is exactly the kind of result that one expects from a non-linear transformation. One can use this fact, setting up a mean-field theory for the approximation of the transformed Hamiltonian. Rewriting it in terms of two spinful fermions $a_{i,\sigma}$, built using the γ-s and the μ-s exactly as the original ones,[2] this new form of the Hamiltonian can be studied with a mean-field approximation. Of course such a Hamiltonian must contain a hybridization between the two fermion species a_1 and a_2, since it appears explicitly in (5.6). The mean-field Hamiltonian, with the same symmetries of the original one, looks like:

$$H_{MF} = -\sum_{\langle i,j\rangle,\sigma}\left\{t_1 a^\dagger_{1,\sigma}(i)a_{1,\sigma}(j) + t_2 a^\dagger_{2,\sigma}(i)a_{2,\sigma}(j)\right\} + \lambda\sum_{i,\sigma}\left(a^\dagger_{1,\sigma}a_{2,\sigma}\right) + h.c., \quad (5.7)$$

where the real variational parameters t_1, t_2, λ have to be determined selfconsistently.[3]

In contrast to a study performed directly on the original Hubbard Hamiltonian this mean-field analysis is not doomed to fail in the high-U limit, since the partial diagonalization of the interaction grants a (partially) exact treatment of the correlations (4.29), which forces $\lambda \neq 0$ in the mean-field Hamiltonian (5.7). Considering that the inclusion of these effects depends upon the transformation V, one expects that optimizing the angles θ_1 and θ_2 it is possible to find a good mean-field candidate ground-state for the Mott phase. In this sense the transformation allows the enlargement of the variational mean-field space, considering more involved trial states. In this respect it is important to stress that the two angles *are not* mean-field parameters, but variational ones. To find the best free-particle candidate ground-state one should therefore look in the variational θ_1, θ_2 space for the best mean-field ground-state. This task is conveniently undertaken by looking for the best local minima of the mean-field energy functional in the space $t_1, t_2, \lambda, \theta_1, \theta_2$: indeed since any mean-field state is a stationary point of the energy functional with respect to t_1, t_2, λ, and since the θ_1, θ_2 space is compact[4] (the energy functional is periodic in both the angles), and moreover it shows no singularities, this procedure is fully justified. The solution identified by this variational procedure retains all the pros of a traditional variational solution and in particular its energy is a variational upper bound to the ground state energy.

The mean-field procedure guarantees that the ground state can be written down in terms of free particles, i.e. it is expressible as a Slater determinant. Such a Slater determinant however is completely different from the ones that can be obtained in the traditional way (otherwise it would be impossible to go beyond the known results). This can be understood looking at the local Green's function of the original electrons G_{11}, written in terms of the a_i Green's functions $\tilde{G}_{11}$, in formula (10) of paper B:

$$\begin{aligned} G_{11} = Z\tilde{G}_{11} + 12B_3B_4\tilde{G}_{22}(\tilde{G}^2_{21} + \tilde{G}^2_{12}) + 12B_4^2\tilde{G}_{11}(\tilde{G}_{11}\tilde{G}_{22} + \tilde{G}_{12}\tilde{G}_{21}) + \quad (5.8) \\ +48B_2^2\bar{h}^2\tilde{G}_{11}(\tilde{G}_{11}\tilde{G}_{22} - \tilde{G}_{12}\tilde{G}_{21}) + 48B_2^2\tilde{G}_{11}(\tilde{G}_{11}\tilde{G}_{22} - \tilde{G}_{12}\tilde{G}_{21})^2, \end{aligned}$$

[2] In the way we wrote the transformation there is actually no formal difference between the physical fermions and the $a_{1,\sigma}$ ones, and the auxiliary fermion and the $a_{2,\sigma}$ ones. This is because we interpreted (and set up) the coordinate transformation as active, instead of passive. There is obviously no difference between the two procedures. Of course any physical operator needs to be transformed accordingly before being used.

[3] The parameter λ must be real and not complex by SO(4) symmetry.

[4] This is a special property, due to the fact that S_1 and S_2 commute with each other. In more general situations this may not be the case, so the analysis should be more careful.

where the B_i, Z and $\bar{h}$ are numerical parameters.[5] The free propagation of an original electron corresponds to the correlated propagation of single-, triple- and penta-electron modes, and vice-versa. Consequently it seems possible that a free state of the transformed fermions, capturing pure multi-particle physics of the original electrons, corresponds to the sum of Slater determinants of the original ones. In paper B we refer to the coefficient Z as "quasi-particle weight"; I will comment in Sec. 5.2 on this choice of words.

It is worth mentioning that it seems inappropriate to speak about a final trial ground *state* for the physical electrons. Indeed the solution found is a Slater determinant written in terms of both species of transformed fermions, which therefore become entangled. Consequently the original physical and auxiliary fermions are entangled. Therefore if one wants to look only at the part comprising the original physical fermions, the information contained in the other species should be integrated out. From this point of view, what we obtain is not a trial state for the physical fermions, but a trial density matrix.

The exact form of this density matrix is irrelevant for most practical purposes,[6] in particular for the computation of the local density of states (DOS) that can be obtained using the spectral representation of the Green's function. To compute the DOS one must take the retarded Green's function $G_{11}(t,i,i)$ of the original physical fermions and transform it via V in the new coordinate system. For example consider the retarded Green's function of the spin up electrons and write it in terms of Majoranas, following for example the convention of formula (22) in paper B:

$$\begin{aligned} G_{1,\uparrow;1,\uparrow}(t,i,i) &= -i\langle \mathrm{T} c_\uparrow(t,i,i) c_\uparrow^\dagger(0,i,i)\rangle \\ &= -\frac{i}{2}\langle \mathrm{T}\gamma_1(t)\gamma_1(0)\rangle - \frac{i}{2}\langle \mathrm{T}\gamma_2(t)\gamma_2(0)\rangle, \end{aligned} \tag{5.9}$$

where the imaginary time convention is used consistently with paper B, even if not necessary for the argument. What one has to compute are therefore the Majorana Green's function:

$$g_{11} = -i\langle \mathrm{T}\gamma_a(t,i,i)\gamma_a(0,i,i)\rangle, \tag{5.10}$$

where a is the Majorana flavor index (which is irrelevant since all the flavors are equivalent because of the $SO(4)$ symmetries) and the average is taken over the variational mean-field ground state. Using V, g_{11} can be expressed in terms of transformed Majorana Green's functions:

$$\tilde{g}_{11}(t,i,j) = -i\langle \mathrm{T}\,\tilde{\gamma}_a(t,i)\tilde{\gamma}_a(0,j)\rangle, \tag{5.11}$$

$$\tilde{g}_{12}(t,i,j) = -i\langle \mathrm{T}\,\tilde{\gamma}_a(t,i)\tilde{\mu}_a(0,j)\rangle, \tag{5.12}$$

$$\tilde{g}_{22}(t,i,j) = -i\langle \mathrm{T}\,\tilde{\mu}_a(t,i)\tilde{\mu}_a(0,j)\rangle, \tag{5.13}$$

by performing explicitly the non-linear transformation

$$g_{11}(t,i,j) = -i\langle \mathrm{T} V\gamma_1(t,i,i)V^\dagger V\gamma_1(0,i,i)V^\dagger\rangle. \tag{5.14}$$

In the previous formulas the tildes remind us when we are working in the transformed space. The result of the transformation $V\gamma_1(t,i,i)V^\dagger$ is given in formula

[5] Of course the spin index should also be indicated, but since it is trivial and cumbersome it is not written explicitly.

[6] An important exception is clearly the computation of the entropy.

(7) of paper B. Given this result one can apply the mean-field approximation to compute all the Wick contractions of the terms that appear in (5.14). In this way one generates the result (5.8), which expresses G_{11} in the new basis as a sum of terms composed by multiple Green's functions $\tilde{G}_{nm}$ of the new free fermions $a_{i,\sigma}$ multiplied together. Clearly the previous recipe can be followed for the computation of any quantum average and not only for the Green's function.

Formula (56) in paper B, or equivalently formula (5.8) in this section, can be used to determine the DOS of the physical part of the system, given that

$$\rho_{11}(\epsilon) = -\frac{1}{\pi}\mathrm{Im}\Big(G_{cc}(\epsilon, i, i)\Big) = -\frac{1}{\pi}\mathrm{Im}\left(G_{11}(\epsilon, i, i)\right), \tag{5.15}$$

and that it is possible to compute exactly the contribution to DOS provided by the incoherent multi-particle part of the transformed Green's function G_{11}, if one knows the Green's function of the $a_{i,\sigma}$ fermions $\tilde{G}_{nm}$ (with $n, m = 1, 2$), which indeed are given in formula (20) of paper B. For example on the Bethe lattice the mean-field Green's function $-\langle \mathrm{T}_\tau a_{1,\sigma}(\tau) a_{1,\sigma}(0)\rangle$ of the a_1 fermion is given in frequency space by:

$$\tilde{G}_{11}(z) = \frac{2z}{z^2 - \lambda^2 + \sqrt{z - z_+}\sqrt{z - z_-}\sqrt{z + z_+}\sqrt{z + z_-}}, \tag{5.16}$$

with $z_\pm = \sqrt{t_1^2 + \lambda^2} \pm |t_1|$ and where we used the imaginary-time and frequency formalism, which considerably simplifies the calculations. Because of the composite structure of $G(\epsilon, i, i)$, it is appropriate to write the Green's function in Lehman representation, so that in general

$$G(z, i, i) = \int_{-\infty}^{+\infty} \frac{\rho(\epsilon)}{z - \epsilon} d\epsilon, \tag{5.17}$$

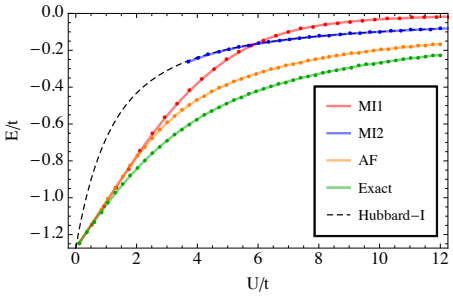
which is exactly (4.38) if $z = \omega + i\delta\mathrm{sign}(\epsilon)$, while it reduces to the retarded Green's function if $z = \omega + i\delta$. This form is particularly useful in the case under consideration, since it allows exact computation of the contribution to the DOS of the multi-particle propagation. In fact, let us assume we know the value of $\rho_{ab}(\epsilon)$ for each Green's function $\tilde{G}_{ab}(\omega)$. Then the contribution $A_3(\epsilon)$ to the DOS of the three-component terms $\tilde{G}_{ab}(t)\tilde{G}_{a'b'}(t)\tilde{G}_{a''b''}(t)$ can be computed exactly via the procedure highlighted in formulae (58)-(59)-(60) in the Supplementary Material of paper B, resulting in the convolution of the three $\rho(\epsilon)$ that appear in the respective Green's functions:

$$A_3(\epsilon) = \frac{1}{\pi}\int\int\int d\epsilon_2 d\epsilon_3 \rho_{ab}(\epsilon - \epsilon_2 - \epsilon_3)\rho_{a'b'}(\epsilon_2)\rho_{a''b''}(\epsilon_3), \tag{5.18}$$

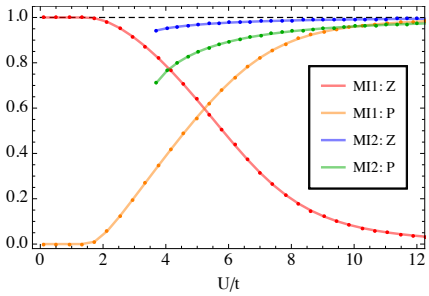
with the additional constraint that all the energies $\epsilon_1, \epsilon_2, \epsilon - \epsilon_2 - \epsilon_3$ must have the same sign. The $\rho(\epsilon)$ for the different Green's functions are easily computed using formula (20) of paper B, so for example on the Bethe lattice

$$\rho_{11}(\epsilon) = \frac{\pi |\epsilon| \sqrt{(z_-^2 - \epsilon^2)(\epsilon^2 - z_+^2)}}{\lambda^4 - 2\lambda^2\epsilon^2 + \epsilon^2 z_+^2 + z_-(\epsilon^2 - z_+^2)}, \tag{5.19}$$

for $-z+ < \epsilon < -z_-$ and $z- < \epsilon < z_+$ and zero otherwise. So the DOS is readily computed, with only extremely light numerics required.



(a) *Evolution of ground-state energy;*



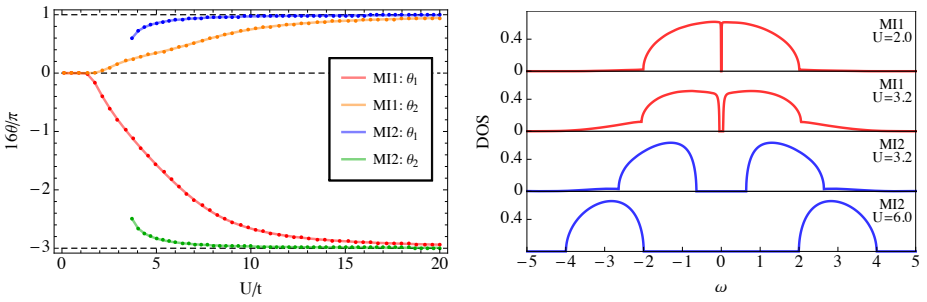
(b) *Parity and quasi-particle weight vs U.*

Figure 5.1: *Both the figures refer to the $d = 1$ study: (a) the evolution of the trial mean-field ground-states with the interaction parameter U, compared with the Hubbard-I solution, the antiferromagnetic ordered ground-state and the exact solution. (b) For MI1 and MI2 the value of the parity operator average $\langle P_1 \rangle$ and the quasi-particle weight Z, computed for different values of U.*

The results obtained with this enlarged mean-field scheme are indeed interesting. We analyzed both the $d = 1$ and $d = \infty$ cases, but analysis can be performed in other dimensions too. However, in both cases, we identified two solutions MI1 and MI2. The first one is the best trial ground state from weak to intermediate U, while the second is a good trial ground state at high U. Both solutions enforce the unit occupancy of the lattice sites with increasing U, although the MI2 solution is able to do it in a more coherent fashion (maximizing Z, the coherent single particle contribution to the Green's function), while MI1 tends to minimize such a contribution. This is shown in Fig. 5.1b. As made evident by Fig. 5.2a, the larger coherence of MI2 is obtained using a different non-linear transformation with respect to MI1; in fact one can see that in $U \to +\infty$ the angles θ_1 and θ_2 are inverted in MI2 with respect to the MI1.

5.2 Results

A discussion of the results is presented in the paper, so in this brief introduction I will just stress the most important one, which is obtained in the Mott insulating phase. The trial mean-field ground state MI2, in both the $d = 1$ and $d = \infty$ cases, proved itself energetically more convenient, with respect to MI1. Interestingly, *it is not* the enforcement of the unit occupancy that makes it our best trial mean-field ground state. This can be understood in the 1d case, comparing Fig. 5.1a and Fig. 5.1b. The first figure shows the evolution of the trial ground state energy (from which we subtracted the leading order $-U/4$ energy shift) with U; in the second are plotted for both MI1 and MI2 the values of the parity operator average $\langle P \rangle$ and the value of quasi-particle weight Z. In this context Z quantifies how much of the original electron Green's function is given by the coherent component of the transformed fermions. The term "quasi-particle weight" is slightly abused in this context. In fact it is always necessary to keep in mind the two different operations that are performed in order to obtain the trial solutions: the non-linear transformation and the mean-field analysis. The first is an exact operation, while the second requires approxima-



(a) *Optimized rotation angles θ_1 and θ_2 in 1d;* **(b)** *Ground-state DOS in the $d = \infty$ case.*

Figure 5.2: *(a) the evolution of the non-linear rotation angles θ_1 and θ_2 with U, for both MI1 and MI2 in the $d = 1$ case. (b) The computed DOS on the best trial mean-field ground-state for different values of U, in the case of a $d = \infty$ Bethe lattice. The Dos is given in natural units, so to compare with Fig. 4.2 one has to multiply the y-ticks by πt; this operation shows that for $U = 0$ the DOS at $\omega = 0$ has the same hight in both figures.*

tions. The non-linear transformation maps the one-particle Green's function of the original electrons into the sum of a one-particle Green's function and many-particle Green's functions for the new fermions. This second part is then approximated within the mean-field approximation, producing the incoherent contributions in (5.8) as well as coherent one that get summed to the original one-particle Green's function. The total coefficient in front of the coherent contribution is Z. The quantity Z measures the "coherency" of the full procedure, since its value depends on both the non-linear transformation and the mean-field approximation. This is why we used the name "quasi-particle weight" to indicate Z.

As evident MI2 at high coupling is energetically favorable to MI1. In particular it seems that for $U \to \infty$ the energy density of MI2 is equal to the energy density of MI1 minus $J/4$. In this sense, and considering the exact map between Hubbard and Heisenberg Hamiltonian at high coupling, it seems that MI2 captures the constant shift $-J/4$ present in the Heisenberg Hamiltonian, together with the constant shift $-U/4$. Instead MI1 captures only this second effect. Looking only at Fig. 5.1a and at the evolution of P_1 in Fig. 5.1b, this behavior is not comprehensible: indeed MI1 is at least as good as MI2 in the enforcement of the single occupancy. The difference between the two states is given by the opposite behavior of Z, which at high coupling goes to zero for MI1 and to one for MI2. This different behavior is allowed by the extremely different non-linear transformations used in the constructions of the two states Fig. 5.2a. The MI2 state is more effective at describing the high coupling ground state because it is able to give a more coherent representation of it, allowing to capture more of the kinetic energy of the electron. In fact the kinetic energy can be computed using $G(0^-, i, j)$ with i, j nearest neighbor indices, which can be approximated in our enlarged mean-field scheme with a formula of the same form of (5.8). In the case of MI2 this means that the kinetic energy depends linearly on the nearest-neighbor Green's function of the new fermions; while in the MI1 case it depends upon the product of three of nearest-neighbor Green's function. It is clear that the value of the nearest-neighbor Green's function of

the new fermions goes down with increasing U, therefore the MI1 state is much less efficient than the MI2 state to optimize the kinetic energy of the electron in the $U \to +\infty$ limit. Thus, the fermions used in MI2 provide optimal eigenstates for building the ground state as a trivial Slater determinant. In this sense we are able to provide a free particle representation of the Mott insulating phase.

The MI1 phase is a bad variational trial ground-state also in the metallic region, as shown in Fig. 5.2b. The density of states of MI1 is gapped for any U also in $d = \infty$, although the gap is unphysical at small coupling. This tendency of the gap to keep a small size can be interpreted as the tendency of the ground state to be "as metallic as possible". To improve the results one should allow for more auxiliary bands, extending the variational space even more.

5.3 Achievements of Paper B

Briefly summarizing the main achievements contained in Paper B:

- a general strategy for the study of correlated models has been proposed;
- the enlarged mean-field analysis of the Hubbard model was performed in different dimensions and in particular in $d = 1$ and $d = \infty$;
- a free particle description of the Mott insulating phase has been identified as the MI2 trial mean-field ground state;
- a full characterization of the main properties of the non-linear mapping that generates the states MI1 and MI2 has been performed.

Part III

Application: the Kondo lattice model

Chapter 6

The Kondo lattice model

The Kondo Lattice (KL) model plays a crucial role in condensed matter physics: it connects two different worlds, lying in the gap between spin models and pure electron models. The competition between the electron and the spin nature of the model generates new interesting physics, that can hardly be explained using only the concepts that belong to either one or the other world. The term KL indicates a system where a quantum spin is located on each atomic site, together with electrons that are free to hop from site to site. Among the spins and the electrons there exist a local spin-spin (Kondo) coupling. Although many exotic variations of the model have been defined, in this manuscript the term "Kondo lattice" will mean the model where the on-site impurity spins have $\mathbf{S}^2 = 3/4$ and there exist only one species of hopping electrons (single channel KL). Depending upon the structure of the lattice, the average number of electrons per site n_c, the temperature T, the Kondo coupling J and the bandwidth t, the properties of the system can change drastically. The Hamiltonian has the compact form:

$$\begin{aligned} H &= -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_\sigma(i)c_\sigma(j) + c^\dagger_\sigma(j)c_\sigma(i)\right) + \\ &\quad + J\sum_i \mathbf{S^c}(i)\cdot\mathbf{S^f}(i) - \mu^* \sum_{i,\sigma} c^\dagger_\sigma(i)c_\sigma(i), \end{aligned} \tag{6.1}$$

where $\mathbf{S^c}$ ($\mathbf{S^f}$) is the spin vector operator of the conduction electrons (impurity spins), μ^* the chemical potential, $\langle i,j\rangle$ denotes nearest neighbors and $\sigma = \pm 1/2$ indicates the two spin orientations respect to the quantization axis (that will always be chosen as $\hat{z}$).

Obviously the interesting physics of the model is generated by the only interaction term present. Because of it, the electrons and the local momenta become correlated, offering a cornucopia of possible configurations for the system, able to describe a huge variety of compounds: from Kondo insulators, to heavy fermions superconductors and ferromagnetic metals. Many of the mechanisms that stabilize these phases (for example the glue of the unconventional superconductors) are still object of research and represent an hot topic (see discussion in Ref. [133] for details).

The minimal understanding of the KL has been elaborated by Doniach [134]. According to his picture, the interaction between electrons and spins generates

two competing effects: the RKKY effect[1] (an effective spin-spin interaction for the impurity spins) and the Kondo effect. At low coupling it seems reasonable that the electrons will not be very much affected by the coupling with the impurity spins, so the effect of the coupling term is summarizable into an effective spin-spin interaction (RKKY); the system will decrease the energy of the ground-state optimizing the spin correlation function, eventually ordering the spins.[2] Increasing the coupling, the Kondo effect takes over, implying a massive change in the electron wavefunction, that becomes entangled with the spin state; of course the Kondo screening mechanism must be slightly different than the one considered in the more famous Kondo model [78], because it must take place coherently on every site. The competition between these two mechanism and the transition between the regimes where one or the other effect is dominant, determines the interesting physics of the KL.

Doniach's picture is considered good enough in two and three dimensions, where it is believed that the transition between the two regimes passes through a quantum phase transition [138–140]. In one dimension instead this minimal picture is known to be inappropriate (except at half filling) and it seems that the the number of competing effects needed to explain the different regions in the phase diagram should be increased enormously, anticipating a probable failure of this kind of approach [141, 142]. For example a first correction to Doniach's picture can be done considering a three-effect scenario, adding to the RKKY and the Kondo effect also the double exchange mechanism. This three-effect picture offers a justification for the ferromagnetic part of the phase diagram, but it is still only an approximation, as will be explained in this chapter.

From now on we will mainly focus on the one-dimensional Kondo lattice model (1dKL), assuming for simplicity only antiferromagnetic coupling $J > 0$. The 1dKL is the only (low dimensional) KL that has been successfully characterized, although some of its properties are still obscure. Vice-versa the scenario is completely different in two and three dimensions where, despite a great debate about the properties of the QPT, just a small part of the physics has been analyzed theoretically. This difference is mostly due to a technical problem: the absence of reliable and efficient methods for the analysis of the two and three dimensional cases. The 1dKL has been treated efficiently making use of two powerful techniques: bosonization (analytical [143, 144]) and DMRG (numerical [145]); both of them are much less effective in two and three dimensions and therefore these are still open problems. Some recent results regarding the ferromagnetic phase in many dimensions [146] throw some shadows on the validity of the Doniach's picture also in two and three dimensions. It is therefore of primary relevance to develop an approach that permits one to deal with these systems. I believe that the approach explained in this manuscript will permit such an analysis and will represent the appropriate way to deal with these open questions; in paper C I try to convince the reader of this fact using the 1dKL as benchmark.

[1] The name comes from the initials of the first authors that considered this effect: Ruderman, Kittel [135], Kasuya [136] and Yosida [137]

[2] Of course this cannot be the case in one dimension; so one speaks typically about quasi-long range orders.

6.1 From real materials to the model

A standard objection that is often raised when a theoretical work is presented regards the applicability, or the "reality" of the models considered. It is possible that already at this stage some worried readers are wondering about the physical significance of the KL, therefore I considered appropriate the inclusion of a preliminary section that deals with the derivation of the model.

f-orbitals

The KL Hamiltonian can represent a big variety of systems, that differ from each other on the origin of the impurity spins. In principle they could have nuclear origin, but in this case the coupling J would be too small to make sense: in fact the form (6.1) assumes implicitly that the electron-spin coupling is the dominant one and that all the other interactions (for example the local Coulomb interaction among the conduction electrons) are negligible; therefore an excessively small J is non-sensical.[3] The spin could also represent more complex structures, like for example a quantum dot: if the parameters of the dot (gate and applied voltage) are properly chosen then the spin trapped in the dot will behave like a spin impurity. However, considering more concrete scenarios instead, the most interesting situation is when the local impurity spins have electronic origin, i.e., they are the low-energy degrees of freedom of electrons that are localized by strong interactions. This situation is encountered in many real materials, in particular in rare-earths[4] (lanthanides plus Yttrium and Scandium) and actinide compounds [7, 78, 133, 147], that means in those elements that have partially filled *f*-shells. In compounds built making use of these ions, it is important to distinguish between two types of the electrons: the f-electrons (often called valence electrons) and the d- or s-electrons[5] (called conduction electrons in the rest of the manuscript). The difference between the two classes is due to the different spatial extent of the wave function: while the s- and d-orbital are (relatively) wide, the f-orbitals are much more compact [7, 148]. This has two consequences: on the one hand the s- and d-orbitals generates broad conduction bands, contrarily to the f-orbitals that remain strongly atomic in character and their negligible hopping leads to almost flat bands; on the other hand the behavior of the valence (f-)electrons becomes completely dominated by Coulomb interaction. Forgetting for the moment the (unavoidable) hybridization between the conduction and the valence electrons, it is clear that the structure of the f-electron system will be that of a Mott insulator. The 14-fold Hubbard Hamiltonian with vanishing hopping is a good (simplified) model to describe the main

[3] This should be studied making use of renormalization group analysis, in order to identify if the couplings flow or not into the KL regime (more appropriately, into a KL fix point) for some energy scale. A discussion of the applicability of the KL to one or another material goes beyond the aim of this work, so I will not argue further along this line.

[4] If the reader does not have a periodic table at hand, I suggest to visit the page `http://www.ptable.com` that contains many important informations, including a list of all the possible compounds.

[5] I omit the principal quantum number, because it is clear that I refer to the s- and d- atomic orbitals energetically in competition with the atomic f-orbitals (4f and 5f for lanthanides and actinides respectively). Are the $(n+1)$s- or the nd- orbitals that compete respectively with almost filled of almost empty nf-orbitals [7].

features of the f-electrons subsystem:

$$H_f = U \sum_i \sum_{\substack{\alpha,\beta=1 \\ \alpha \neq \beta}}^{14} f_\alpha^\dagger(i) f_\alpha(i) f_\beta^\dagger(i) f_\beta(i) + \epsilon_f \sum_i \sum_\alpha^{14} f_\alpha^\dagger(i) f_\alpha(i). \tag{6.2}$$

The spectrum of the valence electrons system will thus be built up by 14 local states (labeled by f^0, f^1, ..., f^{14}, where the number gives the number of electrons per site) spaced by U, starting from the lowest at $E = \epsilon_f$ that is the energy of the ionic level. The 14 comes from the number of degenerate atomic f-orbitals: $(2 \cdot 3 + 1) = 7$ due to the projection of the angular momentum and a factor 2 due to spin. The reader should not be tricked by presence of the N-fold total multiplicity (with N the number of sites). Assuming for simplicity that the configuration with no electrons is the one with minimal energy, one should naively expect that the eigenstates of the system are spaced by steps of height ϵ_f (that later becomes $\epsilon_f + U$) and so that the system could get filled gradually, varying the value of the Fermi level. This is wrong [7], and it depends on the fact that the particle number in the system is determined by the chemical potential, which rules the exchange of electrons among the f-subsystem, the d- or s-band system and the reservoir represented by the rest of the universe. Still neglecting the effect of the hybridization, it is instructive to study what happens changing the chemical potential μ^*. Assuming for example that $\epsilon_f > 0$, which means that the lowest energy f-configuration is with no valence electrons per site (f^0), we can start to increase the chemical potential from the bottom of the conduction band, that we set at $\mu^* = 0$. The density will increase continuously, with the electrons that are hosted into the conduction band, until we reach $\mu^* = \epsilon_f$: only at that point will the electrons start to populate the f-orbitals, filling the N quantum states. It is crucial to note that, although the energy of these configurations is different, the free-energy $H - \mu N$ is the same, so in terms of the free-energy there exist a huge N-fold degeneracy. This means that the number of electrons in the system can be increased enormously without changing the chemical potential, up to the density of one electron per site. In this situation, where only a partial number of f-states are filled, the system is in the so called[6] "mixed-valence" regime $f^0 - f^1$. It seems plausible that the high entropy associated with states at fixed particle number can, in principle, cause an interesting complication of the physics; in particular if the different configurations get mixed by the hybridization with the conduction electrons that for the moment we are still neglecting. The interesting physics described by the KL, as we will see, is a particular case of this kind of phenomena caused by the presence of a huge (thermodynamic) amount of degenerate configurations. Increasing the chemical potential further there will be one valence electron per site and the system will return to an integral-valence regime f^1. When the chemical potential reaches the value $\mu^* = \epsilon_f + U$ again the system enters into a mixed-valence regime, indicated this time as $f^1 - f^2$, etc... In most of the compounds the levels that fall close to the Fermi surface are the f^0, f^1 and f^2, so we will focus only on these possibilities.

[6] The nomenclature is quite wild; referring to the compounds the terms "mixed-valence", "mixed-configurations", "fluctuating-valence" or "fluctuating-configuration" are synonymous. See Ref. [147] for a complete review of the topic.

