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QUANTUM DYNAMICS OF INTEGRABLE SPIN CHAINS

Candidate
Giuseppe Genovese

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Contents

Introduction

Quantum spin chains have been introduced originally as a simple 1-D quantum model for (anti-)ferromagnetism in a paper by Bethe [**7**]. The author introduced the model of nearest neighborhood Heisenberg interaction in one dimension, and found the spectrum of the Hamiltonian, by using the (later on celebrated) Bethe method. Some years later Hùnthel in [**14**] found also the ground state energy for this model. As it is very clearly explained in the seminal paper by Lieb, Mattis and Schultz [**18**], the interest in such models cannot be limited to Bethe and Hùnthel results for several reasons: for example it is not clear how to extent the argument to higher dimensions; more generally, the structure of the model is more rich as it seems, and need further investigation, both in equilibrium, both out from equilibrium.
And indeed the method used for diagonalization in [**18**], *i.e.* the spin-fermion mapping, has revealed a crucial feature, for the study of all the models of spin chains, but also for investigating the relation between quantum spin chains and two dimensional classical spin models, as pointed out by the same authors in [**26**] (for an exhaustive account see also [**10**]). This has given a bridge between one dimensional quantum systems and two dimensional classical ones, in the sense that they can be treated with the same technique: the study of two dimensional spin systems as a problem of many fermions [**19**] is still one of the more interesting questions in mathematical physics and statistical mechanics [**20**].
In this sense, it has been introduced the definition of *integrable* spin chain, as a chain that can be mapped in a free fermion model. In this case the mathematical formalism simplifies crucially, as we will see, but we have to stress that the physical content, from the ferromagnetic point of view, remains very interesting. These models, despite idealized, are very rich, and presents all the features one could aspect from a quantum many body system. In our work we will deal only with this kind of systems.
As simple prototypes of many body quantum systems, in the '70, besides the investigation of their equilibrium properties, an interest was paid also for the dynamics. On this topic, as well as the author knows, up to now there are only results about integrable chains.
Particular attention have been paid to the non ergodic behavior exhibited by such models [**16**]. It has been shown very clearly by the work of Mazur [**21**], Girardeau [**11**], Barouch and McCoy and Dresden [**6**] , that the magnetization as a global obsevable is in fact non ergodic (in further papers Barouch and McCoy extended their results also to correlation functions).

The extension to local observables was done in the study of impurity models. Both Tjon [**27**], and Abraham, Barouch, Gallavotti and Martin-Löf [**1, 2, 3**] have found the same kind of behavior for the XX model with an impurity.
So, definitely, this unusual behavior of such systems could be discouraging, since, as Lebowitz pointed out in [**16**] discussing just these topics: *almost all physical systems are essentially ergodic*. This should mean that *integrable* quantum spin chains are not physical systems, that is they are not well posed models of statistical mechanics. This is at least a controversial idea. It is a certain fact that spin chains, as one dimensional models of magnetic alloys, are very intuitive models, and so common sense would say that they model physical situations. After all, the picture about the dynamics of non integrable chains is rather unclear, so we cannot say if the problem lies just in the integrability of such models. This remains an open question.
It is important to point out that, from a spin chain perspective, we are not dealing with an open quantum system: it is rather a closed system of many particles. On the other hand one could change point of view, and choose to look to a subsystem of the chain; this one remains coupled to the rest, and can be seen as non isolated system. A simple configuration in this sense has been studied by Ho and Araki [**12**] and by Platini [**23**] for the XX chain, and Aschbacher and Pillet for the XY chain [**4**]. They simply divide the chain in several parts, put different temperature on each one, and look for the time evolution: this models a spin system between reservoirs. An analogue point of view will be adopted also in the Chapter 2 of this work; so we have to make a precision: the *environment* in this configuration is *tamed*, in the sense that one can follow its dynamics time by time exactly. This is a sophistication that has origin in the decomposition of a closed system in more open subsystems. On one hand this is a choice that seems physically very natural (one divides the universe in the laboratory plus the rest of the universe); on the other hand a reservoir in which in principle one can easily look inside sounds a little artificial, and one of the main characteristics of the environments, that is putting noise inside the system, seems to be lost by an excessive simplification: mutual exchange of energy in a simple closed system. This is not precisely the case, for example, of the spin-boson model, in which one has at least look for the correct coupling between the two systems [**17**]. So, even if mathematically everything works fine, at least for integrable chains, the physical interpretation of such results is often incomplete and unsatisfactory. We have the feeling that, when studying mathematically the non equilibrium properties arising in such models, trying to develop new instruments in order to get more and more control on the system, one should even take care in interpreting the results.
These considerations have origin also at the light of the different approaches to the dynamics of open quantum systems, often developed in the opposite perspective, *i.e.* figuring the reservoir as a pure source of noise. In this case, however, losing the control on the whole system is simple. This approach has been adopted for open spin chains like systems in a recent work by Horstmann, Cirac and Giedke [**13**].
Nowadays the attention to spin chains is devoted mostly to the quantum information point of view: as a large number of two level systems in mutual interaction, they are in fact a simple model of quantum dots. One of the main problem is the storage and transfer of information (a state) form a point to the other of a given finite chain, that is a cogent problem in quantum information. The literature on the argument is very wide, and we are completely unable to give a full account, neither a significant abstract. But it is worthwhile to notice that in the past years quantum spin chains have been implemented experimentally by quantum simulation [**24, 9, 5**]. Taking apart the debate about quantum simulation be real physics or not, the interesting datum is that we can reproduce in a laboratory a non ergodic system. This point of view open questions and offers other perspectives.
The plan of the work is the following:

The Chapter 1 is introductory. The models of spin chains are presented, and a little deepened where it needs. Particular attention has been paid for the configuration in which we have an integrable chain with an external field in the transversal direction. This is as to say that the amplitude of the transversal direction of the spin operator is small, so two body interaction can be neglected, but not one body interactions (*i.e.* external fields).
So we face the equilibrium properties of the XX chain in presence of an inhomogeneous transverse field. We deal with XX chain for the only reason that it is mathematically simpler, but it preserves all the interesting characteristics of the non rotation invariant XY chain (when there is the field). Our results are often easy to generalize to the XY case, the difficulties being only technical.
The spectrum of the XX chain in presence of impurities is then determined. This calculation has been done in [**2**] for a single impurity, and we have presented and extended that result to the case of arbitrary number of impurities. Of course, as discussed in [**16**], the crucial point is that the spectrum is made in thermodynamic limit by an isolated eigenvalue plus a continuous interval, but at finite size it is discrete: so there is no decay of correlations.
Then we have been concerned on the problem of dynamics. We have shown that the dynamics is given by a one-parameter semigroup of rotation in the Heisenberg picture, for a generic quadratic Fermi Hamiltonian, and we have found the ODE of the semigroup. Then we develop the theory of the *state* and *observables* for such systems. Our results are very similar to the achievements of Narnhofer in [**22**], who studied the problem for a more algebraic point of view. The relation will be further discussed, but it is obvious that a modern perspective on the same subject naturally brings something new about it. So we have developed the theory for integrable spin chains in transverse field, having in mind the non equilibrium configuration of Ho-Araki and Aschbacher-Pillet, and the one treated in the sequent chapter.
In Chapter 2, as a direct application of the theory previously developed, we have dealt with the problem of the forced oscillation of a spin, coupled with an heat bath, namely, the rest of the chain. This is a well known problem in physics, namely the magnetic resonances absorption problem, largely studied in the '40, '50. Here we have the competition of two effects: the oscillation of the spin and the coupling with the rest of the chain. Our approach will be to look at the first one as a perturbation of the second one, and then to treat the problem perturbatively. This is a standard approach.
We solve the equation for the system proposed in Chapter 1, and then we calculate the magnetization. We get information in this way on the structure of resonances.
The conclusion we get is that the coupling with the bath behaves actually as an effective external hight field along the longitudinal direction. The temperature plays the only role to spread the resonance peaks, in full agreement to the theory of Kubo and Tomita [**15**].
In this work, as general reference of quantum mechanics the textbook [**8**] has been used, while for statistical mechanics the classical reference is [**25**], but also [**10**].

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CHAPTER 1

Preliminaries on Quantum Spin Chains

This is an introductory chapter on quantum spin chains. The main models are introduced, pointing out the crucial characteristic of being integrable or not. Furthermore, the analogy with Fermi one dimensional systems by the Jordan-Wigner transformation is deepened. This last will be used to calculate the spectrum of some selected models, namely the XY chain, or the XX chain in a transverse non homogeneous magnetic field. The case with a single impurity was dealt in [**2**], while its generalization to many impurities as well as we know is new. These are some of the few examples of many body quantum systems for which the exact form of the spectrum is known. In the final two sections a theory for the dynamics of general Hamiltonian of Fermi operators is derived, together with some concrete application to spin chain in a transverse field. There are presented (for the first time, at least in this form) equations encoding the dynamics of the chain.