Anderson local moment formation

The reader should start to have an idea of why in these compounds the KL can be a relevant model: if the parameters are chosen in a correct way, it is possible to force the f-subsystem to go into the integral-valence regime f^1, accommodating one electron per site, which then behave like a quantum spins (*local moment regime*). However, in the light of what has been introduced so far, this quantum top should have a 14-fold degeneracy, instead of the (spin-1/2) 2-fold degeneracy. This is due to the fact that up to now we neglected some finer effects due to spin-orbit coupling and crystal-fields (see appendix B), that split[7] the 14-fold orbital degeneracy, leading to a 2-fold degenerate (rarely 4-fold) orbital ground-state, where the two states form a time reversal doublet and can therefore be modeled as a spin-1/2 degree of freedom [7]. Clearly this does not invalidate the previous considerations for the integral- and mixed-valance compounds.

Let us try to characterize the boundaries of this local moment regime [93,133] for an isolated f-impurity, i.e. the interesting regime for the emergence of a KL. In the light of the previous considerations, we are allowed to consider only a 2-fold spin-like degeneracy for the f-electron states, and therefore we can easily enumerate the states that belong to the local Fock space:

$$|0\rangle, \quad |\uparrow_f\rangle = f^\dagger_\uparrow|0\rangle, \quad |\downarrow_f\rangle = f^\dagger_\downarrow|0\rangle, \quad |\uparrow_f\downarrow_f\rangle = f^\dagger_\uparrow f^\dagger_\downarrow|0\rangle,$$

where $|0\rangle$ is the state with no electrons. Considering the interactions of the type (6.2) it is evident that the energies will be

$$\begin{array}{cc} |\uparrow_f\downarrow_f\rangle & \rightarrow 2\epsilon_f + U \\ |\downarrow_f\rangle, |\uparrow_f\rangle & \rightarrow \epsilon_f \\ |0\rangle & \rightarrow 0. \end{array}$$

If we want to obtain a ground state that behaves like a quantum spin, it is necessary to set the parameters ϵ_f and U in such a way that the lowest energy states are $|\downarrow_f\rangle$ and $|\uparrow_f\rangle$; this means also that the energies necessary to add or remove one electron to the single occupied configuration must be positive:

$$\begin{array}{cc} \text{remove} & \rightarrow -\epsilon_f \\ \text{add} & \rightarrow \epsilon_f + U, \end{array}$$

schematically

$$\frac{U}{2} \pm (\epsilon_f + \frac{U}{2}) > 0.$$

The different realizations are drawn in Fig. 6.1a. Clearly it is the smallest value among $|\epsilon_f|$ and $|U+\epsilon_f|$ that sets the energy scale E_s of the analysis. To be in the local moment regime, i.e. no contribution from the vacant or doubly occupied state in order to have in the ground-state f-wavefunction, every other energy scale (for example the temperature) in the system must be smaller than E_s.

These results hold in the case of an isolated impurity, i.e. with no hybridization between the valence and the conduction electrons. In a real situation the

[7] Of course the temperature scale must be lower than the energy scale fixed by the two splitting effects.

f-impurity is embedded into the compound and the hybridization cannot be switched off. The model that fully represents this situation is the Anderson impurity model, if there is only one f-impurity in the system, or the Periodic Anderson Model (PAM), if on each site an f-impurity is present. I write only the latter for future convenience,

$$\begin{aligned} H &= -t\sum_{\langle i,j\rangle,\sigma}\Big\{c^\dagger_\sigma(i)c_\sigma(j)+c^\dagger_\sigma(j)c_\sigma(i)\Big\}+\epsilon_f\sum_{i,\sigma}f^\dagger_\sigma(i)f_\sigma(i) \qquad (6.3)\\ &\quad +V\sum_{i,\sigma}\Big\{c^\dagger_\sigma(i)f_\sigma(i)+f^\dagger_\sigma(i)c_\sigma(i)\Big\}-\mu^*\sum_{i,\sigma}\Big\{c^\dagger_\sigma(i)c_\sigma(i)+f^\dagger_\sigma(i)f_\sigma(i)\Big\},\\ &\quad +U\sum_i f^\dagger_\uparrow(i)f_\uparrow(i)f^\dagger_\downarrow(i)f_\downarrow(i). \end{aligned}$$

The presence of the hybridization modifies the previous results, introducing the new parameter V into the game. If in the isolated case the only competition was among ϵ_f, U and μ^*, now also V sets a new scale in the system. Crudely speaking one expects that the local moment formation will still happen, but only when $V \ll E_s$, i.e. when the Coulomb interaction U and the ionic binding energy ϵ_f dominate over the hybridization V. The latter in fact, mixing the valence and the conduction electrons, adds weight coming from the empty and the doubly occupied configurations to the ground state of the f-electrons. The first contribution becomes inignificant decreasing ϵ_f; the second by increasing U.

The first detailed analysis was carried out by Anderson, in the case of a single impurity. In absence of interactions ($U = 0$), the coupling V determines uniquely how strongly the valence and the conduction electrons are mixed with each other and therefore how big the contribution of the double occupied and vacant f-orbital to the ground-state configuration are. Because the conduction and valence electrons are hybridized, neither of the two classes can be considered an eigenstate of the system. So the singly occupied (pure) f-state can be though of as an unstable state that has finite life-time, and decays into a different states (into the continuum of the conduction electron states). We can estimate the lifetime of this unstable state using the Fermi Golden rule:

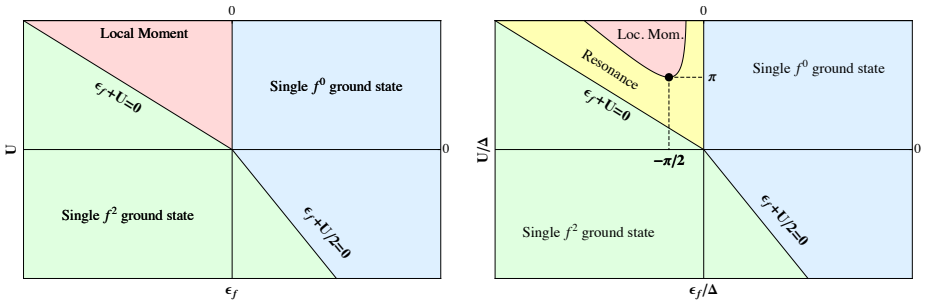
$$\frac{1}{\tau}=\Delta=\frac{2\pi}{\hbar}|\langle in|V_{in,out}|out\rangle|^2\rho_{out}(\epsilon)\delta(E_{in}-E_{out}). \qquad (6.4)$$

Given that the hybridization term conserves the spin polarization,[8] we can treat the up and down spin channels separately. The discussion will be simpler in this way, because only one channel for the decay must be considered: the escape of the valence electron. This is possible because so far we are assuming $U = 0$, and this means that we are neglecting the only term in the Hamiltonian that correlates the two up and down sectors.

In (6.4) the out-states are the states of the continuum and $\rho_{out}(\epsilon)$ is the density of states of the conduction electrons. In Fourier space

$$\begin{aligned} \Delta &= \pi\sum_{\vec{k}}|\langle f^1_\sigma|V(\vec{k})f^\dagger_\sigma c^\dagger_{\vec{k},\sigma}|\vec{k},\sigma\rangle_c|^2\delta(\epsilon_f-\epsilon_{k,\sigma}) \qquad (6.5)\\ &= \pi\int d\epsilon|V(\epsilon)|^2\rho(\epsilon)\delta(\epsilon_f-\epsilon). \qquad (6.6) \end{aligned}$$

[8] Via a unitary transformation this condition can always be achieved.



(a) *Zero hybridization case;* **(b)** *Anderson mean-field analysis;*

Figure 6.1: *The local moment phase diagram without hybridization: (a) without considering the hybridization; (b) with the hybridization, in the the mean-field approximation;* Δ *is the width of the resonance. It is evident that the minimum value of* U/Δ *for the development of the local moment is* π*. The coordinates of the critical point* $U/\Delta = \pi$ *and* $\epsilon_f/\Delta = -\pi/2$ *come from the solution of the equations (6.13) and (6.14), for* $n_f = 1$*.*

This quantity is the width of the resonance and will be denoted by $\Delta(\epsilon_f)$. A more precise derivation and discussion, in terms of Feynman diagrams is given in [93]. According to the previous arguments, the (retarded) propagator in imaginary time for such f-resonance must take the form

$$G_f(\omega + i\delta^+) = \frac{1}{\omega - \epsilon_f - i\Delta(\epsilon_f)},$$

implying for the valence electron the density of states[9]

$$\rho_f(\omega) = -\frac{1}{\pi}\frac{\Delta}{(\omega - \epsilon_f)^2 + \Delta^2}, \tag{6.7}$$

In principle also a V dependent correction to ϵ_f should be considered, but this effect has not been considered in the previous formula, because irrelevant for the following discussion.

Given this density of states it is possible to compute the average number of electrons in the resonance (i.e. in the f-state) by integrating it up to the Fermi level, fixed by μ^*:

$$\langle n_f \rangle = 2\int_{-\infty}^{\mu^*} d\epsilon\, \rho_f(\epsilon) = \frac{2}{\pi}\left[\frac{\pi}{2} - \arctan\left(\frac{\epsilon_f - \mu^*}{\Delta}\right)\right] = \frac{2}{\pi}\mathrm{arccot}\left(\frac{\epsilon_f - \mu^*}{\Delta}\right),$$

where the two comes from the two spin channels. For simplicity μ^* will be set to zero in the following.

Up to this point the f-electrons are fluctuating wildly, because on the one hand they are in a state that is neither empty nor filled, but on the other hand the two spin species are uncorrelated, therefore double occupancy is not suppressed. In this situation one says that the f-electrons exhibit large charge (or valence) fluctuations. To obtain the formation of the local moments, these charge fluctuations must be quenched. Since the valence fluctuations are caused

[9]The explicit the dependence of Δ on ϵ_f has been omitted, to avoid cluttering of the notation.

by the hybridization, the only way to quench them is reducing its effect, making the other parameters dominant and the vacant and double occupied states very inconvenient in terms of energy. This means that the parameters U and ϵ_f must be tuned properly, increasing significantly U and keeping ϵ_f way below the Fermi level. For a critical U_c that depends upon Δ the occupation will collapse to one generating a local moment. To study this effect Anderson used a Hartree-Fock decomposition of the quartic term, interpreting the degeneracy breaking of the up and down f-spin species as the sign of the formation of a magnetic ground state,i.e. of a local moment. This degeneracy breaking becomes apparent in the solution by the development of a magnetic moment for the f-system, that in fact has no magnetization if $U = 0$ because $\langle n_{f,\uparrow}\rangle = \langle n_{f,\downarrow}\rangle$. Proceeding with the Hartree-Fock decomposition, the energies $\epsilon_{f,\uparrow}$ and $\epsilon_{f,\downarrow}$ become dependent upon the average number of electrons that occupy respectively the $f^1_\downarrow$ and $f^1_\uparrow$ states:

$$U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow \to U f^\dagger_\uparrow f_\uparrow \langle f^\dagger_\downarrow f_\downarrow\rangle + U\langle f^\dagger_\uparrow f_\uparrow\rangle f^\dagger_\downarrow f_\downarrow - U\langle f^\dagger_\uparrow f_\uparrow\rangle\langle f^\dagger_\downarrow f_\downarrow\rangle, \tag{6.8}$$

which is equivalent to a spin dependent shift of the f-energy level

$$\epsilon_{f,\sigma} \;\to\; \epsilon_f + U\langle f^\dagger_{\bar\sigma} f_{\bar\sigma}\rangle, \tag{6.9}$$

so

$$\langle n_{f,\sigma}\rangle = \frac{1}{\pi}\mathrm{arccot}\left(\frac{\epsilon_f + U\langle n_{f,\bar\sigma}\rangle}{\Delta}\right).$$

Defining the total density $n_f = \sum_\sigma n_{f,\sigma}$ and the magnetization $M = \langle n_{f,\uparrow}\rangle - \langle n_{f,\downarrow}\rangle$ one gets [93]:

$$n_f = \frac{1}{\pi}\left[\mathrm{arccot}\left(\frac{\epsilon_f + U(n_f - M)/2}{\Delta}\right) + \mathrm{arccot}\left(\frac{\epsilon_f + U(n_f + M)/2}{\Delta}\right)\right], \tag{6.10}$$

$$M = \frac{1}{\pi}\left[\mathrm{arccot}\left(\frac{\epsilon_f + U(n_f - M)/2}{\Delta}\right) - \mathrm{arccot}\left(\frac{\epsilon_f + U(n_f + M)/2}{\Delta}\right)\right]. \tag{6.11}$$

We are interested in characterizing the local moment regime, i.e. the region that supports solutions with $M \neq 0$; this can be done noticing that the second equation is always true if $M = 0$, while the existence of non-trivial solutions implies conditions on the parameters. Up to the second order in M these conditions can be found linearizing (6.11) and the result is [93]:

$$1 = \frac{U}{\pi\Delta}\frac{1}{1 + \left(\frac{\epsilon_f + U n_f/2}{\Delta}\right)^2}. \tag{6.12}$$

If this condition is satisfied, every value of M is solution to the equation (6.11) and the local moment appears; otherwise the only acceptable solution is $M = 0$. Imposing $M \to 0^+$ on the first equation (6.10), one obtains

$$\cot\left[\frac{n_f\pi}{2}\right] = \frac{\epsilon_f + U n_f/2}{\Delta}. \tag{6.13}$$

This result and the previous can be combined to yield

$$1 = \frac{U}{\pi\Delta}\sin^2\left(\frac{\pi n_f}{2}\right). \tag{6.14}$$

This equations creates a relation among the parameters U, Δ and n_f. Evidently there exists a minimum value U_c, below which no non-trivial solution to (6.11) exists. Therefore for

$$U > U_c(n_f) = \frac{\pi\Delta}{\sin^2(\pi n_f/2)}, \tag{6.15}$$

a local moment is formed. This is an improvement of the previous result obtained without the hybridization. The Anderson mean-field phase diagram for the local moment formation is shown in Fig. 6.1b.

The total density n_f is a function of ϵ_f, besides the two parameters Δ and U. The minimum critical value U_c is obtained for $n_f = 1$, i.e. for $U = -2\epsilon_f$. The latter condition is not surprising: if $U = -2\epsilon_f$ the empty and double occupied f-states become degenerate and it is this symmetry that forces the f-system to be exactly half filled. If this symmetry condition is not fulfilled then the total density inside the local moment region can be bigger or smaller than one, depending on which excited configuration has the lowest energy. This property is a feature of the mean-field solution. A recent Gutzwiller analysis of the PAM [149] shows very well the parameter regimes that allows for single occupation and moment formation. The local moment regime in the parameter space, where the valence fluctuations are strongly quenched, is therefore quite big and requires only $\epsilon_f \ll E_F$ and $U \gg \Delta$.

From the PAM to the KL

So far it has been established how the parameters must be chosen in order to obtain the freezing of the charge fluctuations of the valence electrons and the consequent formation of a local moment. In this situation the PAM contains too much information. In fact good part of the physics that it describes is strongly suppressed and is not relevant at sufficiently low energy scales. It would then be appropriate to (properly) remove the quenched, high-energy physics of the charge fluctuations and deal only with the low-energy part of the system, that is composed by conduction electrons and free local spins. In this way what is obtained is the Kondo lattice model (6.1).

It is important to understand the origin of the Kondo interaction term $J\,\mathbf{S_c}\cdot\mathbf{S_f}$. Starting from the considerations of the previous paragraph one could erroneously conclude that there exists no interaction at all between the conduction electrons and the localized spins. In fact the effect of the hybridization has been taken into account and it has been seen that, for properly chosen values of the parameters, its mixing effect becomes completely quenched, strictly implying zero hybridization between f and c electrons deep inside the local moment regime. This conclusion is not correct. In fact, although the valence electrons are forced to the single occupied state, with no contribution to the wavefunction coming from the vacant or double occupied state, they still have the possibility to experience virtual excitations. The f-electron can virtually hop from the f-state to the conduction band and back; or viceversa a conduction electron can fall into the f-orbital, forming a virtual f-singlet, and then jump back into the

conduction band. These processes create a correlation between the spin of the conduction electrons and the localized valence electrons. The correlation must be somehow represented in the effective theory that describes the low energy physics of the PAM in terms of only conduction electrons and local moments; the interaction term $J\,\mathbf{S_c}\cdot\mathbf{S_f}$ is exactly the expression of this correlation, i.e. it represents these virtual second-order hopping processes.

This way of looking at the system is based in the concepts of the renormalization group approach [28, 150–153], where the high energy degrees of freedom are integrated out, down to the energy scale of interest. Their effect can be summarized in the value of the coupling constant of the operators that appear in the low energy Hamiltonian (that by definition is written in terms of low energy degrees of freedom only). In the case of the PAM this procedure can be implemented in a quite straightforward way. In fact in 1966 Schrieffer and Wolff [22] discovered that using a unitary transformation the Hamiltonian of the impurity Anderson Model could be reduced to the one of the Kondo Model. The same transformation holds also for the PAM, that reduces to the KL [77] at low energy.

To set up the Scrieffer-Wolff transformation one has to notice that the hybridization term in (6.3) connects two sectors: the $n_f = 1$ and $n_f = 0, 2$, whose degeneracy is then broken by the interaction, making them the low and high energy sectors. Considering that the only effect of the quartic term is that of creating this energy splitting, it is clear that we can think of the system as a two level one, where the two levels (high and low energy) are connected by a quadratic operator. The Hamiltonian of such system can be written schematically as

$$\begin{bmatrix} H_{low} & V_{low,high} \\ V_{high,low} & H_{high} \end{bmatrix}, \tag{6.16}$$

with $V_{high,low} = V^\dagger_{low,high}$. Such a matrix can be diagonalized by a unitary transformation $\mathcal{U}$:

$$\mathcal{U}\begin{bmatrix} H_{low} & V_{low,high} \\ V_{high,low} & H_{high} \end{bmatrix}\mathcal{U}^\dagger \longrightarrow \begin{bmatrix} H'_{low} & 0 \\ 0 & H'_{high} \end{bmatrix}. \tag{6.17}$$

After this procedure the two sectors will be completely decoupled from each other and the H'_{low} (H'_{high}) will be the effective Hamiltonian for the low (high) energy sector.

On this rationale, Schrieffer and Wolff wrote [22] the formal expression

$$H' = e^S H e^{-S}, \tag{6.18}$$

S is the generator of the unitary transformation $\mathcal{U}$, while H is given by Hamiltonian of the impurity Anderson model

$$H_{IAM} = H_0 + H_1,$$

where

$$\begin{aligned} H_0 &= \sum_{k,\sigma} \epsilon_k c^\dagger_{\sigma,k} c_{\sigma,k} + \epsilon_f \sum_\sigma f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow, \\ H_1 &= \sum_k \left(V_{k,f_\sigma} c^\dagger_{\sigma,k} f_\sigma + V^*_{k,f_\sigma} f^\dagger_\sigma c_{\sigma,k} \right). \end{aligned}$$

They showed that a proper choice of S could be used to cancel every linear operator in V from H', realizing the diagonalization (6.17). Using a known lemma of the Baker-Campbell-Hausdorff formula

$$e^A B e^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + ...$$

it becomes clear that to cancel the first order terms in V of H' it is sufficient to impose

$$[S, H_0] = -H_1, \tag{6.19}$$

which means that S must be first order in V. Applying (6.18):

$$\begin{aligned} H' &= H_0 + H_1 + [S,H_0] + [S,H_1] + \frac{1}{2}[S,[S,H_0]] + \mathcal{O}(V^3) \\ &= H_0 + [S,H_1] + \frac{1}{2}[S,[S,H_0]] + \mathcal{O}(V^3) \\ &= H_0 + [S,H_1] - \frac{1}{2}[S,H_1] + \mathcal{O}(V^3). \end{aligned} \tag{6.20}$$

So

$$H' \approx H_0 + \frac{1}{2}[S,H_1], \tag{6.21}$$

with $\frac{1}{2}[S,H_1]$ an effective interaction that *does not* connect the two sectors. The equation (6.19) has the solution

$$S = \sum_{k,\sigma} \frac{V_{k,f_\sigma}}{\epsilon_k - \epsilon_f}(1 - n_{f,\bar{\sigma}}) c^\dagger_{k,\sigma} f_\sigma + \frac{V_{k,f_\sigma}}{\epsilon_k - \epsilon_f - U} n_{f,\bar{\sigma}} c^\dagger_{k,\sigma} f_\sigma - h.c. \tag{6.22}$$

where $n_{f,\bar{\sigma}} = f^\dagger_{\bar{\sigma}} f_{\bar{\sigma}}$ enters through the definition of two projector operators. This result can be found in the original paper Ref. [22], but an more extensive discussion is done in Ref. [93]. Applying this form of S into (6.21) one gets:

$$\begin{aligned} \frac{1}{2}[S,H_1] \approx \sum_{k,k',\sigma,\sigma'} \Big\{ & c^\dagger_{k,\sigma} f_\sigma f^\dagger_{\sigma'} c_{k',\sigma'} \left[\frac{1}{\epsilon_k - \epsilon_f - U} + \frac{1}{\epsilon_{k'} - \epsilon_f - U} \right] + \\ & + f^\dagger_{\sigma'} c_{k',\sigma'} c^\dagger_{k,\sigma} f_\sigma \left[-\frac{1}{\epsilon_k - \epsilon_f} - \frac{1}{\epsilon_{k'} - \epsilon_f} \right] \Big\} V^*_{k,f_\sigma} V_{k',f_{\sigma'}} (n_{f_\uparrow} - n_{f_\downarrow})^2. \end{aligned} \tag{6.23}$$

The last squared term plays the role of a projector on the $n_f = 1$ subspace, so the effective interaction will operate only on that sector. The first two terms describe the effect of the virtual processes

$$c + f^1 \quad \rightarrow \quad f^2 \quad \rightarrow \quad c + f^1,$$

while the second two represent the virtual processes

$$f^1 \quad \rightarrow \quad f^0 + c \quad \rightarrow \quad f^1.$$

Other terms appear in the calculation, but they can be neglected or reabsorbed into redefinitions of the parameters, *if we assume that* $|\epsilon_f|, U \gg 0$, i.e.

if the system is in the local moment regime and if there is a large separation between the low and high energy sectors. Of course the sums take into account all the possible channels of these processes. By rearranging the fermion creation and annihilation operators, (6.23) can be rewritten as

$$H_{int} = \sum_{k,k'} J_{k,k'} \mathbf{S}^{\mathbf{c}}_{\mathbf{k},\mathbf{k}'} \cdot \mathbf{S}^{\mathbf{f}}, \tag{6.24}$$

where $\mathbf{S}^c$ and $\mathbf{S}^f$ are the spin operators of the conduction and f-electrons respectively, defined as

$$\mathbf{S}^{\mathbf{c}}_{\mathbf{k},\mathbf{k}'} = \frac{1}{2} c^{\dagger}_{k,\sigma} \vec{\tau}_{\sigma,\sigma'} c_{k',\sigma'}, \qquad \mathbf{S}^{\mathbf{f}} = \frac{1}{2} f^{\dagger}_{\sigma} \vec{\tau}_{\sigma,\sigma'} f_{\sigma'},$$

with $\vec{\tau}$ the vector of the Pauli matrices.

The dominant virtual processes occur close to the Fermi surface, so we can approximate $k \approx k' \approx k_F$ and $\epsilon_k \approx E_F$. Therefore if we put $E_F = 0$ (consistently with the convention chosen at the beginning of this section), we can approximate the k, k' dependent interaction by:

$$J = J_{k_F,k_F} = -2|V_{k_F,k_F}|^2 \frac{U}{\epsilon_f(\epsilon_f + U)}.$$

Imposing the symmetric condition $U = -2\epsilon_f$ on the Anderson model, one gets

$$J = J_{k_F,k_F} = -2|V_{k_F,k_F}|^2 \frac{U}{-\frac{U}{2}(-\frac{U}{2} + U)} = 8\frac{|V_{k_F,k_F}|^2}{U},$$

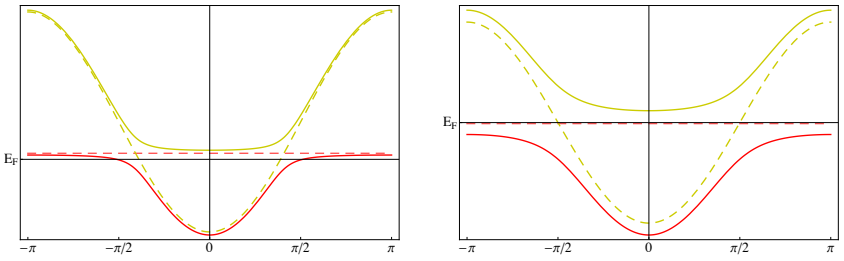
that is the result cited numberless times in the KL literature.

Of course these results were found for the impurity Anderson model, however they can be generalized straightforwardly to the PAM also, leading to the same relation [22, 77]. It must be remembered that this result holds in the limit of high U and it becomes exact when $U \to \infty$. In taking the limit V has to scale as $\sqrt{U}$, in order to obtain a finite J. Though this is an expansion in V, it creates no problems because the higher order commutators in in (6.20) are suppressed by higher powers in U, therefore they have no contribution, if V diverges as prescribed [77]. In principle J could take any value if $V \to \infty$, but in any meaningful system this condition is never fulfilled. A recent numerical study [149] investigated the limits of this condition and showed that there exist a maximum J that cannot be exceeded. In fact, for the Schrieffer-Wolff transformation to be valid, the system has to be in the local moment regime. As it has been discussed, this requires a fine balance between the parameters U, ϵ_f and V. In particular there a exist critical value U_c below which the system is in the mixed valence regime for any ϵ_f. The numerical (Gutzwiller) analysis [149] shows that the critical U_c follows the relation

$$\frac{U_c}{W} \approx 62.56 \left(\frac{V}{W}\right)^{1.54},$$

where W is the conduction electrons bandwidth.[10] Hence for each V there exists a maximum coupling J_{max} that cannot be further increased, because the necessary decreasing of U would imply the transition into the mixed valence regime.

[10]The study was performed assuming a constant density of states. The latter is the only free parameter in the Gutzwiller study incorporating all the properties of the lattice.



(a) *Heavy fermion band structure.* **(b)** *Kondo Insulator band structure.*

Figure 6.2: *The typical band structure of the non interacting PAM. (a) the Fermi surface cuts the f-like band, implying an high effective mass for the Landau quasiparticles; (b) the chemical potential is set inside the gap, so the system is insulating. In both the picture the bands are doubly degenerate and the dashed lines are the original (not hybridized) bands.*

Heavy fermion compounds

Before continuing on the detailed description of the Kondo lattice, I thought appropriate to explain what is the new and exotic physics is exhibited by the KL and the PAM Hamiltonians. These systems are often named as *heavy fermions compounds*. The name comes from the fact that these systems manifest unusual properties, that fits well with the Landau-Fermi liquid picture, but only under the assumption that the effective mass of the carriers is two or three order of magnitudes larger than the bare one. The validity of the Fermi liquid picture, means that the physical quantities follow some phenomenological behavior that is explained by the assumption that the system is well described by Landau's quasiparticle argument. These quantities are: the specific heath C_V, the spin susceptibility χ and the compressibility $\kappa \propto dN/d\mu$, with N the total number of particles and μ the chemical potential; all of them are proportional to the effective mass of the fermionic Landau's quasiparticles, that in turn is proportional to the density of states at the Fermi surface.[11] A detailed discussion can be found in Ref. [104, 154], however it is typically said that a system has a behavior consistent with the Fermi-liquid phenomenology if $C_V \propto m^* k_F T$ at $T \ll T_F$, $\chi \propto m^* k_F$ and $dN/d\mu \propto m^* k_F$, where the last two proportionality constants hide the information of the Landau structure factors (homogeneous antisymmetric and symmetric respectively), besides various physical constants, and k_F is the Fermi momentum. The extremely high value of the mass in the heavy fermion compounds, indicates an extremely high density of states $\nu(E) = d\Omega(\epsilon)/d\epsilon|_E$ at the Fermi surface, where $\Omega(\epsilon)$ is the number of quantum states that are available at the energy ϵ. Of course this quantity can be rewritten in terms of the dispersion laws; in one dimension, where typically there are only a discrete number of states per energy value ϵ, the density of states is proportional to the inverse of the derivate of the dispersion law (or sum of the derivates in more complicated cases). So, in one dimension, the high effective mass can be explained as the consequence of the presence of an almost flat band.

[11] Of course the Landau-Fermi liquid picture assumes the existence of a Fermi surface, i.e. of a discontinuity in the occupation number of the quantum states in the Brillouine zone.

In terms of the PAM this is easily understood: indeed the f-impurity fermions form a flat band. These fermions develop dynamic thanks to the hybridization with the conduction electrons, which changes the shape of the band and redefines the particles that contribute to the quasiparticle of the Landau-Fermi liquid. Putting the interaction term U to zero in (6.3), this mechanism is quite straightforward. In Fig. 6.2a are shown some examples of the typical shapes, for the 1d band structures, that can be obtained. As can be seen a gap, proportional to the hybridization, develops. The bands have an *avoided crossing* structure and the analysis of the eigenvectors shows how both the bands contains eigenstates with both c- and $f-$character. As a rule of thumbs, one can use the distortion of the bands, respect to the original ones, as an indication of the hybridization and the nature of the states: the more a band looks like an original one, the less hybridized those states are. Clearly the maximum of the hybridization happens when the cosine-like curve turns into a flat one.

The location of the chemical potential and of the original flat f-band can greatly affect the physical properties of the system. In fact, if the chemical potential is set in the gap, then the system is insulating. Instead if the Fermi level intersects the lower band (or upper) the system is clearly a Fermi liquid, but evidently the incredibly high density of states implies an incredibly high effective mass.

In the context of the PAM with $U = 0$, the scenario is quite clear. The situation becomes very much different if the interaction is turned on and (for example) sent to infinity. Then, of course, the role (and meaning) of the bands used so far becomes ambiguous and different approaches must be followed (for example the numerical Gutzwiller projection method). The challenge is of course to give a description of these heavy fermion compound only in terms of the degrees of freedom of the KL, without considering the high energy physics of the valence fluctuations of the f-electrons.