1. The Models

In this work we will treat quantum spin systems, ruled by nearest neighborhood two body ferromagnetic interaction on $\mathbb{Z}$. The most complete Hamiltonian for describing such a class of systems is

$$H_N = -\sum_{j=1}^{N^*} (J_j^x S_j^x S_{j+1}^x + J_j^y S_j^y S_{j+1}^y + J_j^z S_j^z S_{j+1}^z) + 1\text{-body interactions.} \tag{1.1}$$

Let us explain everything step by step. Here J_j^x, J_j^y and J_j^z for each site j are real positive numbers, and S_x, S_y, and S_z the spin operators, defined in terms of Pauli matrices as as $S_i = \frac{1}{2}\sigma_i$, $i = x, y, z$, where

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The boundary conditions are defined by the value of N^*: *e.g.* if $N^* = N-1$ we are dealing with open (or free) boundary conditions at extrema, while if $N^* = N$ we are intending that $N+1 = N$, so periodic boundary conditions.

The Hilbert space this operators act on is a tensor product of one spin Hilbert spaces $\mathscr{H}_j$, each spanned by the vectors *spin up* and *spin down* $\left|\sigma_j^{\pm}\right\rangle$:

$$\mathscr{H} = \bigotimes_{j=1}^{N^*} \mathscr{H}_j.$$

This resulting space is usually known as Fock space.
The above Hamiltonian is rather general, and almost anything is known about the model with inhomogenei couplings along all three directions. Actually, even in the homogeneous case the model is very hard. Anyway, save when specified, we will generally deal with model with homogenei couplings:

$$H_N^{XYZ} = -\sum_{j=1}^{N^*} (J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z) + \text{1-body interactions.} \tag{1.2}$$

For different values of J_x, J_y, J_z we get different models of interest. We will treat the simpler case in which one of them, say J_z, is vanishing. In this case we get the XX Hamiltonian if $J_x = J_z = J$

$$\begin{aligned} H_N^{XX} &= -J \sum_{j=1}^{N^*} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \text{1-body interactions} \\ &= -\frac{J}{4} \sum_{j=1}^{N^*} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \text{1-body interactions.} \end{aligned} \tag{1.3}$$

This is the simplest model of quantum spin chain: it has both translational[1] and rotational symmetry, at least in the bulk Hamiltonian, *i.e.* the two body interaction part. Despite these features, the model can be made rather not trivial by adding a suitable one body interaction term in the Hamiltonian. We introduce here transverse fields, *i.e.* one body interaction along the transverse direction (in this case, the z direction). We notice that an homogeneous transverse field like

$$H_N^{\mathrm{h}} = -h \sum_{j=1}^{N} \sigma_j^z$$

(h be a constant) does not affect very much the structure of the chain. This is easily seen by noticing that

$$[H^{XX}, H^{\mathrm{h}}] = 0$$

and so we can diagonalize together the two operators: this means that no new physics arises by the presence of the homogeneous transverse term. What is really interesting is adding an inhomogeneous transverse field of the form

$$H_N^{\mathrm{i}} = -\sum_{j=1}^{N} h_j \sigma_j^z,$$

with generic h_j depending by the site. In this case we have

$$[H^{XX}, H^{\mathrm{i}}] = 2i \sum_{j}^{N} (h_{j+1} - h_j)(\sigma_j^y \sigma_{j+1}^x - \sigma_j^x \sigma_{j+1}^y).$$

Therefore this is the simplest non trivial quantum spin chain.

[1] The translational symmetry depends (mildly) on boundary conditions: for example if we have periodic boundary conditions it is exact, while for open boundaries is recovered only when $N \to \infty$.

Another interesting model is obtained by putting $J_x = J(1+\gamma)$, $J_y = J(1-\gamma)$, $J_z = 0$, $\gamma \in [0,1]$. In this way it results defined the XY chain:

$$\begin{aligned} H_N^{XY} &= -J\sum_{j=1}^{N^*}((1+\gamma)S_j^xS_{j+1}^x + (1-\gamma)S_j^yS_{j+1}^y) + \text{1-body interactions} \\ &= -\frac{J}{4}\sum_{j=1}^{N^*}((1+\gamma)\sigma_j^x\sigma_{j+1}^x + (1-\gamma)\sigma_j^y\sigma_{j+1}^y) + \text{1-body interactions.} \quad (1.4) \end{aligned}$$

In this case the rotational symmetry is broken, and the model is more complicate. For the XY chain, the first not trivial one body interaction one can introduce is the homogeneous field, since it does not commute with the Hamiltonian

$$[H^{XY}, H^h] = 4i\gamma\sum_j^N(\sigma_j^x\sigma_{j+1}^y + \sigma_{j+1}^x\sigma_j^y).$$

From a dynamical perspective, this means that in the XX model the magnetization is always a conserved quantity by the quantum dynamics, but in the XY model this is not the case. This is easy to understand from the point of view of the symmetry of the system, since the magnetization can be view as the generator of a total $SU(2)$ rotation around the z-axis, that is a symmetry for the XX chain and not for the XY one.
In a certain sense, γ is a measure of the degree of rotational symmetry breaking: for $\gamma = 0$ we get the rotational invariant XX model, and for $\gamma = 1$ we get the Ising chain, that is a completely unbalanced model.
If all J_x, J_y, J_z are non zero, we have the XYZ model. The properties of this model are dramatically different with respect to the other two, and a rigorous approach is extremely hard even at equilibrium. The reason of that will be clarified partially in the next section. Anyway we will not deal with XYZ chains in this work.

2. The Fermionic Picture

It turns out that there is a close relationship between spin systems and fermions in one dimension. We have to perform a Jordan Wigner transformation [**14**] in order to transform the spin operators in fermionic operators[2]. We put

$$\begin{cases} c_j &= \frac{1}{2}(\sigma_j^x - i\sigma_j^y)\bigotimes_{k=1}^{j-1}(-\sigma_k^z) \\ c_j^\dagger &= \frac{1}{2}(\sigma_j^x + i\sigma_j^y)\bigotimes_{k=1}^{j-1}(-\sigma_k^z), \end{cases}$$

and their inverses

$$\begin{cases} \sigma_j^x &= (c_j^\dagger + c_j)\bigotimes_{k=1}^{j-1}(-\sigma_k^z) \\ \sigma_j^y &= -i(c_j^\dagger - c_j)\bigotimes_{k=1}^{j-1}(-\sigma_k^z) \\ \sigma_j^z &= 2c_j^\dagger c_j - \mathbb{I}. \end{cases}$$

It is easily seen that the c operators satisfies fermionic anti-commutation relations:

$$\begin{aligned} \{c_j, c_k\} &= 0; \\ \{c_j^\dagger, c_k\} &= \delta_{jk}. \end{aligned}$$

The morphism of algebras naturally induces a morphism of Fock spaces: we have that each c_j ($c_j^\dagger$) acts on a two level Hilbert space $\mathscr{H}_j'$ as an annihilation (creation) operator, spanned by the vectors $|0\rangle_j$ (hole) and $|1\rangle_j$ (particle), as usually in the theory of Fermi systems.

[2]It is suggestive to think at the Jordan Wigner transformation as the quantum analog of the classical transformation for spin variable from ± 1 values to $\{0,1\}$

So the morphism is $\mathscr{H} \to \mathscr{H}' \equiv \bigotimes_{j=1}^{N^*} \mathscr{H}'_j$, but of course not between the single Hilbert spaces (spin and fermion). This is a peculiar feature of quantum mechanics.
However, in what follows it results more convenient to think at fermion operators as anti commuting numbers (*a-numbers*) than an algebra of anti commuting operators acting on $\mathscr{H}'$. In this way, as will be soon clear, the Hamiltonians of spin chain can be seen as (quadratic in our cases) forms of *a-numbers* (that is particularly useful in diagonalization). Therefore, up to a constant term, the Hamiltonian of the XYZ model is the same of the following Hamiltonian for a one dimensional Fermi gas:

$$\begin{aligned} H_N &= -\sum_{j=1}^{N^*} S_{xy}(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger) - A_{xy}\sum_{j=1}^{N^*}(c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) \\ &- J_z \sum_{j=1}^{N^*} c_j^\dagger c_j c_{j+1}^\dagger c_{j+1} + \text{chemical potential}, \end{aligned} \tag{1.5}$$