These heavy fermion compounds, both in the the KL and mixed valence limit, can describe systems with many different properties. For example, if we assume that the final density of state of the KL system will have a shape like the one associated to the bands in Fig. 6.2b, then it is easy to understand that putting the chemical potential in the gap, the system will be an insulator, or better a *Kondo insulator*. This happens in the 1dKL at half-filling and high Kondo coupling, as will be explained in Sec. 6.3.4 and both paper C and paper D. Anyway the simplified picture given by the four band structure of Fig. 6.2a does not typically apply. To understand what happens changing the chemical potential (and the coupling) is the challenge posed by the analysis of the phase-diagram of the 1dKL and the subject of paper C. A great amount of work has been done by the community to solve this problem; the known results will be introduced in the next section. As final note I would like to point out to the reader two interesting studies that show how wide the physics of the KL can be: the nature of the system can change so much that also (unconventional) superconductive phases can be discovered, at least in 2d and 3d systems [155, 156].

6.2 Competing effects in the 1dKL

So far it has been shown why the Kondo lattice is a meaningful model: it describes the interaction of conduction electrons with local spins that are the only active low energy degrees of freedom, remnant of electrons that have been localized by strong local interactions. From now on we can thus forget all the details of the previous derivation and just deal with the Hamiltonian (6.1) that I rewrite here, specializing it to the case of the 1dKL:

$$\begin{aligned} H &= -t\sum_{i,\sigma}\left(c^\dagger_\sigma(i)c_\sigma(i+1)+c^\dagger_\sigma(i+1)c_\sigma(i)\right)+ \\ &\quad +J\sum_i \mathbf{S^c}\cdot\mathbf{S^f}-\mu^*\sum_{i,\sigma}c^\dagger_\sigma(i)c_\sigma(i), \end{aligned} \tag{6.25}$$

One might expect that this problem, which as a matter of fact is just a particular case of the PAM problem, should have an easy solution. This is not the case. In fact the KL presents unique characteristics that put both our formal abilities and our theoretical comprehension at test.

First of all, the degrees of freedom involved in the Hamiltonian are not homogeneous, but belong to two different classes: fermions and spins. From a technical point of view the simultaneous presence of both these classes causes big complications. There exist many tools to treat spin systems and electron systems, but most of them fail (or have big troubles) to describe a system that contains both species. Techniques that are based on the fermionic nature of the operators, have trouble to deal with the spin operators, for which no Wick theorem exist. Tools that are instead used in the context of spins chains have a hard time dealing with the fact that there is no direct interaction between neighboring spins, since it is generated by the correlation between the electrons.

There exist two routes to avoid the pathologies of the different methods and to find a solution to the problem. The first is to introduce a (fictitious) interaction between neighboring spins. This interaction (that is physical and could definitively exist in real materials) creates a new scale in the system. If this scale is dominant, the interacting spin system and its modes (magnons) can be used as starting point in the description of the KL. The drawback is that in the end it becomes very complicated to get rid of this interaction, so the system analyzed is not really the Kondo Lattice model, but the "Heisenberg-Kondo lattice" model. The second possibility is to represent the spins in terms of other particles, for example Schwinger bosons or fermions, as is done more frequently, starting from the PAM and enforcing unit occupancy. Both these possibilities have the problem that it is difficult to implement the constraint on the extra particles, so it is complicated to assure the spin-1/2 character of the local moment: indeed these kind of constraints can typically be fulfilled only on the average and not on an operator level. Moreover, the use of extra particles implies the enlargement of the Hilbert space. This is reflected in the solutions also, that become more difficult to interpret. For example starting from the PAM and enforcing unit f-electron occupancy: the original theory is based on four bands (16-dimensional local Hilbert space), so it is clear that the final solution, after the imposition of the constraint, will also have four bands. The constraint will induce correlations between the fundamental modes and the fillings of the bands, making the final answer not very transparent. Another

drawback is the fact that in any study that starts from the PAM it is hard to guarantee the complete absence of any effect[12] due to charge fluctuations of the f-electrons, and consequently the fact that the results are due uniquely to KL physics [157]. From a formal point of view this means that the energy of the ground states obtained with this approach are not variational upper bounds for the real ground state energy.

These difficulties still represent a serious obstruction in the solution of the KL. For the 1dKL the late nineties had to arrive, before a program of characterization of the phase-diagram was carried out successfully [158]. While for the 2dKL and the 3dKL, although some very interesting effects are subject of debate [103, 133, 159–164], we are still far from a complete characterization of the phase diagrams.

The core of the KL problem is the intimate relation that exist between electrons and spins. In principle, the entanglement between the two species does not allow for a neat separation of these two degrees of freedom and therefore it becomes impossible to look at one part of the system, without considering also the other. Because of this, a perturbative analysis in the limit $J \to 0$ becomes conceptually wrong: in fact the point $J = 0$ is a singular point where not just the interaction, but also the entanglement between the two species is zero. Therefore the $J = 0$ ground state, where the spin system has an extremely high degeneracy (entropy), cannot be used as starting point for a perturbative analysis [150,165]. Despite this, the first considerations on the nature of the KL ground state were carried on in a perturbative fashion, assuming that at small J the effect of the entanglement is small and that a strict separation between electrons and spins holds, while just for larger interactions this assumption becomes wrong. This was the idea behind Doniach's proposal in 1977 [134]. He assumed that in the systems two regimes were in competition; one where the two species can be thought of as separate and the other when the entanglement plays a decisive role. In the first regime the electron-spin interaction term would simply drive the establishment of an RKKY interaction (see Sec. 6.2.1) between the local moments of the lattice, leaving the electron wavefunction approximately untouched; in the second regime instead another kind of physics is the dominant one: the Kondo physics (see Sec. 6.2.2), responsible for the entanglement and implying a drastic change in the structure of the ground state wavefunction. A comparison between the typical energy scales of these two effects enables one to draw the *Doniach phase-diagram*, shown in Fig. 6.3.

This description works well in 2d and 3d KL around half-filling. Indeed it has been proved experimentally that the system passes from one regime to the other via a quantum phase transition [103,133]. In 1d instead it does not work; only at half-filling it does give a qualitative description of the physics, but not as good as in the higher dimensional cases. In particular no quantum phase transition occurs [158]. The peculiarity of the 1d case can find an explanation in the low dimensionality, and therefore the enhanced importance of quantum fluctuations. Moreover, another complication should also be considered. In the 1dKL the ferromagnetic phase is dominant in the phase diagram (covering the majority of it, see Fig. 6.7). Such ferromagnetism is not explained by means of RKKY interaction, but can be instead understood in terms of the double exchange

[12] With this we mean effects due to not instantaneous charge fluctuations. Of course the virtual high-energy (and therefore instantaneous at the time scale of the KL) are necessary to produce the Kondo coupling.

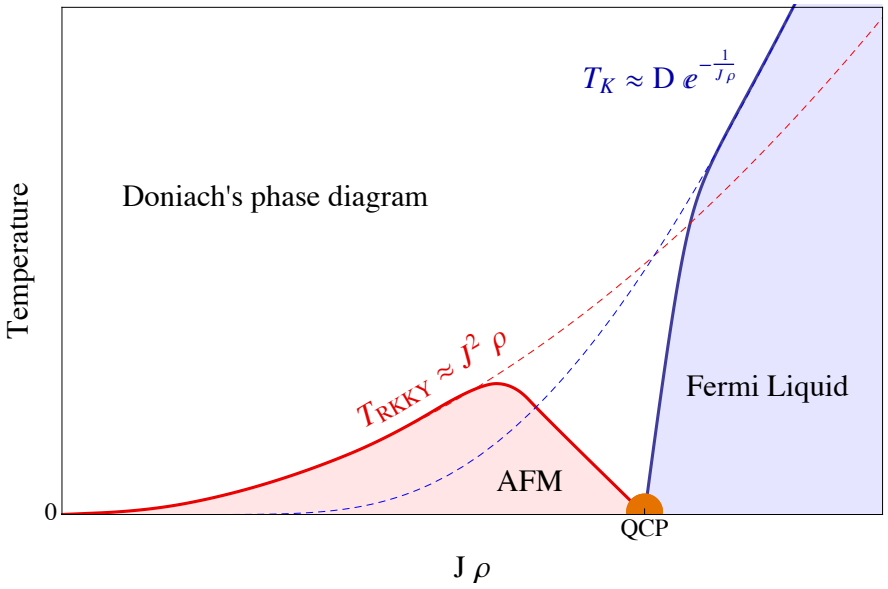


Figure 6.3: *Sketch of Doniach's phase diagram. The two typical energy scales of the RKKY and Kondo effect compete. Reducing the temperature the physics is dominated by the effect with the highest energy scale, while the lowest one plays the role of a perturbation. Where the two scales become very similar a quantum phase transition at zero temperature takes place at the critical point QCP. The "funnel shaped" white region above the QCP is the zone at non zero temperature, affected by the quantum critical behavior.*

effect (see Sec. 6.2.3). A discussion about the relevance of this effect in higher dimension is lacking, because no systematic investigation of the existence of a ferromagnetic phase in the 2dKL and 3dKL has been carried out. Only recently has this topic raised some interest [146,166], but it is still in a preliminary stage.

So far we did not mention a quite important conceptual complication that the KL hides. There exist a rigorous theorem, known as "Luttinger theorem", that says that the volume encapsulated by the Fermi surface depends only upon the density of the electrons. In one dimension it means that the value of the Fermi momentum k_F is proportional to the number of electrons in the system. The question is: "*which electrons?*". In the KL the only electrons are the conduction electrons. But in real compounds the KL represents the low energy physics of the PAM and the two Hamiltonians are adiabatically connected, so it would seem more correct to count the number of c-electrons together with f-electrons. The experiments say [103, 104, 133] that both scenarios apply to the KL where there exist a transition between two regimes: one characterized by a large Fermi surface, where it is the total density of the f- and c-electrons that determines the Fermi volume, and another with a small Fermi surface, where instead it is only the density of the c-electron that matters. How it is possible to justify the Luttinger theorem in the context of the KL, without referring to the PAM, is still source of debate [103, 104, 133, 159, 161, 162, 167–170]. In particular the problem becomes really intriguing if one remembers that the spins could have also nuclear origin.

In the 1dKL most of the phase diagram is characterized by a small Fermi surface, in the phases where a long range or quasi-long range order is present. A large Fermi surface appears in the so called "polaronic liquid" that will be discussed later. Although the work done in the manuscripts C and D does not tackle directly the problem of the size of the Fermi surface, the results contained in paper C shed some light on the low energy interpretation of this Fermi surface collapse, in the sense that the picture that is obtained is consistent with the polaronic liquid one.

To give the reader the possibility to understand the phase diagram of the 1dKL I will dedicate the next sections to the discussion of the three main relevant effects mentioned previously: RKKY interaction, Kondo effect and double exchange.

6.2.1 RKKY Interaction

The concept of RKKY interaction appeared for the first time in the context of magnetic ordering of nuclear spins in metals [135–137]. It is obtained as a second order effect in the coupling constant between the spins and the electrons. The idea is that a spin impurity will polarize the surrounding electron medium, causing an unbalance between the densities of the up and down electrons. These oscillations goes under the name of Friedel oscillations (see Ref. [93]) and can evidently be felt by the other spin impurities embedded into the system. The final effect is that of an effective spin-spin interaction between the impurity spins.[13] The spin polarization of the electron medium is simply the response of the electron liquid to an external perturbation, therefore it is determined by a response function. It is typically assumed that the dynamics of the electrons is much faster than the dynamics of the spin impurities, which as a consequence can be thought of as static; therefore the relevant spin-susceptibility will be the static one. The interaction is magnetic and couples with the spin of the electron, therefore the magnetic response of the electron system is (in linear response approximation and under the assumption of isotropy):

$$\langle M_a(\vec{x})\rangle = -J\chi_{ab}(\vec{x}-\vec{x}')\langle S_b^f(\vec{x}')\rangle, \tag{6.26}$$

where the minus comes from the fact that for antiferromagnetic interaction $J > 0$ one wants antiparallel directions for the two vectors $\mathbf{M}$ and $\mathbf{S^f}$. The definition of the non-local spin dynamical (retarded) susceptibility is

$$\chi_{ab}(\vec{x}-\vec{x}', t-t') = i\langle[\sigma_a(x,t), \sigma_b(\vec{x}', t')]\rangle\theta(t-t'), \tag{6.27}$$

By standard arguments[14], there exist a relation between the Fourier transform of the latter quantity and the Fourier transform of

$$\chi^T_{ab}(\vec{x}-\vec{x}', t-t') = (-i)^2\langle \mathrm{T}\,\sigma_a(x,t)\sigma_b(\vec{x}', t')\rangle = \delta_{ab}\chi^T(\vec{x}-\vec{x}', t-t'), \tag{6.28}$$

[13] This treatment follows Ref. [93] that I suggest the reader to consult for more details.

[14] The time ordered propagator $\chi^T(\omega)$ has poles at $\omega = \omega_e + i\mathrm{sign}(\omega_e)\delta^+$ just above or below the real axis, while the (retarded) dynamical response $\chi(\omega)$ function has poles only below the real axis $\omega = \omega_e + i\delta^+$, where in both cases ω_e is energy of the excitation. It is thus evident that if the poles of $\chi^T(\omega)$ are shifted downwards, then in the limit of $\delta^+ \to 0$ the two functions will be identical (modulo different prefactors in the definitions, that have to be adjusted).

with T the time ordering operator and the $(-i)^2$ comes from the fact that the σ operators are quadratic in the fermions. The relation is

$$\chi(\vec{q},\omega) = \mathrm{Tr}\left[\chi_{ab}(\vec{q},\omega)\right] = -i\chi^T(\vec{q},\omega+i\delta). \tag{6.29}$$

This is very convenient because (6.28) is easily computed using Feynman diagrams, giving as result

$$\chi^T(\vec{q},\omega) = -2i\int_{\vec{k}} \frac{f(\epsilon_{\vec{k}+\vec{q}}) - f(\epsilon_{\vec{k}})}{(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}) - \omega}, \tag{6.30}$$

so using the previous relation and in the limit of static response $\omega \to 0$:

$$\chi(\vec{q}) = 2\int_{\vec{k}} \frac{f(\epsilon_{\vec{k}}) - f(\epsilon_{\vec{k}+\vec{q}})}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}}. \tag{6.31}$$

A second spin impurity located in $\vec{x}$ will interact with the magnetization of the electron gas in the same way, so

$$H_{spin-spin} = J\,\mathbf{S^f}(\vec{x})\mathbf{M}(\vec{x}) = -J^2\chi(\vec{x}-\vec{x}')\mathbf{S^f}(\vec{x})\mathbf{S^f}(\vec{x}'). \tag{6.32}$$

The effective interaction $J_{RKKY}(x-x') = -J^2\chi(\vec{x}-\vec{x}')$ is the RKKY interaction. It has been computed for every dimension in Ref. [171], but the original results in three dimensions can be found in Ref. [135–137]. In the first studies the form of the interaction was found analyzing the effect of the spin-spin coupling at second order in perturbation theory. Of course there is no difference in the final result; in fact it is clear that (6.31) describes the perturbative effect of particle-hole excitations created by the scattering against the spins.

The form of the RKKY interaction in 1D is

$$J_{RKKY}(r = x - x') = -\frac{J^2 m}{2\pi}\left[\mathrm{Si}(2k_F r) - \frac{\pi}{2}\right] \tag{6.33}$$

in real space and

$$\begin{aligned} J_{RKKY}(q) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} J_{RKKY}(r)e^{iqr}dq \\ &= -\frac{8J^2 m}{q}\ln\left|\frac{q-2k_F}{q+2k_F}\right| \end{aligned} \tag{6.34}$$

in Fourier space (see Fig. 6.4). To find these results it is necessary to assume that the dispersion of the electrons is approximated at ϵ_F by a parabola $k^2/2m$. The function in Fourier space is found directly from (6.31) and it is known as the Lindhard function, while the function $\mathrm{Si}(z)$ is the Sine Integral function:

$$\mathrm{Si}(z) = \int_0^z \frac{\sin(t)}{t}dt.$$

The Lindhard function has a weak logarithmic divergence at $q = 2k_F$. This is the sign of a magnetic instability [172], therefore a system with RKKY interaction should develop magnetic order with a typical momentum $2k_F$. This is not the case in 1d because the quantum fluctuations are strong enough to suppress

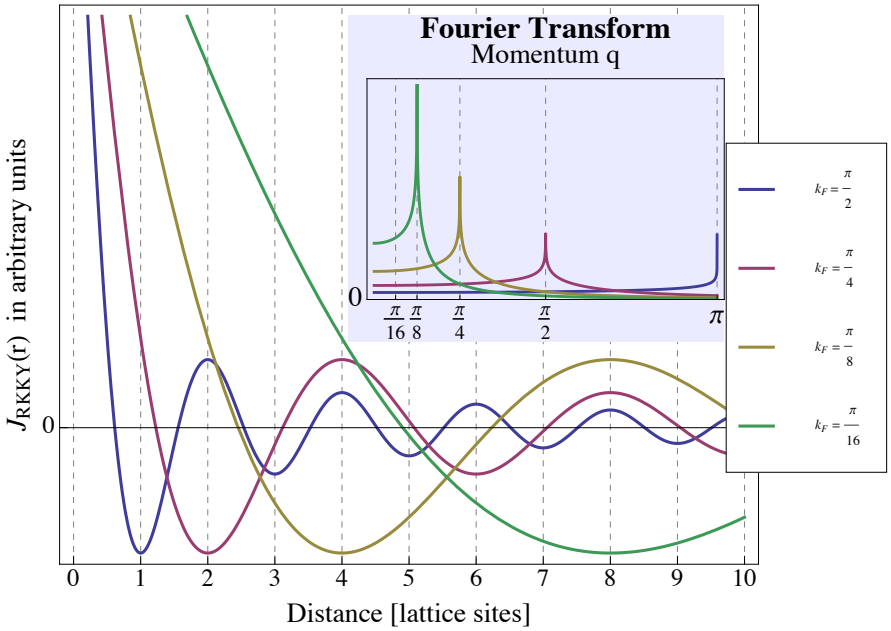


Figure 6.4: *The RKKY interaction $J_{RKKY}(r)$, plotted as function of r for different values of k_F. The gridlines are put in correspondence of the lattice sites. The Fourier transform of the same curves is plotted in the inset, for momenta $q > 0$. Evidently the peak is at $2k_F$; it must be specified that the system is at half-filling when $k_F = \pi/2$.*

ordering. The reader could think that this is a consequence of the Mermin-Wagner theorem that forbids any symmetry ordering in 1d for any temperature. This is not the case, because the RKKY interaction is long range and therefore it is *not* covered by the Mermin-Wagner theorem that is limited to short range interactions. In fact the asymptotic behavior of function $J_{RKKY}(r)$ is given by $\cos(2k_F r)/r^3$. The lack of spin order in 1d and 2d RKKY systems has been proved in a rigorous way only in 2011 [173].

6.2.2 Kondo effect

Considering the vast literature on the topic (in particular Ref. [78]) it is not necessary to write a detailed presentation of the Kondo effect. I will instead focus the attention on the points that are functional for the continuation.

Let us consider a system where only one f-impurity is present. In section (6.1) it has been shown that in order to obtain a local moment, the energy of the single occupied state should be pushed far below the Fermi energy. In this system the valence fluctuations of the f-electron are forbidden and only virtual excitations can occur. The effect of the virtual excitations is summarized in the low energy Hamiltonian by the electron-spin interaction, equation (6.24). As it has been mentioned this interaction entangles the conduction electrons and the impurity spin, that gets quenched and perfectly compensated at low temperatures. Consequentially the final state is paramagnetic and one can think of it

as if the conduction electrons, that continuously scatter against the impurity, effectively accumulate around it generating a sort of spin polarized "cloud" that forms a spin singlet (if $J > 0$) with the local impurity, screening completely the impurity. This phenomenon is known as the Kondo effect.

The japanese physicist Jun Kondo was the first [174] to shed some light on this kind of physics, convincing the world about its existence in 1964. However the full understanding and characterization of the Kondo effect required many years of work and needed also the elaboration of the new fundamental concept of Renormalization Group (RG) by Wilson and Anderson [150, 175].

Kondo discovered that, considering the third perturbative order of the scattering of the electrons on the single spin impurity, it was possible to justify the existence of the resistivity minima found experimentally at low temperature in many conductors [78, 133]. His solution was not perfect, because it predicted a divergence for the resistivity at $T \to 0$, but this pathology was initially considered just a feature of used approximations. Many tried to improve the results, using more precise perturbation expansions, and in particular Abrikosov played a valuable role in the development of the re-summation techniques needed in this problem [78]. However the pathology remained and in particular the typical temperature scale where every expansion broke down was identified:

$$T_K \approx D e^{1/2J\rho_0}, \tag{6.35}$$

where D half of the bandwidth of the conduction electrons and ρ_0 is the density of states at the Fermi level.

The failure of the perturbative approach in the Kondo model is often introduced as a mystery (as it was historically) [78]. Now that the solutions are known we can say that this failure was no mystery at all, indeed it is its success at $T > T_K$ that is surprising. For these (high) temperatures in fact, the electrons and the impurity spins are free and independent from each other. With a not so inappropriate choice of words, we could say that electrons and spins are asymptotically free at high energies. This (very non-trivial) high-energy freedom is the reason behind the success of the perturbative approach at high temperatures: in that regime the non-interacting electron and spin states are convenient degrees of freedom for the representation of the physics, and the interaction can be though of as a correction that causes only small modifications. Below T_K instead they represent a very poor choice; the structure of the ground state changes so much that it is not possible to consider the effect of the interaction as small and therefore the perturbative approach fails. Increasing the temperature a sort of deconfinment of the particles is realized, that at a critical temperature regain their "freedom" destroying the bound state (resonance) that they were forming.[15]

The cause of confusion and problems is that the Hamiltonian of the Kondo model, i.e. the one-site impurity analogous of (6.1)-(6.25), is already written in terms of the high-energy degrees of freedom. This does not mean that it does not describe the low-energy physics, but that it gives of it a very inconvenient representation, so finding any result in the low energy regime becomes extremely complicated. In terms of RG we can say that the free electrons and spins are the eigenstates of the high-energy fix-point Hamiltonian. This fix-point is

[15] This reminds concepts coming from fundamental physics. For a comparison between quark and Kondo physics the reader can start from Ref. [176].

unstable under reduction of the energy scale, therefore the Hamiltonian flows towards a second (infrared stable) fix-point Hamiltonian at low energy, described by completely different eigenstates. The energy T_K represents the cross-over temperature between these two regimes, where one or the other Hamiltonian are good approximations. Curiously both fix-points are Fermi liquid fix points [177].

The temperature-induced freedom of spin and electrons is due to the fact that the Kondo effect is caused by a coherent scattering of the conduction electrons against the impurity spin. This process creates a resonance (the low energy bound state cited previously) at the Fermi level, that was discovered by Abrikosov and Suhl [178] in 1965 and that is now called the "Kondo resonance". The reader should pay attention to not confuse this resonance with the previously discussed (6.7), that was generated by valence-fluctuations, i.e., the excitation of the f-impurity by adding or removing a valence electron. That resonance is located deep into the conduction band, or even below it. Conversely the Abrikosov-Suhl-Kondo resonance does not involve any valence fluctuation (if not in terms of the virtual excitations introduced previously in the discussion of the Schriffer-Wolff transformation), but only the process of spin-flipping of the local spin. Because of the degeneracy of the two spin states, this flipping process has no energy cost; moreover it is evident from (6.24) that each flipping requires the creation of a particle hole pair, so we should expect that the main contribution to the flipping process comes from the electrons close ($\pm T_K$) to the Fermi surface that will be the only ones affected [157, 179]. Because of these reasons it is straightforward to understand that the Kondo resonance will be localized at the Fermi surface, independently upon the energy of the f-state.

With the same line of thought, it is also possible to understand that the width of the resonance will be related to T_K. The resonance represents the bound state of the impurity spins with a collective mode of the Fermi liquid, particularly pronounced at the Fermi surface. Since this is an effect due to the coherent flipping of the impurity spin, induced by the scattering of the conduction electrons, it is clear that if the incoherent flips due to thermal fluctuations become too frequent, then the coherency gets lost and the resonance stops to exist. So T_K fixes the time scale for the critical decoherence. The width gives an approximative idea of the (inverse) life-time of the resonance, i.e. crudely speaking the average time that an electron needs to "escape" from it, or in other words the time needed to loose coherence with the spin because of the hybridization with the rest of the system. Therefore the width of the resonance is approximately given by T_K.

Wilson's numerical RG enabled the exploration of the physical properties below T_K, but wasn't able to give a clear picture of what happens at that scale of energy. It was Nozieres [177] that understood what the structure of the low-energy fixed point at $T \to 0$ is, by realizing that it is described by the Hamiltonian with $J = +\infty$. In this case the problem is simplified because one obtains that one electron gets localized into an unbreakable singlet configuration with the spin on the impurity site. When relaxing the assumptions and assuming the possibility of virtual excitations of this local Kondo singlet, Nozieres found a form for the Hamiltonian of the electron liquid, expanding in t/J. The elastic scattering of the electrons against the Kondo singlets causes an effective interaction among the particles. This effect appears at the fourth order, as a repulsive t^4/J^3 density-density interaction on the sites close to the impurity. Considering higher orders, other sites get involved in the interaction.

This describes the delocalization of the electron involved into the singlet, that becomes increasingly delocalized decreasing J. In this way the screening cloud gets formed.

Clearly the final picture is that of a Fermi liquid of $N-1$ electrons, interacting with each other via a site dependent coupling, that is the effect induced by the scattering agains the Kondo singlet. The existence of the correspondence between the Kondo model and a Fermi liquid with local interaction is typically denoted as "local Fermi liquid picture".

The Kondo effect in the Kondo lattice: the exhaustion problem and the modern perspective on Kondo physics

Besides the important contribution in the understanding of the Kondo effect, Nozieres elaborated also an important critique [157, 179] to the straightforward application of the Kondo effect concepts to the KL. He pointed out that in the Kondo lattice the picture of a Kondo effect realized on each site is quite naive and leads to a problem named "Nozieres exhaustion". The problem can be stated as [180]: "*if T_K is the only energy scale of the problem, only electrons within T_K of the Fermi level are eligible to participate in magnetic screening of impurities [...] the number of such effective electrons is*

$$N_{eff} = \rho T_K \approx N_L \frac{T_K}{E_F} \ll N_L \quad ",$$

with N_L the number of sites, i.e. also the number of impurities. The consequence is that, if the requirement is that the Kondo effect is realized on each site (granting the existence of some sort of paramagnetic global Kondo singlet), then an extremely small number of electrons has to screen an incredible higher number of impurities. Though conceptually possible, the practical realization of such a coherent screening phenomena seems quite improbable. Moreover also the concept of screening cloud is dubious in the context of the KL. In fact the screening cloud should extend spatially over many lattice sites $l = v_f/T_K \approx aE_F/T_K$, so in materials with dense Kondo impurities interference effects should be prominent. So far no experiment ever revealed such effects [133, 157, 180].

A first attempt to solve the problem was performed by Nozieres himself [157], suggesting the existence of a second energy scale, the *coherence Temperature* $T_c \ll T_K$, that would have been the typical temperature necessary for the formation of the coherent Kondo singlet in the lattice. However successive studies [181, 182] demonstrated that T_K remains the only characteristic temperature in the KL. These results can hardly be understood in terms of the standard arguments explained so far [180].

A radically different point of view has been recently proposed by Coleman [133], who considered the possibility that something conceptually wrong is present in the "traditional" picture of the Kondo effect. The conceptually wrong step is to consider as important for the screening only the electrons close to the Fermi surface, instead of all the conduction electron states. This would imply that also the "screening cloud" concept is wrong, or better, it is valid only far from the impurity, where the electrons close to the Fermi surface (i.e. low energy electron-hole scattering states) do rule the physics. This topic is still quite controversial and not everybody agrees on the latter proposal, although it solves the aforementioned conceptual problems and generates a meaningful

background to study the physics of heavy electron compounds (see the vast literature, for example Ref. [103, 133, 160–162, 164, 169, 170, 183]).

The transformations generated in the Papers C and D are conceptually very similar to this latter proposal [133], so I will return to the topic later in Chapter 7. After familiarizing us with the concept of Kondo effect, it is appropriate to continue explaining the third most important effect in the Kondo lattice: the double exchange mechanism.

6.2.3 Double exchange

Double exchange is a mechanism that occurs in metals when propagating electrons are present besides the local spins, and there exist a local interaction between the hopping electrons and the local spins. It is clear that the KL describes this situation perfectly. Naively the effect can be explained as follows: because the electrons like to hop conserving their spin (coherent hopping), then the energy of the ground state will be lowered if two neighboring spin are ordered ferromagnetically (in the absence of direct spin-spin antiferromagnetic interaction). Evidently the latter conclusion is independent upon the sign of the local electron-spin interaction J, a fact that stresses even more the kinetic origin of this spin-spin correlation. It is therefore clear that this mechanism is very different from the RKKY interaction. In the double exchange it is in fact the kinetic energy of the electrons that is optimized by a specific spin ordered state and not vice-versa as in the RKKY, where the energy gain comes form the spin sector of the theory.

The double exchange was discussed for the first time by Zener [184, 185], in the context of manganese oxides compounds, trying to explain the correlation between ferromagnetism and electrical conduction empirically discovered in these materials. Later the microscopic explanation of the effect was formalized by Anderson and Hasegawa [186], in a two-site toy model. The mechanism proved itself valuable in the explanation of some features of magnetic crystals, as was shown by deGennes few years later [187]. In these original works the local spins were treated in a semiclassical (high S) approximation and the local electron-spin interaction was considered ferromagnetic because of Hund's rule (the possibility to have local antiferromagnetic coupling would have been discovered 10 years later, when Anderson discussed the local moment formation, as introduced previously). Under these assumptions, one discovers that the hopping term of the electrons (obtained by direct evaluation of the overlap integrals [186]) develops a parametric dependence on the relative orientation of two consecutive local spins, expressible as [148, 187]:

$$\tilde{t}_{ij} = t_{ij} \cos(\theta_{ij}/2),$$

where t_{ij} was the original hopping matrix and θ_{ij} is the relative angle between the two neighboring spins. Evidently the energy gain due to the delocalization of the electron can be penalized or even cancelled in the extreme case of $\theta = \pi$. From this discussion one immediately understands that, in order for the double exchange to be relevant, the spin impurities must be dense inside the system. Therefore it is an effect relevant in the case of the Kondo lattice, but not in the case of dilute magnetic impurities embedded in a metal.

The name "double exchange" is quite unfortunate. In fact it was clear from the very beginning that this mechanism is quite different from the other ex-

change effects that normally appear in magnetism [186]; in particular it cannot be written as a direct interaction between spins. This difference comes from the origin of the correlation between the spins. In magnetic materials it is typically assumed that the relevant low-energy degrees of freedom, are only those of the quantum spins on each site. These spins must have local origin and therefore come from electrons that are localized[16] by some kind of interaction (most of the cases the Coulomb interaction). The low-energy spin Hamiltonian for the magnetic system, i.e. the effective spin interactions, are thus generated by the original electron processes and derived from the genuine electron models. Depending upon the kind of high-energy process that cause the correlation between the electron states the low-energy effective spin-spin interaction is given different names and, more important, different signs. The typical effects discussed in magnetism are Coulomb exchange (Hund's rule), direct exchange and superexchange (both ferro and antiferromagnetic) [148, 172]. In the double exchange mechanism the scenario is different: the electrons that generate the correlation among the spins are not the same electrons that (after localization) generate the spins. This extra degree of freedom given by the motion of the electrons, creates a difference between the double exchange and all the other exchanges [186], implying the appearance of new physical effects (see Ref. [186, 187]), depending upon the specific circumstances considered.

In the KL the effect of double exchange is a bit more involved, because the spins are quantum 1/2-spins (while the semiclassical approach is valid only with spins where $S^2_{local} = s(s+1)$, $s \gg 1/2$) and the local coupling J is antiferromagnetic, causing the consideration of not only the triplet local state, but also of singlet one. In particular there exist a competition between double exchange ordering and formation of the local singlets. An analysis of the double exchange mechanism in the KL has been performed in Ref. [141, 142] on a two site KL with $J > 0$ and I report it here. The analysis of the two site model is meaningful because it highlights all crucial point, exactly as done in [186] for the $J < 0$ case.

Let us consider two spins-1/2 on two different sites on which one single electron is delocalized and with $J > 0$ and diagonalize the full Hamiltonian:

$$H_{2-sites} = -t \sum_{\sigma} \left(c^{\dagger}_{1,\sigma} c_{2,\sigma} + c^{\dagger}_{2,\sigma} c_{1,\sigma} \right) + J\, \mathbf{S^c_1} \cdot \mathbf{S^f_1} + J\, \mathbf{S^c_2} \cdot \mathbf{S^f_2}.$$

The interaction does not connect the sectors with different total spin projection, therefore the spaces spanned by states with $S^{tot}_z = 3/2$ and $1/2$ can be analyzed separately (obviously the symmetric spaces with $S^{tot}_z \to -S^{tot}_z$ are redundant). The physics in the $S^{tot}_z = 3/2$ is the one described by [186], and it is too high in energy if $J > 0$. The real ground state of the system must therefore lie in the $S^{tot}_z = 1/2$ subspace. Since the one electron Hilbert space is only 16 dimensional, the simplest thing to to is to write down the Hamiltonian in matrix form and diagonalize it. The lowest eigenvalue is

$$E_0 = -\frac{J}{4} - \frac{1}{2}\sqrt{J^2 + 2Jt + 4t^2},$$

[16] If this is not true, but the magnetic properties (typically very tiny) arise in a regime where the electrons are free, the phenomenon is called *itinerant magnetism*.

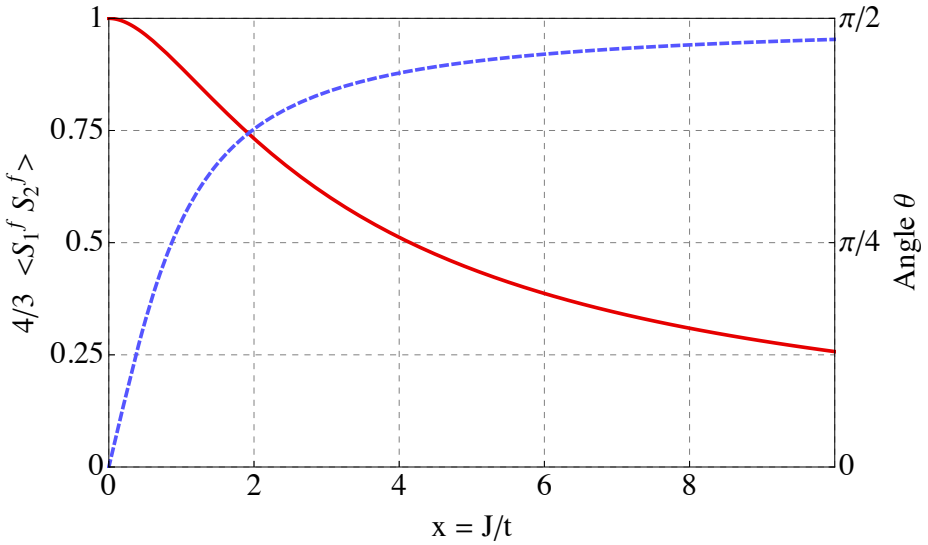


Figure 6.5: *The spin-spin correlation function of equation (6.37), red continuous line. The angle θ of equation (6.38), dashed blue line.*

with a ground state given by

$$Z|\psi_0\rangle = \sqrt{2}\Big\{|KS\rangle_1|\Uparrow\rangle_2 + |\Uparrow\rangle_1|KS\rangle_2\Big\} + \tag{6.36}$$
$$+\frac{t}{J/4-E_0}\Big\{|\downarrow\Uparrow\rangle_1|\Uparrow\rangle_2 + |\Uparrow\rangle_1|\downarrow\Uparrow\rangle_2 - |\uparrow\Uparrow\rangle_1|\Downarrow\rangle_2 - |\Downarrow\rangle_1|\uparrow\Uparrow\rangle_2\Big\}$$

where Z is a normalization constant and, among the two possible degenerate choices, has been chosen the state $S_z^{tot} = +1/2$. Here and in the rest of the manuscript the thick arrows represent the states of impurity spins, while the single arrow are the symbols for the occupied electron states (no thin arrow means that no electron is present). The states $|KS\rangle_i$ indicates the Kondo singlet state $(|\downarrow\Uparrow\rangle_i - |\uparrow\Downarrow\rangle_i)/\sqrt{2}$ on site i.

For $J/t \to +\infty$ the state in the first bracket will be the ground-state of the system, but in the opposite limit it will be the second bracket that dominates. It must be stressed that Kondo singlet components are present also into the second bracket and they must be separated out in order to make manifest the appearance of the double exchange ferromagnetic ordering. This linear combination of the Kondo singlets into the magnetically ordered solution is a recurring theme of the ferromagnetic physics in the 1dKL.

To make manifest the ferromagnetic order induced by double exchange it is appropriate to first compute the spin-spin correlations on the ground-state. The spin-spin correlation (plotted in Fig. 6.5) function is

$$\frac{\langle\psi_0|\mathbf{S_1^f}\cdot\mathbf{S_2^f}|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} = \frac{1}{4}\frac{3\cdot 2y}{y^2+2y+4} \quad \text{with} \quad y = \frac{J}{t} + \sqrt{\frac{J^2}{t^2} + 2\frac{J}{t} + 4}, \tag{6.37}$$

where the 3 comes from the sum over the three components.

It is clear that the more the Kondo singlet contribution becomes important, the less the ferromagnetism is pronounced. It is possible to compute the relative contribution of the singlet $|KS\rangle$ and ferromagnetic ordered $|FE\rangle$ parts on the ground state [141, 142], one gets

$$\begin{aligned} |\psi_0\rangle &= \sin(\theta)|KS\rangle + \cos(\theta)|FE\rangle \\ \tan(\theta) &= \sqrt{\frac{1}{2}}\left(x + \sqrt{x^2+2x+4} - 2\right), \quad \text{with} \quad x = J/t. \end{aligned} \tag{6.38}$$

Evidently the ferromagnetic component becomes dominant at small coupling. The double exchange is fundamental in order to explain the properties of the Kondo lattice model.

6.3 The 1dKL phase-diagram

Now that this long introduction has been done, it is finally possible to focus on the properties of the 1dKL. There are four parameters that control the system: the bandwidth W (i.e. $2t$ for nearest neighbor hopping), the coupling J, the conduction electron density n_c and the temperature T. In the following just the $T = 0$ case will be considered and in that case only two control parameters are needed: the ratio $x = J/t$ between the coupling and the kinetic energy of the electrons (from now on the adimensional parameter x and the parameter J will be indistinctly called *coupling*) and n_c, determined by the chemical potential μ^*. Following the literature I elaborated the phase diagram in Fig. 6.7. The main contributions to the determination of this phase-diagram come from [188–190], where the KL is solved making use of non-Abelian DMRG. These results have been confirmed using exact diagonalization methods [191] and Abelian DMRG [192]. A more detailed analysis can be found in Ref. [141, 142, 190].

In Fig. 6.7 I tried to schematically summarize all the main available results at once. As can be seen there are many ambiguous regions, where also the numerical approach has not yet given definitive answers. The analytical results are limited to few areas, but concentrated at half-filling. There exist five different regimes:

ferromagnetic metal: the blue area on the left that starts at $n_c = 0$ and $J = 0$ and stops at the paramagnetic black transition line;

the RKKY liquid: the paramagnetic red region extended close to $J = 0$ and extends up to the crossover towards the polaronic liquid region and the "wild" regions (these boundaries are still debated and not well determined [141, 142, 190]);

the polaronic liquid: the upper green part of the paramagnetic dome, delimited on left, right and top by two ferromagnetic phases and that crosses over to the RKKY liquid and "wild" phases on the bottom;

the strange ferromagnetic metal: the blue tongue of ferromagnetism inside the paramagnetic dome; its left and right boundaries (black thick lines) have been well characterized; its properties are similar to the other ferromagnetic metal;

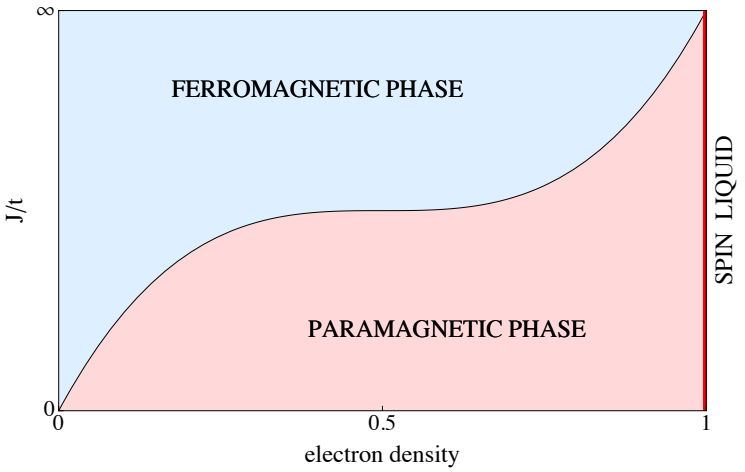


Figure 6.6: *Sketch of the shape of the phase diagram, from the late nineties. Reprinted figure with permission from Ref. [158]. Copyright 1997 by the American Physical Society.*

the "wild zones": the three yellow areas; the physics is not at all understood here, in particular between the ferromagnetic tongue and the RKKY liquid, where some pockets of ferrometallic phase have been discovered [141, 142, 190], suggesting the presence of complicated competitions between different phases;

the spin liquid: this phase behaves like a sharp singularity at $n_c = 1$ in the phase diagram; it is probably the most studied and most understood configuration of the model, although the intermediate parameter region (and therefore how the low coupling physics is connected to the high coupling one) is still unknown; it is considered a prototype of Kondo Insulator.

These phases will be shortly reviewed now, but before a very short historical introduction is necessary. The evolution of the knowledge of the KL phase diagram is quite interesting and rich of twists. The first convincing result was obtained by Fazekas and Müller [193] in 1991, using a mean-field approach. They considered the competition between the magnetically ordered phases and the formation of a *global Kondo singlet*, obtaining that the latter was dominating at coupling $x \gtrsim 0.6$; so no magnetic ordered was present above this critical value of the coupling. Below it instead, they found stable ferromagnetic (at low filling) and spiral spin-ordered mean field states mimicking at mean-field level the pseudo long-range order created by the RKKY effect. In the years after, it became clear that the mean-field result was not satisfactory, in particular at high coupling where it was demonstrated analytically that a ferromagnetic phase must appear [89, 194]. An important step towards the solution came from the Monte Carlo solution [195] of the KL at $n_c = 1/3$ and $2/3$ (where the sign problem is less pronounced). This study proved that ferromagnetism indeed exists in the KL, but is in a completely different region of the phase diagram, with respect to what was predicted by the mean-field approach. The work carried on in the following years, both with analytical and numerical approaches,

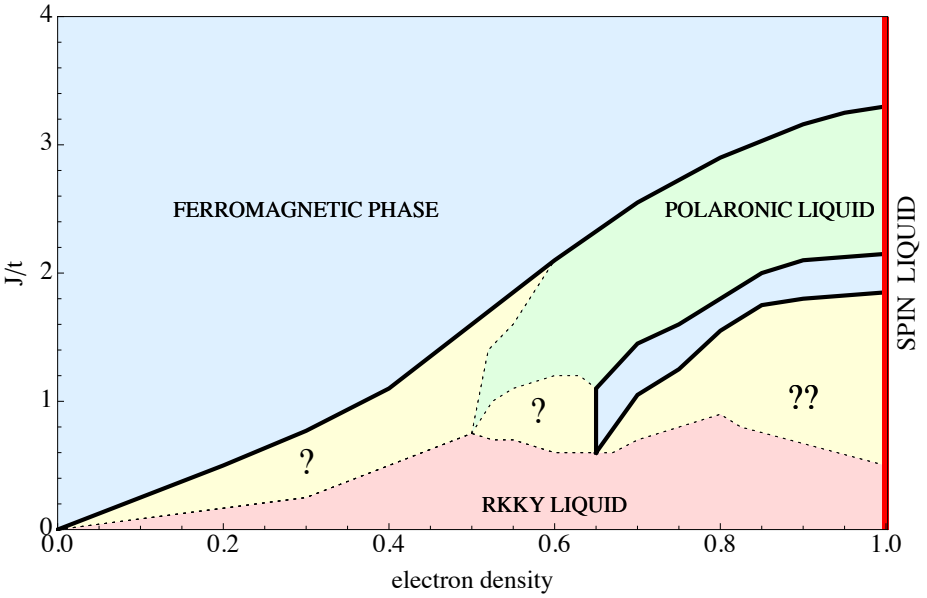


Figure 6.7: *A sketch of the phase diagram of the zero temperature 1dKL, elaborated from the data published in [188, 190]. The different colors represent different phases or regions. The ferromagnetic phase and tongue (light-blue), the polaronic liquid phase (light-green), the RKKY liquid phase (light-red) and the undefined "wild" regions (light-yellow). The thick red line at $n_c = 1$ represents the Kondo insultaing spin liquid phase. The thick dark lines that determines the ferromagnetic-paramagnetic transition are well characterized. The dotted lines sketch instead the boundaries of the zones where a determined phase exist. These boundaries do not have to be associated with any phase transition they just intend to give an idea of where a well determined phase degrades towards a "wild" still not well understood phase. The reader should be warned that close to half filling ($n_c \gtrsim 0.95$) the errors of the numerical simulations grew enormously, so that part of the phase diagram is not well understood. The details will be explained Sec. 6.3.3.*

produced the phase diagram [196] sketched in Fig. 6.6. Three phases are visible: ferromagnetic, paramagnetic and spin-liquid at half filling. This represented a good starting point for the works of the following years, and a review on the known properties up to this point can be found in Ref. [158].

After this blast of results the community had to wait for an important turning point, represented by the two works of Honner and Gulacsi [197, 198], who discovered how to conveniently bosonize the Hamiltonian of the KL away from half filling. Using this technique they elaborated a low-energy effective Hamiltonian for the spins, with which they characterized the ferromagnetic-paramagnetic transition line and the properties of the system close to the transition. The result contrasted with the known phase diagram Fig. 6.6, in particular it put an upper bound to the paramagnetic dome. This result found confirmation in the non-Abelian DMRG analysis carried on few years later [188–190]. A short review of all this kind of physics can be found in Ref. [141, 142].

The last twist in the story happened only in 2012. An interesting DMFT + NRG result in the infinite dimensional KL [146] suggested the existence of a strange "collaboration" between the Kondo effect and ferromagnetism; this "collaborative state" was named spin-selective Kondo insulator (SSKI) and it will be discussed later on. This mechanism represented a novelty in condensed

matter physics and stimulated some of the authors of the work to check if such a machanism was realized also in the 1dKL. The (surprising) results were published by Peters and Kawakami in late 2012 [192]. The SSKI turned out to exist also in one dimension, but (more important) it coincides with the ferromagnetic metallic phase that covers the majority of the KL phase diagram. To this contorted, never ending story the results of paper C add a small twist, that will be the subject of Chapter 7; here is instead more pertinent to continue with the analysis of the KL.

6.3.1 The ferromagnetic metallic phase

Any doubts about the existence of a huge ferromagnetic metallic region, that dominates the majority of the phase diagram, were washed away by two beautiful exact results obtained by Sigrist and collaborators [89, 199]. Those works treat the KL in the limits of infinitesimal density (one-electron only) and of extremely high coupling (perturbative expansion in $1/J$), discovering that in both limits the ground state of the system is ferromagnetic. These two results fixes the boundaries of a ferromagnetic solution that must propagate in the phase space until a magnetic phase transition occurs. The location of the phase transition will be the subject of the next section. Before that, let us first treat the two exact results in the extreme limits and the characterization of the ferromagnetic metallic phase, as done by Peters [192], will be discussed.

The high-coupling limit: the result obtained in Ref. [89] is based on a previous work by Lacroix [194], who noticed the formal and conceptual analogy between the $J = +\infty$ Kondo lattice and the infinite-U Hubbard model. The idea of Lacroix is strongly related to the concepts developed by Nozieres and his idea of "bachelor spins", introduced discussing the exhaustion problem [157, 179, 180]. Let us start from Nozieres picture of the 1dKL at half-filling and $J = +\infty$. The ground state can be obtained from (6.1) putting $t = 0$ and will be composed by a lattice of local Kondo singlets between an impurity spin and a conduction electron (see Fig. 6.8). To go away from half-filling some electrons have to be removed, i.e. some singlets must be broken and an equal number of spins left behind (named *bachelor spins*).

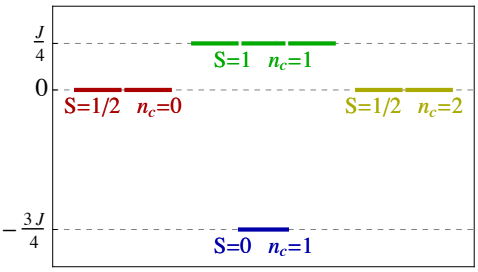


Figure 6.8: *The local quantum levels for $t = 0$ in the KL. S is the total spin, n_c the number of conduction electrons.*

Because of the hopping term the electrons in the Kondo singlets will try to delocalize, breaking their singlet, hopping on the unoccupied sites and forming a new singlet. Clearly this process does not increase the energy and can as well be seen as an effective hopping of the bachelor spins from site to site. Therefore the KL model at filling $n_c < 1$ can be mapped into a model of spin-1/2 holes (so spinful fermions) moving on a lattice, where the density of the holes is $n_h = 1 - n_c$. The only caution one has to take is that two spins cannot be on

the same site, so it is necessary to add an infinite Hubbard repulsion among the holes. The mathematical detail that has to be fixed is the relation between the hopping parameter of the Hubbard model and the parameters of the KL model. The infinite-U Hubbard model [200] can be written compactly as:

$$H_H = b \sum_{i,\sigma} \left\{ d^\dagger_{i,\sigma} d_{i+1,\sigma} (1 - n_{i,\bar{\sigma}})(1 - n_{i+1,\bar{\sigma}}) + h.c. \right\},$$

with b the hopping parameter and $d^\dagger_\sigma$ (d_σ) the creation (annihilation) operator of the spinful hole. Comparing the matrix elements between two states connected by nearest-neighbor hopping processes, using this Hamiltonian and the Kondo lattice Hamiltonian, Lacroix found

$$b = -\frac{t}{2}.$$

As direct consequence all the results of the infinite U Hubbard model apply. In particular the Nagaoka theorem, that predicts the existence of ferromagnetism if only one hole in the Hubbard band is present. Via the mapping it means that a single electron can ferromagnetically order the entire Kondo lattice (at $J = +\infty$). The extent of this ferromagnetic phase in the infinite U Hubbard model is quite debated [7] and the existence of some critical Hubbard hole density (i.e. Kondo electron density) that separates it from a paramagnetic region is expected.

To go beyond these results Sigrist had to follow a similar path, defining a non-linear canonical transformation (similar to Ref. [200]) on the Hamiltonian (6.25), where he represented the spins making use of constrained Abrikosov fermions

$$\mathbf{S}^{\mathbf{f}}_\alpha(i) = \frac{1}{2} \sum_{\sigma,\sigma'} f^\dagger_\sigma(i) \tau^\alpha_{\sigma\sigma'} f_{\sigma'}(i), \quad \sum_\sigma f^\dagger_\sigma f_\sigma = 1, \quad \forall i.$$

The complete derivation of the effective Hamiltonian can be found in the appendix of Ref. [89] and in the appendix[17] A of Ref. [158], so I will not rewrite it here, but simply comment on it. The derivation of the effective Hamiltonian goes through the definition of non-linear operators[18] that *diagonalize the interaction term*. These operators create and annihilate local spin-singlets, spin triplets and double occupied states, therefore they do not have easy (i.e. fermionic) commutation relations. For example the operator

$$b^\dagger_0(i) = \frac{1}{\sqrt{2}} \left[f^\dagger_\uparrow(i) c^\dagger_\downarrow(i) - f^\dagger_\downarrow(i) c^\dagger_\uparrow(i) \right],$$

if applied on an empty site, creates a local singlet on site i. Of course also the constraint on the number of the Abrikosov fermions has to be rewritten considering the presence of these new operators. Anyway the math can be carried out and in particular the kinetic term can be recasted making use of them. Conveniently *new fermion operators* can be defined as

$$\tilde{f}^\dagger_\sigma(i) = \left[1 - c^\dagger_\uparrow(i) c_\uparrow(i) \right] \left[1 - c^\dagger_\downarrow(i) c_\downarrow(i) \right] f^\dagger_\sigma(i).$$

[17] The reader should pay attention to the different notations and conventions used in the two papers and to the presence of some annoying typos.

[18] In the following discussion the vacuum is assumed to be the state with no conduction electrons and no Abrikosov fermions present. The operators defined bring the quantum system from the vacuum to one of the 8 states of the local Kondo Hilbert space.

These operators, when acting on the vacuum, create the state with one spin and no electrons present (the bachelor spin states) and obey fermionic commutation rules (among themself).

The hopping term gets very complicated, but in the high J limit it acts only as a perturbation, and it is the interaction term (that now is diagonal) that dominates. It is the form of the interaction term that drives the choice of the next steps: using the non-linear operators it reads

$$-\frac{3}{4}J\sum_i b_0^\dagger(i)b_0(i) + \frac{J}{4}\sum_i \left(b_1^\dagger(i)b_1(i) + b_2^\dagger(i)b_2(i) + b_3^\dagger(i)b_3(i)\right),$$

where $b_\alpha^\dagger(i)$ creates a triplet state on site. It is evident that if $J \to +\infty$ the ground state, on which the hopping term will act as perturbation, will have occupation number 1, on each site, for the b_0 excitations and zero for b_α. If $n_c \leq 1$ the states without a singlet b_0 will instead contain a bachelor spin, i.e. an $\tilde{f}$-fermion. This is the complete picture at $J \to +\infty$ as Lacroix pointed out, so to obtain the Hamiltonian for the bachelor spins, one has to write an effective Hamiltonian with only these two degrees of freedom $\{b_0^{(\dagger)}, \tilde{f}_\sigma^{(\dagger)}\}$. This can be done using the kinetic term as perturbation on the chosen ground state, or acting on H with a canonical transformation to eliminate any trace of operators that contain different operators rather than b_0 and $\tilde{f}$ (similar to the Schrieffer-Wolff transformation). So

$$\tilde{H} = e^{-S}He^S = H + [H,S] + ...$$

that can be solved asking

$$(H - H') + [H', S] = 0,$$

where H' contains the interaction part plus the operators in the kinetic term that include only operators $\{b_0^{(\dagger)}, \tilde{f}_\sigma^{(\dagger)}\}$. One gets

$$\langle\alpha|S|\beta\rangle = \frac{\langle\alpha|H'|\beta\rangle}{E_\beta - E_\alpha},$$

where $|\alpha\rangle$, $|\beta\rangle$, E_α, E_β are eigenstates and eigenvalues of the (diagonal) interaction part. In this way the effective Hamiltonian obtained is:

$$\tilde{H} = H_0 + H_1 + H_2 + H_3 + H_4, \tag{6.39}$$

with

$$\begin{aligned}
H_0 &= -\frac{t}{2}\sum_{i,\sigma} b_{0,i}^\dagger \tilde{f}_{\sigma,i}\tilde{f}_{\sigma,i+1}^\dagger b_{0,i+1} - \frac{3J}{4}\sum_i b_{0,i}^\dagger b_{0,i} + H.c.,\\
H_1 &= \frac{t^2}{2J}\sum_{i,\sigma} b_{0,i-1}^\dagger \tilde{f}_{\sigma,i-1}\tilde{f}_{\sigma',i}^\dagger \tilde{f}_{\sigma',i}\tilde{f}_{\sigma,i+1}^\dagger b_{0,i+1} + H.c.,\\
H_2 &= -\frac{t^2}{4J}\sum_{i,\sigma} b_{0,i-1}^\dagger \tilde{f}_{\sigma,i-1}\tilde{f}_{\sigma',i}^\dagger \tilde{f}_{\sigma,i}\tilde{f}_{\sigma',i+1}^\dagger b_{0,i+1} + H.c.,\\
H_3 &= \frac{t^2}{6J}\sum_{i,\sigma} b_{0,i-1}^\dagger \tilde{f}_{\sigma,i-1} b_{0,i}^\dagger b_{0,i}\tilde{f}_{\sigma,i+1}^\dagger b_{0,i+1} + H.c.,\\
H_4 &= \frac{3t^2}{4J}\sum_i b_{0,i}^\dagger b_{0,i} - \frac{5t^2}{12J}\sum_i b_{0,i}^\dagger b_{0,i} b_{0,i+1}^\dagger b_{0,i+1} + H.c.,
\end{aligned}$$

Making use of the constraint, that now reads $\sum_\sigma f^\dagger_{i,\sigma} f_{i,\sigma} + b^\dagger_{0,i} b_{0,i} = 1$, one can trade local b-density operators for $\tilde{f}$-density ones. The b_0-operators that sandwich the $\tilde{f}$-operator's structures can be dropped, because the b_0 states can be thought of as holes in a system with $\tilde{f}$-fermions only[19], and the Hamiltonian for such a system looks, after some rearrangement, as the sum of the five parts:

$$
\begin{aligned}
H_0 &= -\frac{t}{2}\sum_{i,\sigma} \tilde{f}_{\sigma,i}\tilde{f}^\dagger_{\sigma,i+1} - \frac{3J}{4}\sum_i 1-\tilde{n}_i + H.c.,\\
H_1 &= \frac{t^2}{2J}\sum_{i,\sigma} \tilde{f}^\dagger_{\sigma,i+1}\tilde{n}_i\tilde{f}_{\sigma,i-1} + H.c.,\\
H_2 &= -\frac{t^2}{4J}\sum_{i,\sigma} \tilde{f}^\dagger_{\sigma',i+1}\tilde{f}^\dagger_{\sigma,i}\tilde{f}_{\sigma',i}\tilde{f}_{\sigma,i-1} + H.c.,\\
H_3 &= \frac{t^2}{6J}\sum_{i,\sigma} \tilde{f}^\dagger_{\sigma,i+1}(1-\tilde{n}_i)\tilde{f}_{\sigma,i-1} + H.c.,\\
H_4 &= \frac{5t^2}{6J}\sum_i \tilde{n}_{i+1}\tilde{n}_i - \frac{t^2}{6J}\sum_i(\tilde{n}_i+4) + H.c.,
\end{aligned}
$$

where $\tilde{n}_i = \sum_\sigma \tilde{f}^\dagger_{\sigma,i} f_{\sigma,i}$ is constrained site-by-site as $\tilde{n}_i \leq 1$.

This is the effective Hamiltonian for the bachelor spins that is created by the motion of conduction electrons, in a system where a local singlet is formed on each site. Clearly H_0 is the dominant term at $t/J \to 0$ and is exactly the same found by Lacroix. The motion of the singlets induces not just an effective hopping for the bachelor spins, but also effective interactions. This Hamiltonian can thus be analyzed [89] and the result is that for every number of bachelor spins the ground-state is the one with the maximum possible spin. So at strong coupling, i.e. at $t/J \to 0$ the spin degeneracy is lifted and the ground state is the *maximally spin polarized* ferromagnetic state, with total spin $S = |n_{\tilde{f}}|/2$, that in KL terms means $|1-n_c|/2$. Surprisingly the latter relation between the density and the total spin polarization holds [196] for any value of J.

One-electron limit: Sigrist, Ueda and Tsunetsugu found the solution to this insidious problem [158,199], although Lacroix's mapping plus the Nagaoka theorem, already gave an exact result for the existence of ferromagnetic order with one electron at $J = +\infty$. To characterize the ground-state one starts considering the KL with only Ising spin coupling.[20] Such model has a trivial ground state, with all the spins aligned and a free plane wave electron with spin antiparallel (assuming $J > 0$ of course) to the local spins, delocalized on the entire lattice. The total projection of the spin vector is $S^{tot}_z = |N-1|/2$. Turning on (slowly) the flipping term, the ground-state will change adiabatically and the resulting

[19] Remember that $b^\dagger_0$ does not create a conduction electron, but the entire singlet. Therefore the operators $b_{0,i}$ does annihilate also the bachelor spin that occupies the site i. Therefore they have no effect in the Hamiltonian, because acting on a state or they generate a zero or the vacuum of the $\tilde{f}$-fermions.

[20] The argument holds in any dimension and for any lattice, but here I focus on the one dimensional case only.

state must be written as:

$$|\Psi\rangle = \sum_{i=1}^{N} \left\{ A^i c^\dagger_{i,\downarrow} + c^\dagger_{i,\uparrow} \sum_{j=1}^{N} A^{ij} S^-_j \right\} |0\rangle \otimes |FM\rangle, \tag{6.40}$$

where $|0\rangle$ is the electron vacuum and $|FM\rangle = \bigotimes_{i=1}^{N} |\Uparrow_i\rangle$. The formula (6.40) represents the linear combination of a plane wave electron with spin down and a delocalized correlated state between an up electron and a magnon.[21] In fact the spin ladder operator generates a local (static) flipped spin, that in this model is the fundamental excitation of the spin system (because no propagation exist in absence of electrons). The magnon (i.e. the flipped spin) is delocalized on the lattice, because the electron that generates it is also delocalized on the lattice. The state (evidently ferromagnetic) is adiabatically connected to the ground state of the previous simplified model, because the Kondo interaction commutes with the total spin operator $\mathbf{S}^2_{tot}$ and its z component S^{tot}_z. Of course the adiabatic connection does not imply that a state like (6.40) is the ground state of the KL. To prove that this is the case, one has to go through the demonstration of the following theorem [199]:

> *The ground state of the Kondo lattice model (in any dimension) with one conduction electron has the total spin quantum number $S_{tot} = (N-1)/2$ and is unique apart from the $(2S_{tot}+1)$-fold spin degeneracy, if the hopping is negative ($-t > 0$) and the coupling is positive $J > 0$ (antiferromagnetic).*

So to obtain the ground state one has to pick up properly the coefficients A^i and A^{ij}, in such a way that (6.40) is an egenstate of $\mathbf{S}^2_{tot}$ with $S_{tot} = (N-1)/2$. Because (6.40) has $S^{tot}_z = (N-1)/2$ the condition to satisfy is $S^+_{tot}|\Psi\rangle = 0$. This generates the constraint $A^i + \sum_j^N A^{ij} = 0$, $\forall i$. Consequently to obtain the ground-state, one has to solve the Schrödinger equation for (6.40), fulfilling the latter constraint. The details can be found in the literature [141, 142, 158, 199] and will not be repeated here.

The problem is solved easily in momentum space, in terms of the Fourier transformed coefficents:

$$\mathcal{A}^K = \frac{1}{\sqrt{N}} \sum_{i=1}^{L} A^i e^{-iKr_i}, \qquad \mathcal{A}^K_q = \frac{1}{N} \sum_{i,j=1}^{L} A^{ij} e^{-iKr_i} e^{-iq(r_i - r_j)}, \tag{6.41}$$

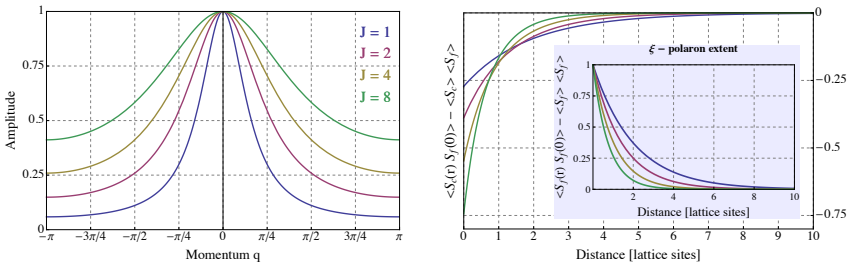
giving as result

$$\mathcal{A}^K_q = -\frac{1}{\sqrt{N}} \frac{E_K - J/4 + t\sum_a e^{iKa}}{E_K - J/4 + t\sum_a e^{i(K+q)a}} \mathcal{A}^K, \tag{6.42}$$

where E_K is the eigenvalue of the Schrödinger equation, that is found solving a non-linear equation and that turns out to have the minima at $K = 0$. The normalization is fixed by $1 = |\mathcal{A}^K|^2 + \sum_q |\mathcal{A}^K_q|^2$.

The details are irrelevant for the purpose of this section, while it is important to focus the attention on one outcome of the discussion: the appearance of the

[21] The existence of some kind of bound state between an electron and a spin flip will be a familiar idea from now on. The mechanism of the SSKI, the physics of the polaronic liquid and at the PM-FM phase transition, the proposal of the composite heavy fermion and the formalism elaborated in paper C, all end up dealing with this idea.



(a) *Magnon momentum distribution;* **(b)** *Spin-electron correlation function.*

Figure 6.9: *(a) Example of the aspect of the modulating function A^0_q in (6.42), for different values of J fixing the momentum of the electron at $K = 0$. The curves represents the shape of the magnon distribution into the polaron bound state. (b) The electron spin-impurity spin correlation functions (main panel) and the function $\xi(J)$ (inset), for the same values of J. The quantity $\xi(J)$ gives the spatial extent (the size) of the polaron.*

polaron, an interesting bound state between a magnon and an electron. As can be seen from (6.41)-(6.42), around an electron propagating with momentum K, there exists a magnon that travels with small deviations q (the value is affected by quantum uncertainty) from K, see Fig. 6.9a. The ground state is a linear combination of a free electron propagating on a ferromagnetic spin chain and a scattered state, and it can be though of as a bound state between a magnon and an electron. This bound state is broad, with a size of many lattice sites and a typical width that is given by the mean free path of the electron. Its spatial extent can be determined by studying the electron-impurity spin correlation function [158, 199] of the ground-state ($K = 0$):

$$\begin{aligned} \chi(r = r_i - r_j) &= \langle \mathbf{S^c}_i \mathbf{S^f}_j \rangle - \langle \mathbf{S^c}_i \rangle \langle \mathbf{S^f}_j \rangle \\ &= \frac{1}{2} |\mathcal{A}^{K=0}|^2 \left[1 - \left(1 - \frac{E_0 - J/4 + 2t}{2t \sinh(1/\xi)} e^{-r/\xi} \right)^2 \right] \end{aligned} \tag{6.43}$$

where

$$\xi^{-1} = \operatorname{arccosh}\left(\frac{J/4 - E_0}{2t} \right), \tag{6.44}$$

gives the extent of the polaron, i.e. the typical distance up to which the electron spin and the impurity spins are correlated. For $J \ll t$ the correlation last for long distances and falls down exponentially with a typical distance $\xi \approx \sqrt{2t/J} \gg 1$, indicating that the electron can travel for long distances before getting scattered. It also means that the electron and the magnon are only weakly bound. In the opposite limit $J \gg t$ the bound state becomes an extremely localized (it becomes a Kondo singlet) and $\xi \approx 1/\ln(J/t)$, implying that $\langle \mathbf{S^c}_i \mathbf{S^f}_i \rangle = -3\delta_{i,j}/4$.

Another important quantity is given by the correlation between the impurity spins. It exhibits exponential behavior in the coherence length:

$$\langle \mathbf{S^f}_i \mathbf{S^f}_j \rangle - \langle \mathbf{S^f}_i \rangle \langle \mathbf{S^f}_j \rangle \propto e^{-\frac{r}{\xi}}. \tag{6.45}$$

Two processes characterize the polaron: the scatternig, that fixes its size, and the propagation of the electron, that determines its internal structure. Inside the

polaron (or between two scattering events, if one thinks in a semiclassical way) the electron travels freely, ordering the spins ferromagnetically, as intuitively understood in terms of double exchange. Therefore the spatial extent of the polaron and the extent of the ferromagnetic correlation between the spins are correlated. This property originates from the free electron component of the wave-function (6.40). A good cartoon picture of the polaron is thus given by an electron surrounded by many spins ordered antiparallel to it. The island of ordered spins has the same extent as the polaron.

Summarizing: the 1dKL with only one electron has been completely solved and characterized. The ground state is ferromagnetic with total spin $S^{tot} = |N-1|/2$ and the electron forms a bound state with the magnon created by its scattering events with the impurity spins. The bound state, i.e., the polaron, is more and more localized with increasing coupling, and in the extreme limit of infinite coupling the electron and the magnon move together as a Kondo singlet. The polaron has a typical extent ξ that characterizes the correlation between magnon and electron and can also be interpreted as the typical length scale of the ferromagnetic correlation between the spins; this can be understood in terms of double exchange. The picture of more and more localized polarons is consistent with the strong coupling limit analyzed previously. In this sense it is easier to imagine J as the controlling parameter of the deconfinement of the polaron (formed by the electron and the magnon). At $J = +\infty$ the two particles are confined, i.e. they form an hardcore particle very well localized in space with the size of a single lattice site, that can undergo hopping processes only keeping the coherence between its two components. Decreasing the coupling the polaron becomes "soft", and the two constituent particles can "deconfine", in the sense that they undergo more independent hopping events. In this way the two bound components (still keeping a certain degree of correlation) increase the size of the polaron, that broadens and occupies many lattice sites; in doing this the correlation between the spin of the conduction electron and the local impurity spins is created.

The central region of the ferromagnetic phase: so far two limiting cases have been analyzed, namely the one electron limit and the infinite coupling one. These limits pave the way for the analysis of the more physical region of the phase diagram at intermediate fillings and coupling. A first step towards the solution was again done by Sigrist, Ueda and Tsunetsugu in Ref. [201]. Although the work was purely numerical, they understood the key of the stabilization of the ferromagnetic phase in the low carrier regime. In presence of more electrons the interaction between the different polarons (i.e. the different ferromagnetically ordered domains) becomes important. As long as the overlap (i.e. the interaction) between the polarons is not too big the system keeps the global ferromagnetic order, although the latter becomes a collective affair between different polarons. As a consequence one should expect some relation between the polaron's extent and the density: some critical density must exist, above which the polarons become too packed, the overlaps too pronounced and a phase transition takes place. These considerations drove Honner and Gulacsi [197, 198] in the characterization of the FM-PM transition line. A nice introduction can be found in Ref. [141, 142]. The physics at the transition will be discussed in the next section.

Although the boundaries of the FM phase were determined accurately in Ref. [188–191], its nature remained somehow a mystery until the work by Peters and Kawakami [192]. In fact the idea of an interaction between polarons is convincing, but the exact microscopic realization is quite obscure. The results in Ref. [192] demonstrate how the stability of the FM phase is granted by the formation of the spin-selective Kondo insulator (SSKI). This mechanism was originally discovered using DMFT+NRG in the infinite dimensional KL [146] in the beginning of 2012. A subsequent DMRG study [192] of the 1d case showed that the same mechanism takes place in the FM phase. This mechanism appears naturally at a mean-field level, thanks to the (Majorana fermion based) map elaborated in paper C. This mean-field picture gives a very nice description of it, in complete agreement with the interpretations in Ref. [192].

The SSKI is naively explained by a cooperation of Kondo effect and double exchange, realized via a highly *asymmetric* treatment of the two spin species of the conduction electrons. The double exchange orders the spins ferromagnetically (majority spins), granting a maximization of the kinetic energy of the electrons, which gets accumulated in one spin species only (the majority electrons). The interaction term contrasts this process, scattering the electrons from one to the other spin species (the minority electrons) and generates flipped spins (minority spins). In order to not loose the high contribution of the kinetic energy, due to the ferromagnetic coordination of the spins, the systems entangles the majority spins and electrons with the minority ones, generating delocalized Kondo singlets. In the wave function there are therefore two main components: conduction (majority) electrons that travel (almost freely) on an highway of ferromagnetically ordered spins, and Kondo singlets that take care of all the troubles represented by the scattering terms. All the minority electrons end up in a Kondo insulating phase, while the majority electrons behave as free (spinless) electrons on a lattice, generating the metallic properties. The spectral function of the minority electrons (see Fig. 8 in Ref. [192]) shows the existence of a gap at the Fermi level, for each value of J and n_c. The gap is not present in the spectral function of the majority electrons.

The situation can be described semiclassically recalling the polaronic picture. Suppose that there are dilute polarons on the lattice. Each of them brings one electron (majority) and a cloud of ferromagnetically (majority) ordered spins. If there exist a small overlap between two polarons, then an exchange of electrons between the two ferromagnetic islands can take place and a larger ferromagnetic region can be stabilized, inhibiting the scattering on the overlapping boundary. But since the existence of the scattering events is responsible for the generation of the minority electron and spin populations, if the number of scattering events is decreased by the coherent overlap of two polarons, clearly an asymmetry between the majority and minority populations will occur.

Semiclassically this mechanism, given an electron density n_c, suppresses the Kondo physics, encapsulating all its effects into the creation of an optimized number of delocalized Kondo singlets. With the formation of the singlets, the majority electrons can propagate freely in the system, without causing any flipping and therefore ordering the spins ferromagnetically. This process generates an unusual correlation between the different quantities of the system. Assuming translational invariance and denoting by $\langle A \rangle$ the average of an operator A on

the ground state and on every site, one gets:

$$2\langle S_z^f \rangle + \langle m_c \rangle = \langle n_c \rangle - 1, \tag{6.46}$$

where $m_c = c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow$ and $n_c = c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow$. This relation takes an even simpler form in terms of Abrikosov fermions, but it becomes straightforward in the formalism introduced in paper C, so I leave the discussion for Chapter 7. It is very important to remark that evidence of the existence of the SSKI has been found in both 1d with DMRG and infinite dimensions with DMFT+NRG. This suggests the existence of a ferromagnetic phase, stabilized by the SSKI formation, in every dimension at low fillings. This results agrees with the RG analysis performed by Yamamoto in the 3dKL [166, 202–204], that suggested the existence of such a phase, although in those studies an Heisenberg coupling between the spins has been added for practical reasons. The SSKI seems therefore to be the key to understand ferromagnetism in the KL and a formalism that is able to describe it in a simple way would be useful in future studies. I argue that the approach developed in paper C fulfills all these criteria.

Concluding I would like to point out an annoying feature of the SSKI. This mechanism is based on a very asymmetric role played by the two electron species. The total wave-function is very complicated (entangling Kondo singlets with the majority electron Fermi liquid) so it is difficult to imagine the structure of the ground state. In order to do it we can think to (approximately) split the wave-function in two parts: the first given by the Kondo singlets, where *all* the minority electrons and some of the majority electrons bound to the spins; the second where the majority electrons, left behind by the formation of the Kondo singlets, behave as free spinless modes. It has been shown that at very strong coupling all the electrons are bound into Kondo singlets and that it is the effective hopping of the bachelor spins that generates the ferromagnetism. Therefore at strong coupling the asymmetry among up and down electron species does not seem to occur. As a consequence it seems improbable that the SSKI can be the mechanism that stabilizes the ferromagnetism at high coupling, if not with some variations to the (simplified) picture just introduced.

6.3.2 The FM-PM phase transition

The exact results at vanishing density and strong coupling, imply the existence of a ferromagnetic-paramagnetic transition at some critical J-dependent electron density. This phase transition represented an enigma, until the publication of the two works by Honner and Gulacsi [197,198]. They followed the idea that the interaction between the polarons, and therefore the double exchange mechanism, is responsible for the stabilization of the ferromagnetic phase. On this assumption they defined a sort of "smooth bosonization" procedure or "coarse grained bosonization". In the standard bosonization techniques the Bose fields, representing the density or current oscillations and their momenta, are canonically conjugate and their commutator vanishes if the two fields are not on the same site. To take into account the fact that the electron is smeared on many sites (due to the broad spatial extent of the polaron) they considered a space cutoff α in the definition of length, fixed by the the typical extent of the polaron. This uncertainty smears the bosonic fields, implying a change in the

commutation relations that they modeled as

$$[\phi_\nu(j), \Pi_{\nu'}(0)] = 2i\delta_{\nu,\nu'} J_j(\alpha),$$

where ν indicates the two possible sectors of charge and spin, j the distance in lattice sites between the two field coordinates, $\phi_\nu(j)$ ($\theta_\nu(j)$) is the Bose density (current) field, $\Pi_{\nu'}(j) = -\partial_x \theta_\nu(j)$ is the momentum of the field and $J_j(\alpha)$ is a smearing function modeled as

$$J_j(\alpha) = \int_0^{+\infty} \cos(kja)\Lambda^2(k,\alpha)dk,$$

where a is the lattice spacing. The function $\Lambda(k,\alpha)$ determines the smearing in k-space. Different forms of the cut-off produce different results (and also the normal Luttinger bosonization procedure, in the limit of $\alpha \to 0$, if J_j is chosen properly), but for smooth cut-offs the authors noted no sensible difference. The details can be found in the original papers and in Ref. [141, 142].

A point that is stressed in the original papers (but not very much in the reviews) is that this "smeared bosonization" is justified as long as the electron is delocalized on many sites. At high coupling, where the localization due to the Kondo effect is dominant, driving to the formation of "compact" Kondo singlets (small size polarons), the procedure is not justified. An estimate in Ref. [197,198] puts this limit at $J/t \approx 5$, i.e. anyway quite far from the paramagnetic transition line. Making use of this smeared bosonization procedure it is possible to expose a term in the Hamiltonian that explicitly takes into account the effect of double exchange effect, which is actually due to the delocalization of the electron inside the polaron. The extra term in the Hamiltonian has the form

$$-\frac{a^2 J^2}{4\pi^2 v_F} \sum_{j,j'} J_{j-j'}(\alpha) S_z^f(j) S_z^f(j'),$$

and appears in the Hamiltonian after a properly chosen unitary transformation [141, 142, 197, 198]. Although this term does not depend upon the Bose fields, other operators in the Hamiltonian do have such dependence. In order to get rid of the Bose field, i.e. to obtain a Hamiltonian for the spins only, they are substituted by their average values on the non-interacting ground state. This substitution is justified in the small coupling regime, where the two fields are smooth. The final effective spin Hamiltonian reads:

$$\begin{aligned} H_{eff} &= -J_{eff} \sum_j S_z^f(j) S_z^f(j+1) + \\ &+ A\frac{Ja}{\alpha} \sum_j \left[\cos(K_j) + \cos(2k_F ja)\right] S_x^f(j) + \\ &- A\frac{Ja}{\alpha} \sum_j \sin(K_j)\sin(2k_F ja) S_z^f(j). \end{aligned} \tag{6.47}$$

where K_j is a function that counts the total S_z^f on the right and subtract the total S_z^f on the left, therefore it is approximately zero in the thermodynamic limit, into and close to the FM phase, and A is a normalization constant. So the physics close to the transition is described by the first term, with

$$J_{eff} = \frac{a^2 J^2}{2\pi^2 v_F} J_1(\alpha),$$

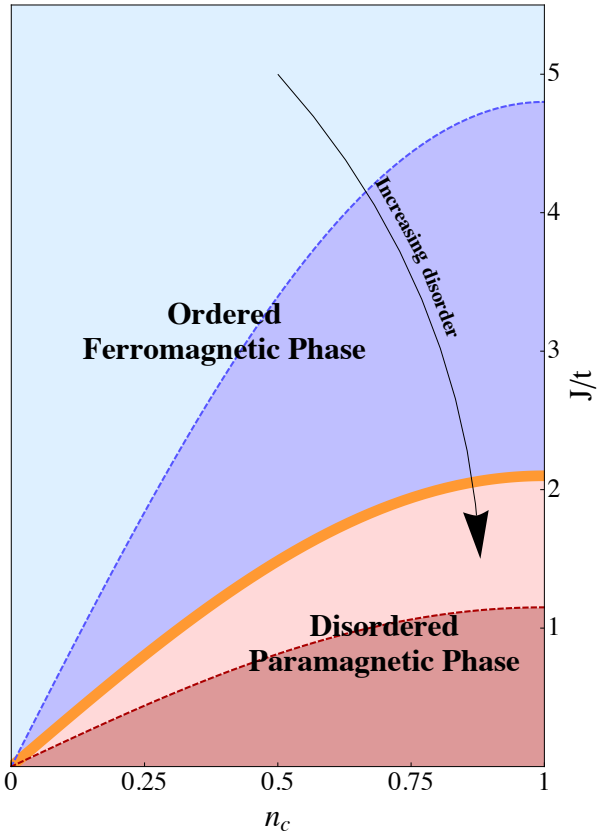


Figure 6.10: *Sketch of the phase diagram of the effective spin Hamiltonian (6.47). The thick orange continuous line is an example of a possible best fit for the FM-PM transition, according to the form given by the formula (6.50). The top (bottom) dashed line represents a corresponding possible boundary where the effect of disorder (order) become negligible. For more details and a complete discussion see Ref. [197], where the best fit is plotted and analyzed in details.*

plus the second one, that becomes $A\frac{Ja}{\alpha}\sum_j \left[1+\cos(2k_F ja)\right] S^f_x(j)$. At incommensurate fillings the term $\cos(2k_F ja)$ oscillates randomly with respect to lattice sites and it can (without any change in the physics) be represented by a random variable h_j described by the distribution function [197, 198]

$$\rho(h) = \frac{\alpha}{\pi AJa}\sqrt{\frac{1}{1-\left[(\alpha h/AJa)-1\right]^2}}. \tag{6.48}$$

This distribution function is not an outcome of the theory, but comes from considerations [197, 198] on the spin flip processes that the random term has to represent. Anyway, the most important final result (i.e. the location of the FM-PM phase transition), is independent upon this choice.

It can be concluded that the (spin) physics at the paramagnetic transition

and close to it, is governed by the effective Hamiltonian

$$H_{eff} = -J_{eff} \sum_j S_z^f(j) S_z^f(j+1) - \sum h_j S_x^f(j), \tag{6.49}$$

which is nothing but the *quantum random transverse-field Ising Hamiltonian* [205], a known model that has a quantum order-disorder transition. In terms of the KL parameters this transition occurs at

$$\frac{J}{t} = \frac{4\pi^2 A \sin(\pi n_c/2)}{\alpha \int_0^{+\infty} dk \, \cos(ka) \Lambda^2(k,\alpha)}. \tag{6.50}$$

Clearly this formula has to be fitted to the (numerically) known critical points, in order to obtain the α dependent prefactor. The result is shown in Fig. 6.10. The choice of the distribution function (6.48) does *not* affect the location of the transition line, but only the physics close to it and the position of the two dashed lines.

The main outcome of this analysis is that the phase transition is expected to happen at finite J even for $n_c \to 1$; this fact was in complete contrast to the beliefs in the late nineties, and had to wait for the DMRG analysis [188–190] to be confirmed. Moreover it gives an idea of the physics close to the transition, although it must be stressed that, except for the location of the phase transition line, the phase diagram of Fig. 6.10 is sensitive to arbitrary choices and approximations, that makes it reliable only close to the phase-transition. In particular at high couplings ($J/t \approx 5$ in the graph) the approximation of the smeared bosonization does not take into account the formation of compact Kondo singlets.

For fixed density n_c the relative effect of the transverse random field becomes more and more relevant, if compared with J_{eff}. This causes an increase of the disorder in the ferromagnetic phase, that culminates at $J_{crit}(n_c)$ with the order-disorder phase transition [104, 139]. The ordered ferromagnet breaks into independent islands of locally ordered spins, which become the low energy degrees of freedom of the theory[22] and generate a total paramagnetic phase. This low energy effective description is well suited for the KL, where the concept of islands of ordered spins appears naturally through the polarons. The appearance of the disordered phase seems therefore perfectly consistent with the known physics of the FM phase. For a critical value of the coupling (or density) a coherent state among all the polarons becomes unstable, because the overlap (so the interactions) among them increases too much. The globally ordered state (the SSKI) breaks and the polarons "melt" by beginning to move independently making the system paramagnetic.

Considering that the polarons are the low energy degrees of freedom, it is appropriate to name this phase *polaronic liquid*. A quite interesting observation from the DMRG analysis is that the Fermi surface in this polaronic liquid phase is *large*. This result is obtained measuring the peak of the impurity spin structure factor, shown in Fig. 6.11.

[22] The low energy of the dynamics is generated by the fact that any interaction among the polarons has to flip the spin of an entire region, therefore it is a quite improbable and slow process.

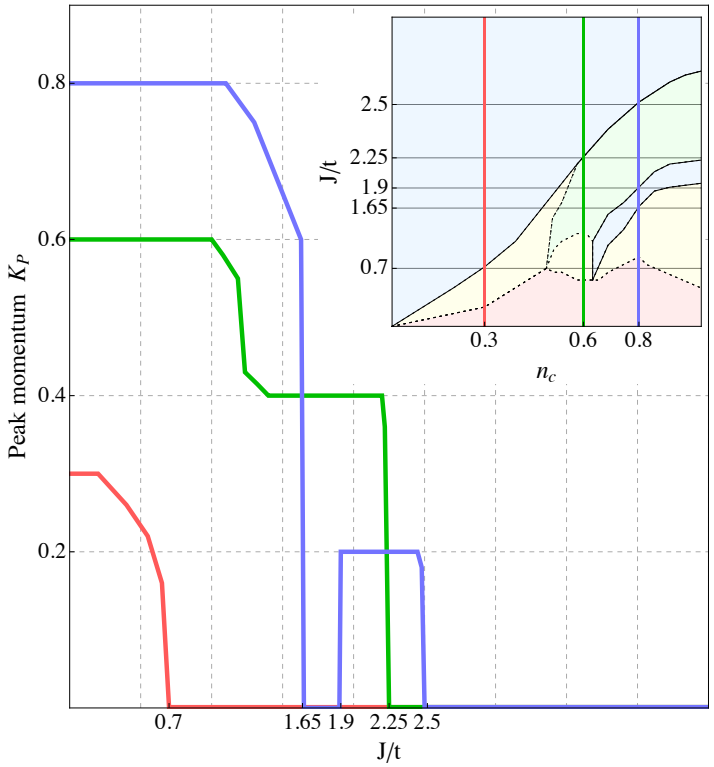


Figure 6.11: *Sketch of the evolution of the peak of the spin-spin correlation function for electron densities $n_c = 0.3$, $n_c = 0.6$, $n_c = 0.8$ (respectively red, green and blue lines in both the main panel and the inset) and varying coupling. Using the DMRG approach [188], the spin-spin correlation function can be computed and its peak determined. The evolution of the peak is plotted in the main panel. As evident from this sketch, when the system goes form one zone of the phase diagram to another, the location of the peak changes. At $J/t = 0$ it is equal to $2k_F$ (where in these units $2k_F = n_c$) for each curve and that value remains as long as the system is in the RKKY liquid phase (first plateaux of each curve). In correspondence of the polaronic liquid the value of the peak falls to $2k_F - \pi$, showing the existence of a large Fermi surface (second plateaux of the green and blue lines). Instead in the ferromagnetic phases the peak is located at zero; all the curves fall to zero beyond a critical coupling that corresponds to the PM-FM transition, but the blue curve has an extra region where the peak falls to zero, in correspondence of the ferromagnetic tongue. In the wild zones the peak is instead in a transient regime, that is very visible in the red curve of the main panel. The exact datas can be found in Ref. [142, 188], from which this sketch has been inspired.*

6.3.3 The RKKY liquid, wild zones and ferromagnetic tongue

In the phase diagram, inside the paramagnetic dome, there are some regions that still represent a challenge: the RKKY liquid phase, the wild regions and the ferromagnetic tounge, that can be seen in red, yellow and blue in Fig. 6.7. With the term RKKY liquid is meant the paramagnetic region of the phase diagram where the RKKY behavior is dominant and causes a peak in the structure factor $S(k)$ of the impurity spins. This peak is the remnant of the divergence (6.34), that is suppressed by the 1d quantum fluctuations. As can be seen in Fig. 6.11 below $n_c = 1/2$ the peak of $S(k)$ is always localized at $2k_F$ for each $J < J_c$,

marking the dominance of RKKY physics, and then at $k = 0$, indicating a phase transition to the ferromagnetic phase. Increasing n_c the evolution of the peak marks two transitions: from $2k_F$ to $2k_F - \pi$ and from $2k_F - \pi$ to zero; this indicates that the system passes first from the RKKY liquid phase to a heavy fermion one (polaronic liquid) and then, at higher J, from the polaronic liquid phase to the ferromagnetic one (PM-FM disorder-order transition). At higher fillings, the transition between the RKKY and polaronic liquid is separated by another ferromagnetic phase, i.e. the "tongue", indicated by the dashed line in Fig. 6.11. About this tongue FM phase not so much can be said, except the fact that it looks similar to the other FM one.

As pointed out in Ref. [141, 142, 190], the boundaries between these different regions are not very well marked (see data plots in Ref. [141, 142, 190] and Fig. 6.7). Under the ferromagnetic tongue there exist a region where a competition between the RKKY effect and the FM ordering becomes more significant and makes the phase diagram complicated, causing the appearance of other ferromagnetic pockets. Moreover the transition between the RKKY liquid and the polaronic liquid, as well as the $n_c < 1/2$ transition between the RKKY liquid and the FM phase, go through a set of intermediate states.

All this confusion can be explained by an important consideration, present already in Ref. [158]: *there is no nontrivial limit where the conduction electrons and the localized spins can be considered independently in the 1dKL.* This seems particularly true in the case of the competition between the RKKY and the Kondo effect. The first seems dominating only in the very weak J regime, but quickly looses its importance and becomes seriously affected by the Kondo physics.

The evidence suggests that in the 1dKL the concept of the RKKY effect is not very well defined, because the regime of parameters where it is dominating and (almost) unaffected by the Kondo physics is eventually very small (or maybe absent). The only exception is given by the special phase that appears at $n_c = 1$, where the RKKY effect, tries to order the system antiferromagnetically. Up to now the physics that comes from the collaboration of the RKKY and the Kondo effect is still quite debated and not fully understood [103, 104].

6.3.4 The spin-liquid phase at half-filling

This is probably the most studied phase of the 1dKL. What makes the value $n_c = 1$ different from all the others is the particle-hole symmetry. In fact on bipartite lattices, if the Hamiltonian is particle hole symmetric as in the case of the KL, the physics at $n_c > 1$ is obtained from to the one at $n_c < 1$, through particle-hole transformation. This makes $n_c = 1$ a very special point, characterized not just by the invariance with respect to the operators $S^{tot}_{x,y,z}$, generators of the rotation symmetry group $SU(2)$, but also to the pseudospin operators $I_{x,y,z}$ of the conduction electrons [158, 206–208] (see also appendix C for a quick introduction to the pseudospin concept). The latter symmetry is broken away from half-filling, because the chemical potential enters multiplied by I_z.

The existence of this extra symmetry changes completely the physics of the system, forcing it into a so called "spin liquid phase". A spin liquid phase is a quite general term that indicates a huge variety of systems without any long range spin order [153]. Typically a spin liquid is obtained starting from a (Neél)

ordered state and adding frustration via next-nearest-neighbour spin-spin interactions. When the classically ordered ground state becomes degenerate with other states that differ by local spin flips, then one expects that the quantum fluctuations will destroy the order, leaving the system in a globally paramagnetic state. A classical example of spin liquid is given by Anderson's resonant valence bond system.

In the case of the 1dKL it is the Kondo interaction that induces the frustration on the spins, preventing the formation of long range order. It also causes the development of gaps in both the charge and the spin sectors, making the 1dKL a prototypical Kondo insulator. The physics of this phase is not trivial, so it is a very good idea to carefully define what is meant by "gap". In the literature four main gaps have been defined in the half-filled KL [158], but just three are important for the rest of the discussion:

i. *the spin gap:* the spin gap $\Delta_s[J]$ is the energy required to excite the lowest energy quantum state with total *spin* different from zero, *without* changing the number of electrons

$$\Delta_s[J] = E_{gs}(J, N_c = L, I = 0, S = 1) - E_{gs}(J, N_c = L, I = 0, S = 0),$$

where L is the number of sites and N_c the number of electrons; this can be done exciting a local spin triplet for example;

ii. *the charge gap:* the charge gap $\Delta_c[J]$ is the energy required to excite the lowest energy quantum state with total *pseudospin* different from zero, *without* changing the number of electrons

$$\Delta_c[J] = E_{gs}(J, N_c = L, I = 1, S = 0) - E_{gs}(J, N_c = L, I = 0, S = 0);$$

this state is for example realized by exciting a particle-hole pair, i.e. a linear combination of $|0\rangle$ and $|\uparrow\downarrow\rangle$;

iii. *the quasiparticle gap:* this is the energy required to *remove one electron* from the system, independently upon the spin or isospin configuration of the $N_c - 1$ state.

$$\Delta_{qp}[J] = E_{N_c-1}(J, N_c = L - 1) - E_{gs}(J, N_c = L, I = 0, S = 0);$$

by definition this is the important quantity that has to be studied when one wants to break the Kondo insulating state varying the chemical potential, in the fashion of the normal band insulators, that become conducting only if a critical value for the chemical potential is reached.

The origin of the gaps is the crucial question that physicists have tried to answer. A complete analysis requires the characterization of the structure of the ground state. This is an issue because of the absence of a phase transition between the behavior at low and high coupling, that are instead connected by a smooth crossover [145, 158, 208–210]. To understand how the properties of the high coupling limit are smoothly connected with those at low coupling (where for example it exist a local antiferromagnetic spin order) is quite a challenge. This is the umpteenth return of the unsolved riddle encountered away from half-filling: *how is it possible to understand the combined effect of the RKKY and Kondo*

mechanisms? The difference at $n_c = 1$ is that the ferromagnetism is excluded from the picture, because of the unbroken pseudospin symmetry, and just the other two main characters are left. This makes the problem more treatable and allows for the derivation of some exact results, that are fundamental for the understanding of the nature of the ground state. The most important feature is that the the ground state is a total singlet. This is formalized by the following theorem

> *The ground state of the half-filled Kondo lattice model is unique and has* $S = 0$ *for any* $J > 0$ *and in any dimension if the lattice is bipartite.*

The original forms of the theorem and the proof can be found in Ref. [158, 211–213]. This theorem immediately complicates the task, because it implies the presence of no long-range magnetic order in the system. However it does not exclude the existence of a local magnetic order, that in fact exist as proved by a second rigorous result. The theorem is demonstrated in Ref. [214] for the PAM, but holds also in the KL limit:

> *Consider the ground state of the symmetric PAM at half filling* $|GS\rangle$ (on a bipartite lattice). *At any* $U \geq 0$ [with U defined in (6.3)] *and in any dimension, the equal-time spin-spin correlation function between two "supersites"* $(\vec{r}, \gamma)$, $(\vec{r'}, \gamma')$
>
> $$S^{\gamma,\gamma'} = \langle GS|\mathbf{S}_{\gamma}(\vec{r})\mathbf{S}_{\gamma'}(\vec{r'})|GS\rangle,$$
>
> with $\gamma, \gamma' = c, f$ *is*
>
> *i. positive or zero, if* $\gamma = \gamma'$ *and* $\vec{r}$, $\vec{r'}$ *are in the same sublattice,*
>
> *ii. negative or zero otherwise.*

As shown in Ref. [158] this theorem means that in the 1dKL we have to expect a maximum for both the impurities and electron spin-spin structure factor at $q = \pi$. In practice it means that the system is locally ordered antiferromagnetically and that the correlation between local impurity and electron spins is negative (i.e. if the impurity spin points up, then the local electron spin will point down). Of course this is not in contrast with the previous theorem, because it does not imply the development of any long range order. This result was anticipated numerically by the results published in Ref. [215].

Although these two rigorous theorems give the exact structure of the ground state, they do not give any information about the nature of the gaps. To disclose these properties it is necessary to decrease the ambitions and use some approximation. The strong coupling limit permits a study of the gaps and their dependence upon J/t, using a perturbative expansion around the limit $J/t \to +\infty$. The details can be found in Ref. [158, 207, 210] and here I will report only the formulas for the gaps, valid at second order in the perturbative expansion.

i. $\Delta_s(J \to +\infty) = J - 20t^2/3J$, where the spin excitation are given by the creation of local triplets [210].

ii. $\Delta_c(J \to +\infty) = 3J/2 - 2t + t^2/3J$, is different from the spin gap. This is an interesting feature that does not appear in normal band insulators. In Ref. [158] the appearance of these two energy scales were interpreted as a manifestation of charge-spin separation in 1d, but in Ref. [216, 217]

it is instead proved that such separation does not happen in the 1dKL, implying that the reason for the development of the two different energy scales must be different.

iii. $\Delta_{qp}(J \to +\infty) = 3J/4 - t + t^2/6J = \Delta_c/2$, this result is quite interesting. In particular the factor $3J/4$ that is due to the breaking of a local singlet that has to be done in order to add or remove a particle to the system. The importance of this fact will be remarked later discussing [165, 218] and paper C, suggesting a close relation between the formation of Cooper pairs in BCS and of Kondo singlets in the KL.

These results do not extend down to $J/t \to 0$ and unfortunately a perturbative expansion program at $J/t \to 0$ cannot be carried out, because the ground state at $J = 0$ does not share the structure of the KL one, as mentioned previously. Other strategies must be used, both from an analytical and numerical point of view. In fact the problem gets more complicated also numerically, because of the non-local correlation existing among the spins. Anyway at low coupling the gap has been characterized succesfully [145, 158, 206–210], disclosing an unusual behavior. Of course all the gaps tend to zero approaching the non-interacting regime, but they do so in different ways [158]. The spin gap evolves as

$$\Delta_s(J \to 0) \propto \exp\left(-\frac{8\pi t}{3aJ}\right).$$

This energy scale should be compared with the Kondo temperature of the single impurity (6.35), which turns out to be smaller. This means that the characteristic spin energy scale of the KL is higher than the one of the single impurity system, indicating that physics different form the usual Kondo effect is important to describe the system. The charge gap evolves instead as [158]

$$\Delta_c(J \to 0) \approx \frac{J}{2},$$

i.e. it goes to zero much slower than the spin gap, implying a divergent ratio between the two quantities [207].

The analysis at low filling, has been carried out successfully by Le Hur [216, 217], making use of non-Abelian bosonization, and Tsvelik [219], creating a mapping on the $O(3)$ non-linear sigma model. Although beautiful, these two approaches have limitations. In fact the non-Abelian bosonization scheme describes extremely well the low energy physics, but relies on perturbative treatment of the interactions, so for large J it is not reliable. The map to the non-linear sigma model instead is based on semiclassical arguments that are acceptable at $J \ll 1$, but becomes suspicious otherwise.

Chronologically the latter analysis was performed first. It is based on the continuos path-integral representation of the Euclidean action for the spins [152, 153, 220], that relies on the identification of the Berry phase for the local spin field. The spin field is then decomposed[23] in slow and fast components, where the latter are then integrated out. In this way an effective Lagrangian, that describes the slow varying components interacting with the fermions, is

[23] This is the semiclassical step, taking into account an antiferromagnetic predisposition of the spins, so that the fast varying components of the field are the ferromagnetic ones, while the slow ones give the antiferromagnetic structure

obtained. The electron field is subsequently integrated out, but its determinant is computed *exactly*, thanks to a formal equivalence with the effective action of the gapless excitations of the Gross-Neveu model with $U(M) \times SU(N)$ symmetry [219]. In turn this permits to write down an effective action for the slow varying components of the spin field only. This generates a modification in the effective Lagrangian for spin chains, adding an extra topological term to the usual Haldane term [152, 153]. The final effect is that the spin excitations become massive (gapped), in agreement with the numerical results [219]. It also shows that at small coupling the excitations are massive triplets and that the correlation lengths are very large, indicative of the fact that the RKKY effect dominates at small J.

A problem of this solution is that it gives no indication about the behavior of the electrons, because it focuses on the effective Lagrangian for the spin field. The results of Le Hur [216, 217] do not share this limitation. The use of non-Abelian bosonization enables to treat spin currents in a more rigorous way, taking into consideration the involved commutation relation that the Lie group algebraic structure of the spin operators induce on the spin currents. Besides this (non-trivial) complication it proceeds as the usual bosonization, identifying the charge and spin current operators for left an right movers. The derivation is rather technical and can be found in the original papers. The results instead are very neat and interesting.

What is found is that the KL at half filling is gapped in both the spin and charge sectors, with a gap that varies linearly with the coupling, accompanied by a weak (local) antiferromagnetic order. The reason for the appearance of the gap for the electrons is quite natural: although the antiferromagnetic order for the spin is not long ranged, the electrons feel the *local* staggered potential and they scatter coherently as if the system was a perfect antiferromagnet. The charge gap opens and the electrons develop a spin density wave structure, triggered by the local spin order. This process also suppresses the typical charge-spin separation.

The scenario at low coupling seems therefore quite clear and it follows well the description given by the RKKY picture, if one considers also the backscattering of the electrons on the locally antiferromagnetic spin configuration. Instead at high coupling everything change and a new ideas must come out. An interesting prospective has been developed by Eder and collaborators in [165, 218].

In those works the authors started considering the ground state of the infinite coupling Kondo lattice $|KI\rangle$, that is given by a set of Kondo singlets: one for each lattice site. On this ground state the excitations are of the particle-hole kind: an electron is taken from a site and put to a nearest one, leaving behind a bachelor spin and forming on the new site a local singlet with the electron already present there. These excitations are evidently stimulated moving away from the $J \to +\infty$ limit and can be modeled using two fermionic operators $a_\sigma(j)$ and $b_\sigma(j)$: with $a^\dagger_\sigma(j)|KI\rangle$ a bachelor spin state $|\sigma\rangle$ is created on the site j; performing instead with $b^\dagger_\sigma(j)|KI\rangle$ the state $|\uparrow\downarrow\rangle \otimes |\sigma\rangle$ is created. Evidently a charge fluctuation of the vacuum pairs a fermion a with a fermion b, which have to be created or annihilated in pairs. The conduction electron hopping term allows these fermions to propagate in the lattice, in the same fashion explained in Sec. 6.3.1.

Under the assumption that the hopping of a and b *does not* leave behind an excited state (i.e. a triplet state like for example $|\uparrow\Uparrow\rangle$), then the motion

of these two fermionic excitations is coherent, which means that the particles do not loose energy decaying into different states. This makes the description of the charge fluctuations possible in terms of fermionic operators only and a general effective Hamiltonian (valid only under these hypothesis and enforcing no double occupancy of any site) for the fermions a and b can be written down as:

$$\begin{aligned} H &= \sum_{i,\sigma} \Delta a^\dagger_\sigma(i) a_\sigma(i) + \bar{\Delta} a^\dagger_\sigma(i) a_\sigma(i) + \sum_{i,j,\sigma} V_{i,j} b^\dagger_\sigma(j) a^\dagger_\sigma(i) + h.c. + \\ &\quad + \sum_{i,j,\sigma} V'_{i,j} a^\dagger_\sigma(j) a_\sigma(i) + V''_{i,j} b^\dagger_\sigma(j) b_\sigma(i). \end{aligned} \tag{6.51}$$

The coefficient has to be fixed comparing the matrix elements of this matrix with those of the KL Hamiltonian. The result is [165,218] $V_{i,j} = -V'_{i,j} = V''_{i,j} = t_{i,j}/2$ and $\Delta = \bar{\Delta} = 3J/4$, leading to

$$E_\pm = \frac{\epsilon(k) \pm \sqrt{4\Delta^2 + \epsilon(k)^2}}{2}, \tag{6.52}$$

with $\epsilon(k)$ a free electron band with bandwidth $2t$. This is exactly the same result obtained hybridizing a flat band f with a cosine like c band and that leads to the avoided crossing typical of the Kondo Insulators, shown in Fig. 6.2b. The most interesting result of this analysis is the origin of the gap, that resemble very much a superconductive gap, due to the fact that to create an excitation it is necessary to break a Cooper pair; in this case the role of the Cooper pairs is played by the Kondo singlets, while the condensate is the ground state $|KI\rangle$.

The reader should keep in mind this picture analyzing the paper C, because the result at half filling have exactly the same character. Moreover also the SSKI state away from half filling suggest an analogy with the physics of superconductivity.

Chapter 7

Introduction to Paper C

7.1 Majorana fermions and the Kondo lattice

A SPIN-1/2 SYSTEM can be represented and studied in terms of Majorana fermions [37, 38, 74, 221–224] and attempts to use the same approach have been made also in the Kondo lattice [36,225–227], in the two channel Kondo model [75] and in the t-J model [84]. As mentioned in Chapter 3 and explained thoroughly in paper A, $su(2)$ spin operators can be represented using three Majorana fermions μ_1, μ_2 and μ_3 as $S_k = -i\epsilon_{ijk}\mu_i\mu_j$. The description of low energy spin-1/2 degrees of freedom is very convenient in the three Majorana description, since it gives a faithful representation of them: *no constraint* must be enforced on the Majoranas in order to obtain that $S^2 = 3/4$. This is quite different than (for example) slave fermions techniques, where the spins are represented in terms of projected f-impurity fermions [172]. Because of this reason, an optimized trial state constructed using the Majorana representation of the spins is a *strict variational upper bound* to the true ground state energy [226], although some care has to be taken when studying the system [228]. Although interesting this is not how the Majroana representation has been thought and used in paper C, where instead the spirit of paper A has been followed.

In paper C the three Majorana representation of the spins, applied to the KL model, is seen as the result of the Schrieffer-Wolff transformation. This is easily understood using the example (3.2.2), since the term (3.17) appears in the symmetric PAM as in (6.3) and it is the limit of its coupling constant $U \to +\infty$ that gives rise to the KL model. In fact, the local interacting term of the f-electrons in the symmetric PAM is:

$$U\left(f_\uparrow^\dagger f_\uparrow - \frac{1}{2}\right)\left(f_\downarrow^\dagger f_\downarrow - \frac{1}{2}\right) = U\mu_1\mu_2\mu_3\mu_4, \tag{7.1}$$

where

$$f^\dagger = \begin{pmatrix} \frac{\mu_1 + i\mu_2}{\sqrt{2}} \\ \\ \frac{-\mu_3 + i\mu_4}{\sqrt{2}} \end{pmatrix}. \tag{7.2}$$

In the light of the concepts explained in paper A and Section 3.2, it is clear that if the f-impurity fermions are represented in terms of their holon and hyperspin

components, then it is straightforward to identify the energy separation of the Hilbert space of the local f-electrons into two sectors: the low energy sector at $-U/4$, containing the states with one f-holon (i.e. one f-fermion)

$$h_f^\dagger = \left[(2i\mu_1\mu_2\mu_3) + i\mu_4\right]/\sqrt{2}$$

on each site, and the high energy at $U/4$ containing those with no holon present (i.e. empty or doubly occupied). The rationale behind of the shift $-U/4$ in (7.1) thus becomes clear, so it is convenient to cancel it adding an extra $U/4$ to the symmetric PAM Hamiltonian, retrieving its typical form (6.3). As explained previously, the local low energy space of the f-impurity sector of the theory is two dimensional, because of the hyperspin sector of the Hilbert space:

$$\mathcal{H}_{f,\text{low}} = |1_{f,\text{holon}}\rangle \otimes \{|\Uparrow\rangle_f, |\Downarrow\rangle_f\} = \{|\uparrow\rangle_f, |\downarrow\rangle_f\}.$$

It is clear that these states are associated with the local quantum levels of the impurity spins. The total local Hilbert space is therefore obtained multiplying $\mathcal{H}_{f,\text{low}}$ by the (local) conduction electron Hilbert space, spanned by

$$\{|0\rangle_c, |\uparrow\rangle_c, |\downarrow\rangle_c, |\uparrow\downarrow\rangle_c\}.$$

As a consequence, the KL Hamiltonian can be rewritten in terms of the four Majoranas of the conduction electrons $\gamma_1, \gamma_2, \gamma_3, \gamma_4$, plus the three Majoranas μ_1, μ_2, μ_3 that appear in the $su(2)$ spin operators, which in the U infinite limit coincide exactly with the hyperspin ones. This Majorana form of the Hamiltonian can be obtained also without any prior knowledge about the non-linear transformations of the Hilbert space, starting from the original KL model and using the Majorana based representation of the impurity spin operators [74]. Choosing the same gauge (7.2) for the representation of both the f and c spinors, the KL Hamiltonian represented on the Majorana fermions is thus:

$$\begin{aligned} H_{KL} \;=\; & -it\sum_i \left(\gamma_{2,i}\gamma_{1,i+1} - \gamma_{1,i}\gamma_{2,i+1} - \gamma_{4,i}\gamma_{3,i+i} + \gamma_{3,i}\gamma_{4,i+i}\right) + \\ & -\mu^* \sum_i (1 - i\gamma_1\gamma_2 + i\gamma_3\gamma_4) + J\sum_i \sum_\alpha S^\alpha_{c,i} S^\alpha_{f,i}, \end{aligned} \tag{7.3}$$

where the $S^\alpha_{f,i}$ are the $su(2)$ operators of the holon-spinon representation of the f-fermions operators (the sum on the indices is suppressed):

$$S^\alpha_f = -i\epsilon_{\alpha\beta\sigma}\mu_\beta\mu_\sigma,$$

and the S^α_c are instead the spin operators of the conduction electrons. Using the usual fermionic representation

$$S^\alpha_c = \frac{1}{2}\left(c^\dagger_\uparrow, c^\dagger_\downarrow\right)\sigma^\alpha_{a,b}\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}, \tag{7.4}$$

one discovers that

$$S^x_c = -i\frac{\gamma_2\gamma_3 + \gamma_1\gamma_4}{2}, \quad S^y_c = -i\frac{\gamma_3\gamma_1 + \gamma_2\gamma_4}{2}, \quad S^z_c = -i\frac{\gamma_1\gamma_2 + \gamma_3\gamma_4}{2}. \tag{7.5}$$

The different form of these operators, with respect to the f-impurity ones, is due to the fact that in the case of the f-impurity fermions the constraint of unit

occupancy of the holon is fulfilled exactly in the Hilbert space of the KL, so the hyperspin operators coincide with the spin ones. This is clearly not true for the c-fermions, where the dynamic of the c-holon is not (in general) frozen by the interaction. So all four γ_i Majoranas are still present.

Looking at (7.3) one can understand that there is an annoying feature hidden within this representation: the presence of the extra third Majorana in the spin representation, i.e. the fact that seven Majoranas and not six are in the Hamiltonian. This feature was present also in the original works by Coleman, Miranda and Tsvelik [225–227], who tried to follow this path. An innovative way to look at it was developed few years ago and can be found in Ref. [229]. In that work it was pointed out that an exchange of the Majorana γ_4 with the three-composite $2i\mu_1\mu_2\mu_3$ is a proper unitary transformation, that leaves the Hamiltonian with six Majoranas; *in other words it was proved that one of the Majoranas is actually redundant, so in this representation a half-fermion degree of freedom is unnecessary.* Performing this exchange, the six Majoranas left can be recombined into three spinless fermion which are enough to describe the local Hilbert spaces of the KL. Of course there exists quite an arbitrariness in the definition of these three fermions, since the six Majoranas can be combined in many different ways. The original proof makes use of the numerical procedure described in Ref. [26]; in paper C a mapping that permits verification of the validity of the transformation by direct inspection is elaborated and then the new three fermion representation is used in the analysis of the KL.

Formally the exchange

$$\gamma_4 \longleftrightarrow 2i\mu_1\mu_2\mu_3, \tag{7.6}$$

is performed by a non-linear transformation of the degrees of freedom. This transformation is generated by an object of the kind shown in (3.14); in terms of Majoranas the transformation[1] is given by

$$R = \exp\left\{-i\frac{\pi}{2}\gamma_4\mu_1\mu_2\mu_3\right\}. \tag{7.7}$$

Clearly this transformation is not at all different from the transformation (3.14). The real difference between the two situations is that in this case the Hilbert space is the 8 dimensional Kondo one, so the effect of these kinds of non-linear transformations is not as trivial as in the Hubbard case. One can consider this transformation as a final part of the Schrieffer-Wolff one, able to turn it into a canonical transformation, i.e. a transformation that starts from a fermionic description of the PAM and gives a fermionic representation of its low energy sector (the KL).

It is important to stress that the final representation of the local KL Hilbert space is in terms of *three unconstrained fermionic* degrees of freedom. This goes much beyond the previous purely fermionic representations of the KL, that instead required the presence of four *constrained* fermions. Our representation is instead *constraint free* and faithful, generating no extra states in the Hilbert space. Equivalently, our transformation realizes an *analytically exact* implementation of the constraint of unit occupancy of the f-electron states. The final form

[1] For sake of elegance in this formula the convention of (3.14) is used, where the Majoranas have the property $\gamma^2 = 1$, so the generated exchange is $\gamma_4 \longleftrightarrow i\mu_1\mu_2\mu_3$. In the other convention instead it becomes $4i\gamma_4\mu_1\mu_2\mu_3$, which also squares to -1.

of the Hamiltonian is:

$$\begin{aligned} H_M &= -it\sum_n \left(\gamma_{2,n}\gamma_{1,n+1} - \gamma_{1,n}\gamma_{2,n+1} + \gamma_{3,n}\gamma_{0,n+1} - \gamma_{0,i}\gamma_{3,n+1}\right) + \\ &+\frac{J}{4}\sum_n i\left(\gamma_{1,n}\mu_{1,n} + \gamma_{2,n}\mu_{2,n} + \gamma_{3,n}\mu_{3,n}\right) + \\ &+\frac{J}{2}\sum_n \left(\gamma_{2,n}\mu_{2,n}\gamma_{3,n}\mu_{3,n} + \gamma_{1,n}\mu_{1,n}\gamma_{3,n}\mu_{3,n} + \gamma_{1,n}\mu_{1,n}\gamma_{2,n}\mu_{2,n}\right) + \\ &-\mu^*\sum_n \left(1 - i\gamma_{1,n}\gamma_{1,n} - i\gamma_{0,n}\gamma_{3,n}\right), \end{aligned} \tag{7.8}$$

with

$$\gamma_0 = 2i\mu_1\mu_2\mu_3,$$

used as short-hand notation. Of course the final non-linear transformation makes the kinetic term more involved, exactly as the similar ones used in the Hubbard [25,83] and t-J model [85–88] do; the interacting term becomes instead partially quadratic. Moreover it is interesting to point out the nature of the final c-density term, which is now partially quartic.

The studies in papers C and D tackle the previous Hamiltonian in two different ways. In paper C the fact the final Hamiltonian can be represented in terms of fermions only is used; in paper D an approach that instead relies only on the Majorana representation is developed.

7.1.1 Non-Linear Mean-Field study

In paper C we used the fact that the the Hamiltonian (7.8) can be represented in terms of three fermions only. Starting from the six Majoranas $\gamma_1, \gamma_2, \gamma_3$, μ_1, μ_2, μ_3, the (ad hoc) built fermionic operators are:

$$c^\dagger = \frac{\gamma_1 + i\gamma_2}{\sqrt{2}}, \quad f^\dagger = \frac{\mu_1 + i\mu_2}{\sqrt{2}}, \quad g^\dagger = \frac{\gamma_3 + i\mu_3}{\sqrt{2}}. \tag{7.9}$$

With these definitions the eight states of the local Hilbert space of the KL acquire a fermionic structure and an exact map, shown in Section III of paper C, between the new representation and the old one (in terms of conduction electrons and impurity spins) is established. For the sake of completeness I report here also the representation of the the cgf-fermions creation and annihilation operators in terms of the previous conduction electrons and impurity spin operators.

$$c^\dagger = c^\dagger_\uparrow, \tag{7.10}$$

$$g^\dagger = -\frac{1}{2}\left(c^\dagger_\downarrow + c_\downarrow + (c^\dagger_\downarrow - c_\downarrow)2S^z_f\right), \tag{7.11}$$

$$f^\dagger = -i(c_\downarrow - c^\dagger_\downarrow)S^+. \tag{7.12}$$

From a formal point of view, this mapping creates a new spinor, based on the $SU(3)$ symmetry group. In fact the three singly occupied states form an irreducible representation of the $SU(3)$ group, whose generators can be expressed

in terms of combinations of bilinear and quadrilinear Majorana[2] operators. Although interesting, this aspect is is not developed in the paper.

Of course the map established in (7.9), from now on called *cgf-map*, is not unique, but this particular choice is quite appropriate for the description of the ferromagnetic phases of the KL. This can be understood by representing and studying the Hamiltonian in terms of the cgf-fermions:

$$H_{cgf} = H_c + H_{de} + H_J + H_{\text{chem}}, \tag{7.13}$$

with

$$H_c = -t \sum_{n,\delta} \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right), \tag{7.14}$$

$$\begin{aligned} H_{de} \;=\; & +t \sum_{n,\delta} \Big\{ \Big(\frac{1}{2} - f_n^\dagger f_n \Big) \Big(g_n^\dagger - g_n \Big) \Big(g_{n+1}^\dagger + g_{n+1} \Big) + \\ & - \Big(\frac{1}{2} - f_{n+1}^\dagger f_{n+1} \Big) \Big(g_n^\dagger + g_n \Big) \Big(g_{n+1}^\dagger - g_{n+1} \Big) \Big\}, \end{aligned} \tag{7.15}$$

$$\begin{aligned} H_J \;=\; & \frac{J}{4} \sum_n \left(1 - c_n^\dagger c_n - f_n^\dagger f_n - g_n^\dagger g_n + 2 c_n^\dagger c_n f_n^\dagger f_n \right) + \\ & + \frac{J}{4} \sum_n 2 g_n^\dagger g_n \left\{ i (c_n^\dagger f_n - f_n^\dagger c_n) \right\}. \end{aligned} \tag{7.16}$$

The last term H_{chem} is given by the chemical potential:

$$H_{\text{chem}} = -\mu^* \sum_n \left(c_n^\dagger c_n - f_n^\dagger f_n - g_n^\dagger g_n + 2 f_n^\dagger f_n g_n^\dagger g_n + 1 \right).$$

There are two unusual features in this Hamiltonian: the presence of an involved hopping term H_{de}, that correlates the hopping of the fermion g with the density of the fermion f; the partial quartic form of the conduction electron density operator.

Of course to treat this Hamiltonian some approximations must be used. In paper C the simplest possible treatment is undertaken: a mean-field approximation. In order to do this, a symmetry that simplifies the problem is identified and imposed. It is in fact easy to check that the operator

$$\sum_n A_3(n) = \sum_n \left\{ i \gamma_1(n) \gamma_2(n) + i \mu_1(n) \mu_2(n) \right\}, \tag{7.17}$$

commutes with the Hamiltonian (7.13). We decided to keep this symmetry, enforcing it also at the mean-field level, and so simplifying significantly the problem. In fact all the hybridization channels between the g-fermions and the other two get closed, together with all the superconducting c-f hybridization channels. The mean field Hamiltonian gets thus separated into two parts: a c-f part and a g part, and no quantum process, but only semiclassical ones (via

[2]Of course these operators can also be written in the original conduction electron creation and annihilation operators, together with the impurity spin ones.

the mean-fields), connect these two sectors. These two parts can be found in Section IV of paper C and I rewrite here only the kinetic term of the g-fermions, that comes from H_{de}:

$$H_g^{MF-de} = t\sum_n \Big\{ \Big(\frac{1}{2} - \mathcal{F}_n\Big)\Big(g_n^\dagger - g_n\Big)\Big(g_{n+1}^\dagger + g_{n+1}\Big) + \\ -\Big(\frac{1}{2} - \mathcal{F}_{n+1}\Big)\Big(g_n^\dagger + g_n\Big)\Big(g_{n+1}^\dagger - g_{n+1}\Big)\Big\}. \tag{7.18}$$

Evidently if the mean-field $\mathcal{F}_n = \langle f_n^\dagger f_n\rangle$ has no spatial modulation (i.e. it is the same on each site n), then a common factor can be gathered in front of the sum, leading to

$$H_g^{MF-de} = \left(\frac{1}{2} - \mathcal{F}\right) 2t \sum_n \left(g^\dagger \tilde{g} + \tilde{g}^\dagger g\right), \tag{7.19}$$

that is a normal fermion hopping term, with a renormalized bandwidth. If now one notices that according to (7.12)

$$\frac{1}{2} - \mathcal{F}_n = \frac{1}{2} - \langle f^\dagger(n) f(n)\rangle = \langle -S^z(n)\rangle, \tag{7.20}$$

with $S^z(n)$ the spin operator of the impurity spin on the nth site, then it becomes clear that the renormalization term in front of H_g^{MF-de} has purely magnetic origin. If the KL is ordered ferromagnetically and fully polarized, then the kinetic term of the g-fermions is maximal; instead if the polarization is partial, because some spins are reversed by the Kondo scattering, then the hopping of the g-fermions becomes (on the average) more difficult and the kinetic term looses efficiency. *This looks very much like the double exchange effect.* This interpretation is also supported by a quick look at (7.11) where it is evident that if $\langle S^z(n)\rangle = 1/2$, then $g^\dagger = c_\downarrow^\dagger$. So if the impurity spins are fully polarized and have ferromagnetic order then the g- and $c_\downarrow$-fermions coincide. Therefore the g-sector of the mean-field Hamiltonian describes the majority electrons.

It is worth pointing out that a renormalization effect of the conduction band is obtained naturally, *at mean field level*, in our formalism. Typically, to observe such effects, much more involved techniques (such as Gutzwiller projection) must be used. This is an indication of the large number of physical effects that can be addressed when studying a system using Majoranas and non-linear transformations.

Another interesting property that strongly suggests that this formalism is very much suited to the study of the ferromagnetic region of the KL, is the fact that the symmetry operator (7.17), can be rewritten as

$$\sum_n A_3(n) = \frac{1}{2}\left(2S_f^z + \hat{n}_c + \hat{m} - 1\right), \tag{7.21}$$

with $\hat{n}_c = c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow$, $\hat{m} = c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow$. So at mean-field level, this necessarily implies that

$$C = 2\langle S_f^z\rangle + \langle n_c\rangle + \langle m\rangle - 1, \tag{7.22}$$

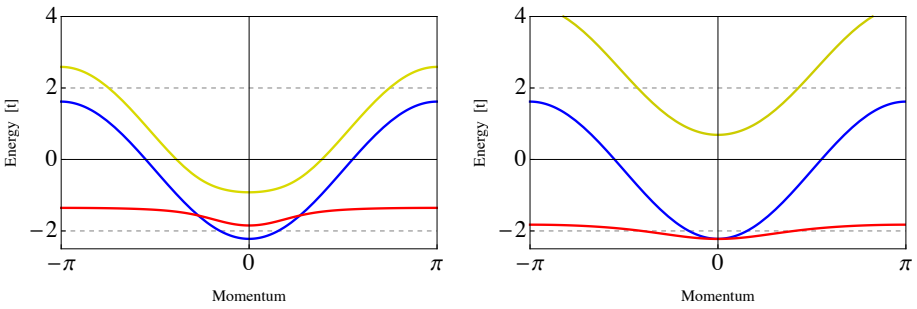
with C a real constant. This is *exactly* the same unusual commensurability operator (6.46) discovered in 2012 [192]. The mean-field analysis of the solutions

(see paper C) reveals that there exists a large region of the mean-field phase diagram that occupies the same position of the SSKI and that also has $C = 0$, in *perfect agreement* with the DMRG results.

The detailed characterization of the mean-field solutions can be found in the appended paper, so I will not repeat it here. The analysis shows, at low coupling J, the existence of two translational invariant, magnetic, possible configurations of the ground state. The first (FM-I) has the characteristics of the SSKI, so the local spins have ferromangnetic order, the commensurability parameter is zero, the total spin polarization follows a linear dependence with the electron density[3] and there exist a big imbalance between the populations of $c_\uparrow$ (minority) and $c_\downarrow$ (majority) electron species. For a critical, J-dependent, value of the electron density $n_{crit}(J)$ the FM-I phase experiences a second order phase transition and turns into a second ferromagnetic phase FM-II, which survives up to half-filling. The transition line, for $J \lesssim 2$, is quite close to the known FM-PM transition line characterized by the DMRG studies, so the FM-II phase is located inside the paramagnetic dome. This phase competes with the spiral spin ordered mean-field solutions (which are the best mean field realization of the RKKY liquid phase), and (surprisingly) outperforms them also at very low couplings, showing the importance of the entanglement between the spins and the electrons, which evidently is more important than effect of non-local ordering. The FM-II is therefore a possible ferromagnetic trial ground state, which beats the spiral ordered mean-field solution and that extends up to half-filling. Indeed it seems a *perfect natural mean-field candidate for ground state of the phase in the ferromagnetic tongue*. Moreover, exactly as the ferromagnetic tongue, this FM-II phase disappears for $J \gtrsim 2$. To my knowledge, there are no other theoretical proposals that are able to justify the ferromagnetic tongue, i.e. that are able to describe a low energy ferromagnetic state (able to outperform energetically the spiral spin ordered mean-field state) at fillings $n_c \gtrsim 1/2$. Of course this state should compete also with non-translationally invariant states, i.e. where the mean-fields have a space modulation. Such states should be energetically much better than the usual spiral spin ordered mean-field state, because they take into account more of the Kondo interaction, and I expect that they should represent the phase of the wild zones. Moreover they cannot be studied efficiently following the same procedure chosen for the translationally invariant phase, but it is our belief that following some of the ideas of paper D, something about such RKKY-Kondo competition could be learnt.

Returning to the FM-I and FM-II phases, the difference between the two is found in the different nature of the electronic wave functions. In the FM-I phase, as can be seen in paper C, the $c_\downarrow$ (majority) electrons have a Fermi surface, while the $c_\uparrow$ electrons do not. This is due to the fact that the $c_\uparrow$ (minority) electrons exist in the FM-I (SKKI) phase only as *part of a delocalized Kondo singlet*; there are *no free* minority electrons, but only the ones bound to a spin-flip processes. This is the nature of the spin-selective Kondo insulator, that is captured very well by the cgf-mapping. In fact the c and f bands have the typical shape of the Kondo singlet bands (the same shape that appears at half filling, see discussion in paper C and Sec. 6.1), which is the typical avoided crossing structure common

[3] As proved in Ref. [192] this is a direct consequence of the value of the commensurability parameter. Moreover I must point out that we have chosen a different convention for the direction of the $\hat{z}$ polarization axis, so the commensurability operator discussed by Peters is mapped into (7.22) by the inversion operation $s^z \to -S^z$, $m \to -m$.



(a) *FM-II,* $x = 1.4$ *and* $n_c = 0.95$*;* **(b)** *FM-I,* $x = 2.8$ *and* $n_c = 0.67$*;*

Figure 7.1: *The mean-field band structure of the* cgf*-Hamiltonian. The blue line represents the g-fermions, while the red an yellow one are the f-like and c-like bands. As can be seen only the g-fermions cross the chemical potential, set at the level zero. In the two examples: (a) FM-II mean-field band structure; (b) FM-I mean-field band-structure. Both figures are taken from paper C.*

to any heavy fermion theory (see figures 7.1a, 7.1b and 6.2b). It must be kept in mind that only a part of the $c_\downarrow$ (majority) electrons is represented in the g-fermions in this phase. A part is into the f-fermion, and in fact a part of the $c_\downarrow$ electron wave function is necessary to create the Kondo singlets.

This configuration, which requires a high imbalance between the majority and minority electron densities, becomes unstable if the total density is too big. For $n_c > n_{crit}(J)$ some $c_\uparrow$ electrons are able to escape from the bonding process and create a Fermi surface (Fig. 7.1a). The SSKI is still partially present, but becomes less and less pronounced upon increasing the density, in the sense that less and less minority electrons form the Kondo singlets.

The success of the cgf-map in the description of the FM phases of the KL at low coupling is due to the asymmetric treatment of the the electron species, which fits very well with what is realized in nature with the asymmetry of the minority and majority electrons. The cgf-map links the breaking of the spin symmetry (ferromagnetic ordering) with the breaking of the electron symmetry between the two spin species. This can be seen in (7.19): evidently the same physics is obtained for both $\mathcal{F} > 1/2$ and $\mathcal{F} < 1/2$. In fact, even if the latter condition implies an upside-down g-band, it also causes an inversion in the meaning of the $g^\dagger$ operator that if $\mathcal{F} = 0$ is equal to $c_\downarrow$. So the transformation that inverts all the spins gets linked with the one that inverts creation-annihilation operators in the majority electron channel, changing the vacuum of g and implying a total null effect. As long as the asymmetry in the spin and electron species is kept, one expect the cgf-map to work well. Instead when this asymmetry is at stake, i.e. when $\mathcal{F}$ approaches $1/2$, meaning that the filled f-like band (red line in 7.1a) approaches the Fermi level, the cgf-map cannot work. This is why for $J \gtrsim 2$ the mean field solution is not able to describe the polaronic liquid phase, but it can only see a first order phase transition between the half-filled solution and the one at $n_{crit}(J)$. This transition is consistent with the picture of polarons that melt into the polaronic liquid, but since the latter is a true paramagnetic phase it cannot be described by this cgf mean-field analysis. Allowing

for the hybridization of the g fermion with the other two this problem could be, in principle, solved. However we have not yet examined this possibility.

Increasing further still the coupling ($J \gtrsim 6$), the solutions become quite meaningless. I believe that this is due to the fact that, although at high coupling the ground state is ferromagnetic for every filling, the SSKI (as it has been described in the previous paragraphs) is not anymore the mechanism that stabilizes it, but something different must happen.

This mean field analysis produces interesting results also at half filling. In that zone of the phase diagram two ground-states for $J < 2$ and $J > 2$ can be found. The first is the ferromagnetic FM-II one, while the second is the Kondo Insulating (KI) one, which tends asymptotically to the state with one Kondo singlet per site at $J \to +\infty$. The ferromagnetic one is expected to be overtaken by an analogous antiferromagnetic one, so it is not worth further considerations. More interesting is the KI solution, which shows how the weight of the ground state wavefunction is moved from the triplet to the singlet sector increasing J. In the cgf-framework it is possible to characterize very well the quasi-particle gap of the KI state, which can be measured studying how the critical μ^*, which determines the breakdown (the disappearence) of the half-filled solution, evolves with J. This result is consistent with the perturbative approximations around the $J \to +\infty$ ground state, but differently from those, it does not share the unphysical behavior for small J. Moreover the physical picture is very similar to that explained in Ref. [165, 218] and in Sec. 6.3.

Although vaguely successful the mean-field analysis of the cgf Hamiltonian is not the best way to study the half-filled ground state. This is due to the fact that the important competition is between the RKKY effect and the Kondo effect. In the mean-field analysis the RKKY effect was suppressed; keeping the mean field approach it could be possible to consider it, enlarging the unit cell used for the analysis. This causes many computational problems (related to an excessive number of the mean-field solutions and an excessively high dimensional mean-field parameter space), so probably it does not represent the best way to proceed. A different approach has been attempted in paper D. To understand how to join the RKKY and the Kondo effect is important for the study of the wild zones in the phase diagram away from half-filling, so it seems natural to perform a complete study of the half-filled case, where the ferromagnetism is not present and there exists a cross-over between a local antiferromagnetic regime and the KI phase, and then later to apply the same techniques away from it.

7.1.2 Analogies with previous studies

The composite fermion: It is appropriate to point out an interesting connection existing between the fermionic degrees of freedom defined by the cgf-map and those successfully used in other studies of similar systems. I refer in particular to the composite heavy fermion picture developed by Coleman [133]. In that approach the local spins are represented making use of the "pseudo-fermions",

$$\sigma_{\alpha,\beta} f^\dagger_\alpha(j) f_\beta(j), \tag{7.23}$$

with $\sigma_{\alpha,\beta}$ an N-dimensional representation of the Pauli matrices; in the normal KL case $N = 2$. It becomes possible to decompose the Kondo interaction, now

in the form of the four fermion interaction

$$H_J = \frac{J}{2}\sigma_{\alpha,\beta} f^\dagger_\alpha(j) f_\beta(j) c^\dagger_\beta(j) c_\alpha(j), \tag{7.24}$$

with an Hubbard-Stratonovich transformation, introducing a dynamical complex bosonic field $V(j)$:

$$H_J \to H_J[V,j] = V^*(j)\left(c^\dagger_\beta(j) f_\beta(j)\right) + V(j)\left(f^\dagger_\alpha(j) c_\alpha(j)\right) + 2\frac{V^*(j)V(j)}{J}.$$

Typically this operation is carried out in path-integral formalism, so the bosonic (quantum[4]) field that decouples the interaction describes the fluctuating hybridization between the conduction electrons and the pseudo-fermion (i.e., the spins, if the constraint of unity occupancy is enforced). Typically it is difficult to study the full Hamiltonian, so only the large N-limit is considered (*large N-approximation*; in the previous formulas the 2 gets substituted by an N), where N is the number of possible projections of the total spin of the local impurities (which becomes the number of N species of f-electrons). In that approximation the path integral becomes dominated by the saddle points of the V Lagranigian. The large N approximation also solves another complicated issue. In fact a constraint has to be enforced on the pseudo-fermions, in order to imply the unit occupancy in the case of $N = 2$. In the case of larger N the different constraint $\langle n^f_{tot}\rangle = N/2$ has to be imposed [133], in order to obtain results that should mimic the physics of the $N = 2$ case. To enforce this occupancy a dynamic chemical potential (which must become an integration variable in the path integral) can be used. In the large N approximation the contribution from this term is also dominated by its saddle point configuration and so it is easy to handle.

The final picture that arises from this treatment is that of a "composite fermion", built by the conduction electron bound to a spin-flip of the local moment [133]

$$\frac{1}{N}\sigma_{\alpha\beta} c_\alpha \to \left(\frac{V^*}{J}\right) f_\beta, \tag{7.25}$$

so there exists a correlation between adding an electron and causing a spin flip on the same site. These objects behave as fermions and come from a mix of the spin impurity and the conduction electron operators. The parallelism with the f-fermion of the cgf-map:

$$f^\dagger = -i(c_\downarrow - c^\dagger_\downarrow)S^+, \tag{7.26}$$

is interesting and realizes almost the same operation. Clearly it is different from the composite fermion introduced by Coleman, but it is also true that the f-fermion of the cgf-map is a proper fermionic degree of freedom at $N = 2$, while the same assertion is more problematic for the composite fermion. This is of course due to the fact the the cgf-map requires no constraint to be enforced.

Confined and deconfined particles: I would like to suggest to the reader another parallelism existing between this work and a nice result obtained by

[4]This means that the field is one of the integration variables of the path-intagral.

Pépin in Ref. [164]. That paper deals with the description of the quantum critical point, between the AFM phase and the Fermi liquid with large Fermi surface (Kondo phase), that exists in the Kondo-Heisenberg model in more than one dimension. In that case the author used the Schwinger boson representation of the local impurity spins and suggested that a fermion is "released" when the Kondo singlets experience, reducing the coupling J, a process of deconfinment. The net result of this deconfinement process is the appearance of a spinless gapless fermion. My personal feeling is that this fermion is (somehow) related to the g fermion; I expect that a similar picture could hold also in the 1d KL at half filling. At high J the g fermion band is "frozen" because it is fully occupied; decreasing the coupling, the shape of the band changes, getting renormalized, and moves upon approaching the Fermi surface. So at some J I would expect some states to become unfilled and that the g-fermions will become relevant for the dynamics.

The proposal in Ref. [164] has many similarities with this picture, although it is clearly very different (and still suffers from an approximate realization of the constraint on the Schwinger bosons). Anyway, this kind of deconfinment process, that were also encountered reviewing the properties of the 1dKL, appear to be more and more meaningful and this idea is present in many works [103, 162, 169, 183] that deal with the transition from the Kondo phase to the magnetically ordered one. It is however interesting that this concept also appeared in some works dealing with the t-J model [85–88], as a consequence of a non-linear unitary transformation of the Hilbert space. This generates an immediate consideration about the fact that in our Majorana based description of the KL, we deal with the object γ_0, that is formed by "gluing together" three Majoranas. *Is it possible that the process that moves weight from the "compact" object γ_0, to its components μ_1, μ_2, μ_3, describes naturally these kinds of deconfining processes?* This was the question that we sought to answer in Paper D.

7.2 Achievements of paper C

It is appropriate to summarize briefly and schematically the main achievements described in the appended manuscript:

- definition of the cgf-map, i.e., of an unconstrained purely fermionic description of the Kondo Lattice model;
- alternative demonstration, by direct inspection, of the faithful representation of the KL Hamiltonian in the Majorana representation;
- identification in the cgf-form of the 1dKL Hamiltonian of a term responsible for double exchange mechanism;
- discovery of the symmetry responsible for the definition of the "commensurability parameter";
- justification of the ferromagnetic phase in the 1dKL phase diagram, via simple mean-field analysis; this considerably improves the existing known mean-field solutions;

- identification of the phase FM-I with the SSKI phase; moreover a simple interpretation of the latter and of its physics was provided;
- discovery of a mean-field ground state that could be a prototypical state for the description of the ferromagnetic tongue inside the paramagnetic dome; so far (to the best of my knowledge) this represents the only mean field theoretical proposal able to justify this ferromagnetic phase;
- characterization of the ferromagnetic tongue and identification of the reasons behind its high stability;
- recognition of the important role of the confinement of the fermionic degrees of freedom into composite particles; this is evidenced by the SSKI phase, and by the KI phase at half-filling, which matches the known properties $J \to +\infty$;
- characterization of the quasiparticle gap in the half-filled case, consistent with known perturbative results;
- confirmation of the Doniach picture at half-filling, where the AF and KI phases are (at mean-field level) dominant at $J \to 0$ and $J \to +\infty$ respectively.

Chapter 8

Introduction to paper D

In paper D we deal with the half-filled KL only, focusing on the magnetic and energetic properties of the ground state. In contrast to papers B and C the focus of this work is on the spatial correlations in the system, which we tried to capture using a very non trivial non-linear transformation in the Brillouin zone. Optimizing this transformation with respect to the energy of the ground state, we identified a process of "deconfinement" of the composite Majorana, which was introduced in the previous chapter. The paper is divided into two parts: in the first one we perform a variational study of the ground state, building on the idea of the existence of a deconfinement process for the Majoranas; in the second we develop some easy-to-handle rules to work with Majorana fermion Hamiltonians, in the path integral formalism, and to deal with the confinement/deconfinement process hypothesized in the first part in terms of the path integral.

8.1 Deconfinement of emergent Majoranas

The paper is a follow-up of Ref. [229], where a (Majorana based) variational optimization of the ground state was performed. In that work all the (good) low coupling variational ground states were magnetically ordered, so the spin rotation symmetry was broken. This is unacceptable for any prototype ground state of the 1dKL, and so the result needed significant improvements. In order to realize them, we started from the quadratic part of the Majorana Hamiltonian (7.8), analyzing it in Fourier space. It must be pointed out that we chose a different gauge for the Majoranas with respect to paper C. The gauge transformation used is

$$c^\dagger_\uparrow(r_i) \to e^{i\frac{\pi}{2}r_i} c^\dagger_\uparrow(r_i), \qquad c^\dagger_\downarrow(r_i) \to e^{i\frac{\pi}{2}r_i} c^\dagger_\downarrow(r_i).$$

This affects the form of the kinetic term that becomes

$$H = it \sum_{a=0}^{3} \sum_i \gamma_a(i+1)\gamma_a(i), \tag{8.1}$$

where γ_0 is still $2i\mu_1\mu_2\mu_3$, so the kinetic term contains three quadratic terms ($a = 1, 2, 3$) and one six-fermion term ($a = 0$). The three quadratic parts,

together with the quadratic operators coming from the J-dependent interaction part, form a quadratic Hamiltonian $H^{(2)}$.

It is straightforward to see that $H^{(2)}$ is diagonalized by a linear combination of the Majorana operators in the halved BZ. We parametrized the unitary transformation[1] with a k-dependent angle α_k.

$$\begin{aligned}\tilde{\mu}_a(k) = &\quad \cos(\alpha_k/2)\mu_a(k) + i\sin(\alpha_k/2)\gamma_a(k),\\ \tilde{\gamma}_a(k) = &\quad \cos(\alpha_k/2)\gamma_a(k) + i\sin(\alpha_k/2)\mu_a(k).\end{aligned}$$

Anyway we did not chose the angle α_k to diagonalize the quadratic part of the Hamiltonian, but we kept it as a free variational (functional) parameter, that has to be optimized to minimize the total energy, taking into account also the effect of the four- and six-fermion terms.

In order to do this we studied how the rotation in the BZ affects the Majoranas in real space and we discovered that the new set of Majoranas was formed making a linear combination of μ and γ that belong to different sites. So performing the rotation in the halved BZ, one obtains a non-local transformation of the original Majorana set. We then rewrote the total Hamiltonian in terms of this new set of Majoranas, and then computed its average on two different trial ground states.

In the first trial state we consider that

$$\begin{aligned}\langle\tilde{\gamma}_a^\dagger(k)\tilde{\gamma}_a(k)\rangle = 0 \text{ or } 1 \quad &\text{for } a = 0,1,2,3,\\ \langle\tilde{S}_a(r_i)S_b(r_j)\rangle = \delta_{ab}\delta_{ij}/4, \quad &\text{with} \quad \tilde{S}_a(r_i) = -i\epsilon_{abc}\tilde{\mu}_a(r_i)\tilde{\mu}_b(r_i). \qquad (8.2)\end{aligned}$$

These conditions mean that we considered the Majorana $\tilde{\gamma}_0$, together with the other ones, as the fundamental degrees of freedom. In practice we assumed that this Majorana fermion is like a well defined single particle. Since $\tilde{\gamma}_0(r_i) = 2i\tilde{\mu}_1(r_i)\tilde{\mu}_2(r_i)\tilde{\mu}_3(r_i)$ it is natural to think of this particle as a confined state of three Majoranas. At $J \to 0$ the angle α_k goes to zero, so

$$\tilde{\gamma}_0(r_i) \to 2i\mu_1(r_i)\mu_2(r_i)\mu_3(r_i).$$

Vice versa, increasing the angle, the contribution to $\tilde{\gamma}_0$ of the Majoranas that belong to different sites, becomes more and more important. At the same time it can be seen that this causes a reduction of the renormalization factor in front of the kinetic term, that in turn implies a decrease of the kinetic energy gained by the hopping processes of the γ_0 Majorana. We used these features to mimic the deconfinement process of the Majoranas μ_1, μ_2 and μ_3. At $J \to 0$ the three Majoranas can be thought of as forming a sort of "hard" bound state γ_0, that behaves as a single whole object, coherently hopping from site to site. Increasing the coupling more and more, the size of the γ_0 object becomes bigger and bigger and its hopping, generated by a less and less coherent hopping of the constituent Majoranas, becomes less efficient. This effective "soft" bound state is represented by the local $\tilde{\gamma}_0$ that in fact is built using Majoranas from different sites (and of course mixing μ and γ components). In this process the configuration of the rotated spin operators $\tilde{S}_a(r_i) = -i\epsilon_{abc}\tilde{\mu}_a(r_i)\tilde{\mu}_b(r_i)$ simply helps to optimize the final configuration, whose energy depends also on the internal structure of

[1] I remind the reader that in the halved BZ the Majorana operators behave as standard fermion operators.

the soft bound state $\tilde{\gamma}_0$. To impose a correlation (or complete de-correlation in this case) on the rotated spin correlation function has the physical meaning of imposing a correlation between the impurity spins on different sites and with the electron spins. However, the optimized solution reveals a predisposition towards antiferromagnetic correlation functions also imposing no correlation on the rotated spins. It is important to stress that this is very different with respect to the imposition of an order; as a consequence our state is able to be non-magnetic, although magnetic correlations exist.

The result of the optimization can be found in the paper. The angle α_k has been optimized on the set of the continuous functions, i.e., Taylor expanding the function around $k = \pi/2$ and leaving the coefficients as free parameters; a good convergence of the results was obtained using only three or four orders in the k^n expansion. Qualitatively all the main features of the result are obtained already, simply with the k^0, i.e. $\alpha_k = \alpha = const$, approximation. As is shown in the paper the energy of our variational ground state has the correct (free) limit at $J \to 0$ and approaches it with the same behavior as the Neél ordered one, i.e., as J^2/t up to logarithmic corrections. *It is fundamental to stress that our trial ground state does not break the spin rotational symmetry*, but all the antiferromagnetic spin-spin correlation appear naturally and are short ranged. This is clearly in strong contrast with the Neél ordered state, where the antiferromagnetism is an input and the spin rotation symmetry is broken. In this sense our variational state is qualitatively closer to the real ground state, which also is a global singlet.

The variational result obtained in paper D improves significantly the previous, non-magnetic one, found in Ref. [229] and that instead describes the dynamics of the system considering the Majoranas μ_1, μ_2 and μ_3 as propagating independently. It is therefore natural that such a state becomes the energetically most favorable at high coupling, where one could imagine that the deconfinement process is so advanced and the $\tilde{\gamma}_0$ Majorana so soft, that the three Majoranas behave independently. This deconfined state is obtained imposing

$$\begin{aligned} \langle \tilde{\gamma}_a^\dagger(k)\tilde{\gamma}_a(k)\rangle &= 0 \quad \text{for } a = 1,2,3, \\ \langle \tilde{\mu}_a^\dagger(k)\tilde{\mu}_a(k)\rangle &= 1 \quad \text{for } a = 1,2,3. \end{aligned}$$

Although a bit exotic, the features of our confined Majoranas ground state are not completely new. In fact we obtain a variational band structure that resembles closely the one hypothesized by Coleman, Miranda and Tsvelik in Ref. [225–227]. These authors suggest also the persistence of a gapless Majorana band in the half-filled Kondo lattice. Besides the different techniques chosen for the calculation, the path followed by the two analyses is similar. Although in Ref. [225–227] the initial Hamiltonian is redundant (seven Majoranas are present), the three Majorana fermions representing the spins are integrated out. This operation causes the opening of a gap in three of the four Majorana modes coming from the free electron, while one remains gapless. It is not my purpose to create a bridge between these works and paper D, but anyway such a resemblance is suggestive.

8.2 Majorana Path Integral

A problem of the first part of the paper is that in principle the results can be significantly improved by considering different correlation functions between the rotated spins. In practice, however, this turns out to be complicated, because it is difficult to obtain a reliable perturbative recipe to order the (many) interaction terms. We understood that our analysis would have benefited by a change in the formalism used. In particular the path integral representation of the quantum mechanics seemed very convenient for our purposes.

Unfortunately we were not able to find any reference in the literature that explained how to use, in a practical way, the path integral formalism in imaginary time with Majorana Hamiltonians. We were aware of the fact that mathematically the path integral for Majorana Hamiltonians is as well defined as the one that deals with standard fermionic Hamiltonians (i.e. making use of Grassmann numbers), as demonstrated by Casalbuoni in Ref. [230] and Berezin and Marinov in Ref. [231]. These results have been applied to analyze spin systems represented in terms of Majorana fermions, in particular by Vieira and collaborators [36–38, 221–224], who developed interesting perturbative analysis and diagrammatic rules for their studies. Some standard literature mentions the possibility of building such path integrals to represent general fermionic Hamiltonians [232] and also uses the path-integral representation [233, 234], but without pointing out any clear standard recipe. A very complete, but extremely mathematical, reference can be found in Ref. [235], where it is clearly stated that there exists two possible ways to deal with Majorana path integrals: fermion halving, where the Majoranas in the Hamiltonian are paired up to form fermions, and fermion doubling where instead to the n Majoranas in the Hamiltonian are paired to another n Majoranas, forming in this different way the fermionic degrees of freedom on which the standard formalism can be applied.

All the previously cited literature follows the principle of fermion halving, and few among those works focus on the development of a formalism useful in condensed matter systems (where path integrals are often used to compute thermal averages). We tried instead to use the method of *fermion doubling*, in the imaginary time path integral. In doing so we obtained a general set of rules that can be followed to treat Hamiltonians written in terms of Majorana fermions. Our way to proceed seems very well suited for condensed matter problems and it requires no change in the existing technique. The reason behind the success of our approach lies in the fact that the addition of the n extra Majoranas permits us to rewrite everything in terms of Grassmann numbers using the standard definition of the Majorana variables: the Majorana operators are

$$\gamma_\alpha = \frac{c_\alpha + c_\alpha^\dagger}{\sqrt{2}}, \quad \mu_\alpha = i\frac{c_\alpha - c_\alpha^\dagger}{\sqrt{2}}, \tag{8.3}$$

where the set γ is formed by the original Majoranas, while the μ are those inserted by the doubling operation. So, since the Grassmann variables related to the operators c and $c^\dagger$ are ξ and ξ^*, then the Majorana variable of the path integral can be written as

$$\zeta = \frac{\xi + \xi^*}{\sqrt{2}}, \quad \text{and} \quad \nu = \frac{\xi - \xi^*}{\sqrt{2}} \tag{8.4}$$

and the measure form

$$d\xi d\xi^* = d\nu d\zeta, \tag{8.5}$$

with ξ, ξ^* two normal Grassmann numbers. The Majorana variables are a simple shorthand notation for these two linear combinations of the two independent Grassmann numbers; hence they must have Grassmann character too. Consequently we can use the standard formalism of Grassmann variables path integral. Of course, we expect that the (unphysical) ν-s do not enter into the dynamics, and in fact it is possible to integrate them out exactly, leaving an action that contains only the Grassmann variables ζ. The only difference in the final result, between the standard fermionic Lagrangians and the Majoranas Lagrangians, in our path integral formulation, is given by a modified time evolution.

We performed the continuum limit of our results, obtaining consistently the formulation described in Ref. [234]. Moreover we also performed a consistency check computing some trivial averages for a free Hamiltonian.

These results proved the reliability of our procedure, so we decided that an interesting test could be the direct application to the KL Hamiltonian in the confined phase. In that situation a more involved analysis is needed. In fact, as we have seen previously, the process that characterizes the ground state is a sort of deconfinement of the three Majoranas that form the γ_0. The operation of "gluing together" the three Majoranas is not straightforward, because it implies some kind of correlation between the propagators of the three different species, because the three (rotated) Majoranas have to propagate together in space and time. A nice way to deal with this effect is to perform a fermionic Hubbard-Stratonovich (FHS) transformation (exotic, but also used in Ref. [164]) to separate the two $\tilde{\gamma}_0$ terms of the kinetic term, i.e., the two three-Majorana components of the six fermion term. The new fermion field ξ, introduced by the FHS, is coupled (locally in space and time) to the $\tilde{\gamma}_0$ term and represents it effectively. Performing later a second Hubbard-Stratonovich using this time a $\mathbb{Z}_2$ gauge field to separate the $\mu_1\mu_2$ Majoranas from μ_3, it becomes possible to integrate out both μ_1 and μ_2, whose effect becomes summarized by the $\mathbb{Z}_2$ gauge field. The latter behaves like a phase multiplying the μ_3 Majorana and has no dynamics, so it can be gauged away, transforming the variables associated with μ_3. Finally the ξ field also can be integrated out, so the only term left gives back a simple action for the Majorana μ_3.

In practice all these passages permit description of the motion of $\tilde{\gamma}_0$ by the motion by μ_3. This is possible because it has been assumed that the rotated spin-spin correlation function is (8.2). If this is not the case the final action becomes more involved.

Once all of these passages have been done, it becomes possible to compute the average value of the Hamiltonian and the entropy contribution to the Free energy (which is the correct quantity to minimize in the case of finite temperature calculations). Keeping the α_k parametrization of the rotation, the Free energy can be optimized exactly as in the first part of the paper. However, differently from that situation, now it is possible to study in a more ordered and systematic way the effect of the other terms of the Hamiltonian and of different correlation between rotated spins. In this sense, we seem to have arrived at the discovery of a powerful tool in the fermion ξ introduced by the FHS, which will be subject of future studies.

8.3 Achievements of paper D

Here again, it is appropriate to summarize briefly and schematically the main achievements described in the appended manuscript:

- introduction of the deconfinement mechanism of the three composite Majorana object and definition of its connection with the physics of the 1dKL;
- realization of a variational trial state that is able to take into account the effect of the deconfinement;
- identification of non-magnetic trial ground states for the 1dKL at half filling, with the correct asymptotic behavior at $J \to 0$;
- determination of practical and general rules for the representation and analysis of Hamiltonians (actions) written in terms of Majoranas, in the path integral formalism;
- definition of strategies able to describe and treat the deconfinement process in the path integral formalism.

Part IV

Outlook and Appendices

Chapter 9

Conclusions

In this thesis I analyzed the possibilities offered by the study of Strongly Correlated Electron Systems in terms of Majorana fermions. Using this representation of the quantum degrees of freedom it becomes easy to understand the origin of the group of canonical transformations, in particular of its non-linear components. One could object that in many circumstances, in past decades, non-linear transformation have been used to simplify or to treat quantum problems and therefore that the analysis here reported is simply a not novel application of those concepts. I believe that such an objection is ill-posed, since it is undeniable that the justification, the origin and the meanings of the non-linear canonical transformations become clear only in the light of the work of this thesis and, in particular, only thanks to the Majorana fermion representation of the quantum operators. It is the understanding of the formal symmetry that exists between Majoranas and Emergent Majoranas that makes possible the identification of the full canonical group and that allows the optimization of such transformations, in clear contrast with (almost [26]) any prior study where some singular, ad hoc, non-linear transformations have been defined and used. The novelty offered by the technology developed in this thesis is the possibility to use and interpret the *full continuos* group of canonical transformations, connecting it also with the possibility to have non-canonical transformations and to apply in a more straightforward way concepts and ideas of Dynamical Symmetries and Spectrum Generating algebras. With respect to the previous existing literature, this thesis creates a context in which the role of the non-linear transformations can be clearly identified and justified.

I tried to convince the reader that the combined use of Majorana representation and non-linear transformation may help in the study of SCES. These systems are typically characterized by the fight between the local and non-local nature of the electron. The use of non-linear transformations can help in this context, since it allows to define new fermions that hop with more difficulty and therefore can mimic the increasing importance of the local physics. This can be helpful in the study of a SCES model, since it can improve the efficiency of our methods. Indeed the reader should never lose sight of the practical dimension of this discussion. The idea that I tried to defend in this thesis *is not* that any SCES can be perfectly represented in terms of fermions only, which can be generated via a non-linear transformation of the original ones. Such a statement goes much beyond what has been proved and it is also of question-

able truth. The position that I defend is much less radical, since I just want to bring attention to the fact that it is plausible that in the SCES the original description of the Hamiltonian in terms of electron creation-annihilation operators may not be optimal. Therefore a change of coordinates may affect positively the study of quantum systems. Coordinate changes are realized very well by non-linear coordinate transformations, since they preserve the fermionic nature of the quantum operators and define new fermions able to capture, at zeroth approximation order, part of the electron's correlations (and so many non-trivial effects). In this sense the present analysis is not in conflict with any other (analytical or numerical) method, but instead it is a valuable tool that complements them.

We obtained evidence of the effectiveness of analysis based on non-linear transformation in the case of the Hubbard and 1d Kondo lattice models. Although both the analysis are not satisfactory from many points of view, it is safe to say that the qualitative (and often quantitative) agreement between the known results and our mean-field results in the non-trivial Mott insulating and Spin Selective Kondo Insulating phases represent important non-trivial achievements, which justify a more detailed study of these non-linear (or Majorana based) techniques. In both cases the analysis shows some regimes where the transformations considered did not performed particularly well; in particular the low coupling regime of the Hubbard model and the high-coupling regime of the Kondo lattice model. It is my opinion that in both situations the inefficiency is due to the not maximally general approach used. In the case of the Hubbard model just one auxiliary band has been added, while in the Kondo lattice the cgf fermions were not at all optimized, since we applied no non-linear transformation on them. Future studies should focus on this issue, understanding the best way to implement and select the "best" way to use the non-linear transformations in the study of a generic system.

As final consideration I would like to stress how this work strongly reevaluates the importance of Majorana fermions, stressing even more the fragility of the concept of the electron in condensed matter systems. In the case of strongly correlated systems, where the Landau-Fermi liquid of dressed electrons is at question, it seems more and more appropriate to give up the idea of electron modes. This can be done only if one accepts the possibility that the electrons are not (in condensed matter systems) the most fundamental degree of freedom. The Majorana fermions are (at least from an algebraic point of view) a much more meaningful fundamental degree of freedom, suitable in many different context. This of course does not mean that to them should be recognized the status of fundamental modes (as a matter of fact it makes no sense to "add a Majorana to a system"), but that they naturally occupy the space of fundamental (algebraic) degrees of freedom and, as such, they represent the most logic and fundamental unit on which our analysis should be based.

Appendix A

Clifford algebras

Complete introductions to Clifford algebras can be found in the literature,[1] so the role of this appendix is not that of providing a full review on this (huge) subject, but to introduce the basic concepts that are related to this Thesis. In the following will be assumed a minimal knowledge of differential geometry.

It is convenient to start in a very informal way as done in [236], considering three symbols e_1, e_2, e_3 and setting up a simple game giving the rules:

- we can form new symbols (words) multiplying (writing close to each other) the symbols;
- we can linearly combine such symbols (words) also scaling them by a number;
- the symbol (word) $e_i e_j$ can always be replaced by $-e_j e_i$ (and viceversa), with $i, j = 1, 2, 3$;
- the symbol (word) $e_i e_i$ can always be replaced by the special symbol 1 (empty word).

Setting these rules between the symbols we have just defined an *algebra*. There are of course infinite symbols (words) that are in this algebra (dictionary), but just 8 of them are linearly independent (have different meanings) and all the others can be obtained combining these 8 symbols:

$$1, \quad e_1,\, e_2,\, e_3, \quad e_1e_2,\, e_1e_3,\, e_2e_3, \quad e_1e_2e_3. \tag{A.1}$$

Clearly the choice of these "basic symbols" is not unique. If we start to play this game, we would immediately see some familiar features. Let us for example multiply the symbol

$$A = a_1e_1 + a_2e_2 + a_3e_3, \quad a_i \in \mathbb{R}, \tag{A.2}$$

by itself. One one obtains is

$$A^2 = a_1^2 + a_2^2 + a_3^2. \tag{A.3}$$

[1] I personally found these two pedagogical reviews [69, 236] quite complete, so I recommend them to any reader that is new to this topic.

Multiplying instead A by the symbol $B = b_1 e_1 + b_2 e_2 + b_3 e_3$ one gets:

$$\begin{aligned} AB &= (a_1 b_1 + a_2 b_2 + a_3 b_3) + \\ &\quad + (a_2 b_3 - a_3 b_2) e_2 e_3 + (a_3 b_1 - a_1 b_3) e_3 e_1 + (a_1 b_2 - a_2 b_1) e_1 e_2. \end{aligned} \tag{A.4}$$

It's difficult to not notice the similarities of these operations with the standard operations on vector spaces. In fact, if one interprets e_1, e_2, e_3 as the orthogonal unit vectors $\hat{x}, \hat{y}, \hat{z}$ one sees that:

$$A \to \vec{A}, \quad A^2 = \vec{A} \cdot \vec{A},$$

where $\cdot$ is the scalar product, while in AB there is a part that is $\vec{A} \cdot \vec{B}$ summed to another that looks like the cross product of $\vec{A} \times \vec{B}$. Indeed if one embraces the more general formalism offered by the tensor algebra built on a vector space, it is not difficult to realize that the second term in AB is given by $\vec{A} \wedge \vec{B}$, so the three symbols $e_2 e_3, e_3 e_1, e_1 e_2$ represent the three linearly independent component of a rank 2 skew-symmetric tensor on a (Euclidean) 3d vector space.

The connection with the exterior (Grassmann) algebra is *not* a concidence. Indeed, consider a vector space V of dimension d and its exterior algebra[2] $\bigwedge V = \bigoplus_{n=1}^{d} \bigwedge^{(n)} V$, built using the antisymmetriezed tensor product $\wedge$ to build all the possible non-trivial skew-symmetric tensors (of rank $n \leq d$). Then if one considers the elements of $\bigwedge V$ algebra as basis of a vector space W and defines the product:

$$vw = v \cdot w + v \wedge v, \tag{A.5}$$

with $v \cdot w = (v \otimes w + w \otimes v)/2$ the operation equivalent of the scalar product in (A.4), one obtains an algebra over W, which is called *Clifford algebra*, and the previous product is named *Clifford product*. Typically, fixed a set of basic objects $e_1, ..., e_n$, the elements of W are divided into blades, depending upon the number of basic objects that must be multiplied together to obtain them. So the elements e_i belong to the first blade, and correspond in the Grassman representation to the vectors of V; the elements $e_i e_j$ (with $i \neq j$) belong to the second blade and correspond to skew-symmetric rank two tensors in $\bigwedge^{(2)} V$; and so on.

This way to introduce the Clifford algebra is quite convenient, since it allows one to associate to the elements of the algebra (the words) a geometrical meaning. Indeed, associating the basis vectors of V with basis vectors of the Euclidean space, the formalism of the external algebra (and in particular the concept of multi-forms) associate with the antisymmetric tensors of rank 2 a surface element, to the antisymmetric tensors of rank 3 a volume element, and so on [237]. The maximally antisymmetric tensor (of rank d if V is d-dimensional) is called *pseudoscalar* and it gives the maximal-dimensional volume element of the manifold, determining the orientation of the manifold (which can be positive or negative, depending upon the sign of this form).

To represent a Clifford algebra in terms of exterior elements on a vector space has some advantages and some disadvantages. The main advantage is that some basic operations can be understood in terms of rotations of the basis vectors of

[2] We are assuming an Euclidean metric, so the difference between covariant and contravariant tensors is irrelevant.

V. For example take the Clifford algebra: $Cl(\mathbb{R}^2) = \{1, e_1, e_2, \mathcal{I} = e_1 e_2\}$. This corresponds to the external algebra W of $V = \{e_1 \to \hat{x} = (1,0); e_2 \to \hat{y} = (0,1)\}$, where evidently $e_1 e_2$ is interpreted as $\hat{x} \wedge \hat{y}$, which in turn is the 2-form that gives the surface element of the plane defined by V. Simply using in a straightforward fashion the rules of the Clifford product, one can see that a generic element a of V defined as $a = a_1 e_1 + a_2 e_2$ becomes $\bar{a} = a_2 e_1 - a_1 e_2$ when multiplied on the right by $\mathcal{I}$. Clearly a and $\bar{a}$ are orthogonal to each other. So the multiplication by the pseudoscalar realizes a rotation of $\pm\pi/2$, where the $\pm$ depends upon the application of the $\mathcal{I}$ on the left or on the right. More in general one can see that since $\mathcal{I}^2 = -1$ then

$$b = a e^{\theta \mathcal{I}} = a \left[cos(\theta) + \mathcal{I} sin(\theta) \right], \tag{A.6}$$

corresponds to a rotation of a by an angle θ. A more general way to define this operation is as

$$b = e^{-\frac{\theta}{2}\mathcal{I}} a e^{\frac{\theta}{2}\mathcal{I}}, \tag{A.7}$$

that removes the problem of having to distinguish between left and right application (beside having some extra advantages when handling larger algebras). This is indeed a very practical way to represent rotations in a high-dimensional space.

The previous paragraphs clarifies why it is trivial to say that the set of bilinear objects obtained by $2n$ Majoranas generates closes to the Lie algebra of $so(2n)$: indeed each Majorana can be thought of as a unit vector in a $2n$-dimensional vector space V and the bilinears generate the rotations in planes spanned by pairs of unit vectors

The main disadvantage of this geometric interpretation of the element of the Clifford algebra as elements of the exterior algebra of V is that the geometric intuition is completely lost when one considers combinations of elements belonging to different blades of W. Clearly an object like

$$A = a_0 + a_1 e_1 + a_3 e_1 e_2, \tag{A.8}$$

has no clear geometrical meaning and also as tensor it does not make sense. Although this object still belongs to the vector space W on which we have built the Clifford algebra, defining the product (A.5), it is not possible to understand it if one simply sticks to geometric interpretation and the multi-form representation. The geometric representation brings us implicitly to think not in terms of W, but in terms of a set of separate subspaces $\{\bigwedge^{(p)} V\}$, $p = 1, ..., d$, which cannot be mixed in a straightforward way. Indeed, if one considers on the Clifford algebra only the operations that have a geometrical meaning, only few operations between different elements of W are allowed: rotations, dilatations (multiplying the vectors by a scalar) and inversions (multiplying the vectors by -1). It is important to give up such a geometric picture to use the Clifford algebra in its full generality, which is exactly what we have done in the this Thesis.

Although much more could be said about the structure of the Clifford algebras, it is not necessary to add any further detail to understand the content of this Thesis.

Appendix B

Crystal Fields and effective spin

Let me start making clear that this appendix cannot and does not want to give complete and comprehensive discussion of the complicated role that the crystal fields play in condensed matter physics. Nor does it want to be a mathematical introduction to group theory in physics. The aim of this appendix is just to justify the degeneracy reduction in the ground state of the f-impurities, explaining the rationale behind it. The discussion will be kept as informal as possible, although I must assume a (not superficial) knowledge and understanding of the notion of symmetry in quantum mechanics and some basic concepts of group theory (like representation and irreducible representation), that anyway are typically common to any solid state or high energy physicist. As references for the most formal part I strongly suggest the classical book by Weyl [238] and the (more modern) popular book by Cornwell [239]. Anyway many different books contain the main notions, included the standard reference on quantum mechanics as Ref. [240,241]. Instead for a comprehensive discussion about the role of crystal fields a strongly recommend the book by Fazekas [7], that will be the main reference for this entire chapter.

Let us consider the most used element in heavy fermion compounds: the lanthanide Cerium (Ce). This element has, in its atomic form, two electrons in the highest unfilled shells one, in the orbitals 4f and one in 5d. However when embedded into a compound the orbitals are rearranged and some electrons are donated to the other ions of the compound, so effectively the embedded Cerium ion important in condensed matter physics is Ce^{3+} that has only one active electron in the unfilled shell 4f, so its configuration is f^1, following the notation of Chapter 6.

In principle, as has been pointed out already, the state f^1 is 14-times degenerate. However this degeneracy is broken two times: the first time at atomic level, considering the (atomic) spin-orbit effect; the second time instead it is the lattice that plays an important role, breaking the rotational symmetry of the atomic Hamiltonian via the generation of crystal fields. Let us analyze these concepts step by step.

The first split due to spin-orbit coupling[1] is easy to understand in the case of one electron only:

$$\begin{aligned} \Delta E_{SO} &= \mathcal{G}_{SO}(L,S)\,\vec{L}\cdot\vec{S} \\ &= \frac{\mathcal{G}_{SO}(S,L)}{2}\left\{J(J+1)-L(L+1)-S(S+1)\right\}. \end{aligned} \tag{B.1}$$

With only one electron in an f^1 state $S = 1/2$, $L = 3$ and $J = 5/2$ or $7/2$. In the Cerium $\mathcal{G}_{SO}(1/2,3) > 0$ [7] and this implies that the energetically more convenient states have $J = 5/2$. So this effect already splits the degeneracy of the initial 14 dimensional space into two subspaces of dimension 6 (low energy) and 8 (high energy). Let us focus on the low energy subspace, symbolically written as $\mathcal{H}_6$.

By construction the $\mathcal{H}_6$ is a six dimensional irreducible representation (IRREP) of the rotation symmetry group, generated by the total angular momentum operator.[2] So far it has been assumed that all these states are degenerate; this assumption is unneccesary, because the reason for the degeneracy is given by the form of the Hamiltonian. Indeed lets take an Hamiltonian that is symmetric respect to a group G, i.e., that commutes with all the operators (unitary or antiunitary) $P(g)$ that represent the action of every $g \in G$ on the Hilbert space.[3] Then

$$[H, P(g)] = 0, \quad g \in G, \tag{B.2}$$

so it is straightforward to realize that any eigenstate of H is also an eigenstate of the symmetry operation $P(g)$. This *does not* mean of course that

$$[P(g), P(g')] = 0, \quad \forall g, g' G; \tag{B.3}$$

indeed the latter is true only for abelian groups. As a consequence, given a generic eigenstate Φ_n of H that belongs to an IRREP of G, it must happen that

$$HP(g)\Phi_n = P(g)H\Phi_n = E_n P(g)\Psi_n. \tag{B.4}$$

This means that if G is a symmetry of the Hamiltonian and Φ_n and eigenstate, then also all the states obtained as $\Psi_{n,g} = P(g)\Phi_n$, $\forall g \in G$, are eigenstates of the Hamiltonian *with the same eigenvalue*. So all the states that belong to the same IRREP are degenerate and the dimension of the IRREP must be the dimension of the multiplet:[4] to break this kind of degeneracy it is necessary to break the symmetry. This is exactly the role of the crystal fields.

[1] In some cases this is explained as an effect of the Hund's third rule, that originates exactly from the formula (B.1), but for many-electron states.

[2] Evidently the original 14 dimensional space is not an irreducible representation; indeed it is the direct product of the two IRREPs of dimension seven and two. Although very confusing, I am forced to use the notation, common to physics literature, that uses the term "representation" to indicate both the vector (Hilbert in this case) space on which the group acts and the matrix form of the operation that performs the action.

[3] Personally I believe that this is the most beautiful page of physics, but here there is no space to discuss it deeply. Therefore I must summarize the results and also take a perspective on the concept of symmetry that is more mathematical than conceptual.

[4] If the degeneracy is not enforced by the symmetry it is typically called *accidental*. The most notorious example is give by the accidental degeneracy of the electronic levels of the hydrogen atom if the spin-orbit interaction is neglected.

The crystal fields represent the effect that the surrounding ions of an atom embedded on a lattice site, have on the electrons of that particular atom. So they play the role of an external potential on the local (on site) electron Hamiltonian. Clearly this potential does not share the complete rotational symmetry of the atomic Coulomb potential, but is instead characterized by the symmetry of the lattice. Rephrasing, this means that the electron on an atom embedded in a compound feels not only the (atomic) Coulomb potential, but also the effect of an electric field that has the symmetry of the lattice. The total Hamiltonian is therefore not anymore symmetric under the full rotational group, but only under the action of the *point group* (the group of operations that does not change the position of the atom considered, but transforms all the others sending the lattice into itself), that is evidently just a finite subgroup. The crystal fields therefore break the symmetry and so one should expect that they break the degeneracy of the multiplet $\mathcal{H}_6$.

If the dimension of the original multiplet is odd the discussion is then straightforward. In fact there exist a very accurate mathematical machinery [7] that permits to decompose every finite dimensional IRREP of the rotation group $SO(3)$ on the IRREPs of finite subgroups. This does not sound so exotic: as a matter of fact we are just saying that if in a Hamiltonian that is symmetric under rotation is inserted a term that makes one direction preferable, then the state that orients the electron wavefunction along that direction will have a lower in energy.

The situation is a bit more involved in the case of even dimensional IREPs, hence characterized by a fractional value of the total angular momentum J. As known from basic quantum mechanics the even dimensional representations require the accurate identification of the rotation group, that in quantum mechanics is not given by $SO(3)$, but by $SU(2)$. This permits to consider also even dimensional IRREPs and the difference between the two cases is quite fundamental: the action of the 2π rotation element on a state that belongs to an odd dimensional IRREP, sends the states into itself; the same operation, if performed on a state that belongs to an even IRREP, sends the state into *minus* itself, and instead a rotation of 4π is required to send the state into itself. To solve the problem one could pretend [7] that the group of rotations, when acting on even dimensional IRREPs, is double (this requires the introduction of another group element that makes the rotations between 0 and 2π different from those from 2π and 4π) and in this way allowing for the use of the same mathematical machinery that permits to split the multiplets into IRREPS of the subgroups. The peculiarity is that also the new IRREPs must be *even dimensional*. This fact is not accidental, but it has deep origins. In fact it can be proved that for any system with an odd number of electrons (in general fractional spin particles), i.e. for each even dimensional IRREP of the rotation group because an even number of electrons cannot generate a fractional total angular momentum, the states appear in pairs. These pairs are connected by the operation of time inversion [7] and the two states are degenerate *if the Hamiltonian has the time reversal symmetry.* This has as consequence the so called *Kramer's theorem* [7], and in this case it implies *that there exist a minimal double degeneracy enforced by the time reversal symmetry and that cannot be broken by any geometrical electrostatic effect.*

This affects the embedded Cerium atom in the following way. Assume for example to embed it in a lattice with an octahedron point group. Then it is

mathematically known that the multiplet $\mathcal{H}_6$ is split into two IRREPS of dimension 2 and 4. Typically (but not always) the interaction parameters of the crystal field favors the two dimensional IRREP, making it the ground state. Therefore the ground state of the embedded Ce atom, where the only valence electron will be naturally hosted, is formed by two degenerate states, connected by time-reversal symmetry operation and both eigenstates of an angular momentum operator. Therefore they have the characteristics of spin states and the degeneracy can be thought of as (but it is anyway mathematically isomorphic to) a spin $S = 1/2$ doublet.

Appendix C

Spin and pseudospin

As discussed also in Chapter 3 there exist many ways to represent the states of the Hilbert space. One way is in terms of fermionic operators that, acting on a vacuum, generate the entire Hilbert space. Another is to make use of group theory and organize the states according to the IRREPS of the chosen symmetry groups.

Let us consider the local Hilbert space of the Hubbard model:

$$\begin{gathered} |0\rangle, \\ c_{\uparrow}^{\dagger}|0\rangle = |\uparrow\rangle, \quad c_{\downarrow}^{\dagger}|0\rangle = |\downarrow\rangle, \\ c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}|0\rangle = |\uparrow\downarrow\rangle, \end{gathered} \tag{C.1}$$

where I made use of the fermionic representation of the Hilbert space. The representation can be changed, for example it is very well known (see also Appendix B) that the subspace

$$c_{\uparrow}^{\dagger}|0\rangle = |\uparrow\rangle, \quad c_{\downarrow}^{\dagger}|0\rangle = |\downarrow\rangle, \tag{C.2}$$

forms a two dimensional IRREP of the rotation group, i.e. $SU(2)$. As mentioned in Appendix B and better in Ref. [7] this group can be thought of as a double $SO(3)$ group, where an element that discriminates between rotations of $0 - 2\pi$ and $2\pi - 4\pi$ has been added in order to obtain this double size of the group.[1] The physical meaning of "spin" does not come from the mathematical structure, but it must be provided by the microscopical derivation of the quantum states, which imply the effect of the (physical) action of the rotation group on the states of the space (C.1). On the base of this interpretation it becomes also possible to define the representation of the time reversal operator, mentioned in appendix B.

The interpretation of the group $SU(2)$ that can act on (C.2) as the group of rotations, and with its generators S^z, S^+ and S^- as the spin operators is *fundamental*, when the physical interaction of the different degrees of freedom among themselves and with the external perturbations have to be model. But is is absolutely irrelevant from the point of view of the structure of the Hilbert

[1] $SO(3)$ has as universal (double) cover the group $SU(2)$, or in practice $SO(3) \cong SU(2)/\{1 \simeq -1\}$, so for each element of $SO(3)$ there exist two elements of $SU(2)$.

space. As a matter of fact, if just the space (C.1) is given, and no information about the Hamiltonian nor how the Hamiltonian has been derived from the microscopical properties of the matter are give, then the different states, operators and indices in (C.1) have no physical meaning, but only a mathematical one.

From this point of view it is evident how many more general symmetry groups can be defined and used to classify the states of the Hilbert space (C.1) or any other Hilbert space. Lets consider the particular example of (C.1), and in particular on the part of the Hilbert space that was not considered during the discussion of the spin operators:

$$|0\rangle, \quad |\uparrow\downarrow\rangle. \tag{C.3}$$

In principle these two states can also form an irreducible representation of a group $SU(2)$. Of course this group cannot be put in correspondence to the physical operation of rotation, but anyway it is a group that describes the structure of this subspace. There must exist three generators

$$I^z, \quad I^+, \quad I^-, \tag{C.4}$$

such that

$$\begin{gathered} I^z|0\rangle = -\tfrac{1}{2}|0\rangle, \quad I^z|\uparrow\downarrow\rangle = +\tfrac{1}{2}|\uparrow\downarrow\rangle, \\ I^+|0\rangle = |\uparrow\downarrow\rangle, \quad I^+|\uparrow\downarrow\rangle = 0, \quad I^-|\uparrow\downarrow\rangle = |0\rangle, \quad I^-|0\rangle = 0. \end{gathered} \tag{C.5}$$

These operators are the *pseudospin operators* and the symmetry group is called *group of the pseudospin rotations*. In perfect analogy with the spin case, also here there must exist an operator that represents the action of the $\mathbb{Z}_2$ group (previously associate to time inversion, now still undetermined), that pairs up the states of the even IRREPs. The connection with a symmetry group and with a physical meaning can be discovered writing the operators I^α in terms of the fermionic operators $c^\dagger_\sigma$ (assuming that to have identified them as electron modes, i.e. to have identified the physical degrees of freedom of charge and spin, meant as intrinsic angular momentum). The result is

$$I^z = \frac{1}{2}\left(c^\dagger_\uparrow c^\dagger_\downarrow c_\downarrow c_\uparrow - c_\downarrow c_\uparrow c^\dagger_\uparrow c^\dagger_\downarrow\right), \quad I^+ = c^\dagger_\uparrow c^\dagger_\downarrow, \quad I^- = c_\downarrow c_\uparrow. \tag{C.6}$$

The equivalent of the time inversion operator can be found easily remembering that the time inversion is given by the operator $\mathcal{T} = iS^y\mathcal{K}$ on the two dimensional IRREP, so its pseudospin analogous $\mathcal{C}$ is

$$\mathcal{C} = \left(c_\downarrow c_\uparrow - c^\dagger_\uparrow c^\dagger_\downarrow\right)\mathcal{K}, \tag{C.7}$$

with $\mathcal{K}$ the complex conjugation operation. So far it seems that this group and these operators are completely unphysical. I would like to point out to the reader that it is actually possible (easy) to produce physical interactions that act on the pseudospin operators and that try to polarize the pseudospin (break the pseudospin symmetry), exactly as the magnetic field polarizes the spin. In fact if in the Hamiltonian is present a pairing term

$$\Delta c^\dagger_\uparrow c^\dagger_\downarrow + \Delta^* c_\downarrow c_\uparrow, \tag{C.8}$$

it is easy to see that such a term is simply

$$\Delta I^+ + \Delta I^- = Re(\Delta) I^x + Im(\Delta) I^- = \vec{\Delta} \cdot \vec{I}, \tag{C.9}$$

with $\vec{\Delta} = (Re(\Delta), Im(\Delta), 0)$.

This should convince the reader that the "physical sense" of the symmetry groups defined "ad hoc" to describe the structure of the Hilbert space is a matter of personal taste, because anyway these operations can always be very well characterized in terms of physical (measurable) quantities.

Much more could be said about it, but the complete discussion of these topics is not part of this thesis, so I leave it for the future.

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Paper A

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(in manuscript), arXiv:1405.5176.

Paper B

Free fermion description of a paramagnetic Mott insulator

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(in manuscript), arXiv:1407.4310.

Paper C

Ferromagnetism in the one-dimensional Kondo lattice: mean-field approach via Majorana fermion canonical transformation

Matteo Bazzanella and Johan Nilsson

Phys. Rev. B **89**, 035121 (2014).

Paper D

Majorana fermion description of the Kondo lattice: Variational and path integral approach

Johan Nilsson and Matteo Bazzanella

Phys. Rev. B **88**, 045112 (2013).