where $S_{xy} = \frac{J_x+J_y}{2}$ and $A_{xy} = \frac{J_x-J_y}{2}$. This is a very complicate object, since it describes a Fermi gas with particles interacting each others, where the interaction is given by the quartic term in the Fermi operators in the Hamiltonian.
We also notice that the one body interaction, *i.e.* the transverse field, is nothing but the chemical potential for the Fermi gas, since it fixes the number of modes for every j $\sigma_j^z = 2n_j - \mathbb{I}$. Thus the magnetization becomes the total number of fermions

$$\frac{1+m_N}{2} = \sum_{j=1}^{N} \sigma_j^z = \sum_{j=1}^{N} n_j. \tag{1.6}$$

It is interesting to notice that in the XYZ model a chemical potential with strength proportional to J_z arises without any transverse field in the original spin model. For example, if we choose periodic boundary conditions, we get just the additional term

$$J_z \sum_{j=1}^{N} n_j$$

that can be easily eliminated by a suitable counter-term in the spin Hamiltonian

$$-\frac{J_z}{2}\sum_{j=1}^{N} \sigma_j^z.$$

In this case the model has been exactly solved in [**6**].
Anyway, as previously said, we shall limit ourself to study the free fermion theory, in which one has $J_z = 0$. In particular, in the units in which $J_x = 1$ and $J_y = \gamma$ we get the fermionic analog of the XY chain in a transverse constant field:

$$2H_N(\gamma,h) = -\sum_{j=1}^{N}(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger) - \gamma\sum_{j=1}^{N}(c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) - 2\sum_{j=1}^{N} h_j c_j^\dagger c_j. \tag{1.7}$$

This last will be the starting point of all our consideration during the whole work.

3. Diagonalization of the XY Hamiltonian

The first step for investigating the properties of this model is to recall the procedure of diagonalization developed in [**15**] (see also [**5**]). Hereafter will use mainly the fermions. Let us perform a Fourier transform on the Fermi operators:

$$\begin{cases} a_q &= \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{iqj} c_j \\ a_q^\dagger &= \frac{1}{\sqrt{N}}\sum_j e^{-iqj} c_j^\dagger \end{cases} \tag{1.8}$$

where $q = -\pi, ..., \pi$, with the inverses

$$\left\{ \begin{array}{rcl} c_j & = & \frac{1}{\sqrt{N}} \sum_q e^{-iqj} a_q \\ c_j^\dagger & = & \frac{1}{\sqrt{N}} \sum_q e^{iqj} a_q^\dagger \end{array} \right. \tag{1.9}$$

In terms of these new operator the Hamiltonian becomes (up to the irrelevant addendum $\sum_q e^{iq} = 1$)

$$\begin{aligned} 2H_N(\gamma, h) &= -\sum_q (2\cos q + 2h) a_q^\dagger a_q + e^{-iq} a_q^\dagger a_{-q}^\dagger - e^{iq} a_q a_{-q} \\ &= -\sum_q \Big[(\cos q + h)(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - i\gamma \sin q (a_q^\dagger a_{-q}^\dagger + a_q a_{-q}) \Big] \\ &= -\sum_q H_q(\gamma, h), \end{aligned} \tag{1.10}$$

bearing in mind that

$$\begin{aligned} \sum_q g(q) \alpha_q \alpha_{-q} &= \frac{1}{2} \sum_q (g(q) - g(-q)) \alpha_q \alpha_{-q} \\ \sum_q g(q) \alpha_q \beta_q &= \frac{1}{2} \sum_q g(q) \alpha_q \beta_q + g(-q) \alpha_{-q} \beta_{-q} \\ \alpha_q \beta_q &= \frac{1}{2} [\alpha_q, \beta_q] + \frac{\delta_{qp} \delta_{\alpha \beta^\dagger}}{2}, \end{aligned} \tag{1.11}$$

for every couple of a-numbers $\{\alpha_q, \beta_p\} = \delta_{qp}$ (the last line will be useful in the next considerations).
We notice that all the H_q acts in independent subspaces, that is

$$2H_q = \mathbb{I} \otimes ... \otimes \Big[(\cos q + h)(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - i\gamma \sin q (a_q^\dagger a_{-q}^\dagger + a_q a_{-q}) \Big] \otimes ... \otimes \mathbb{I}$$

and so we always have $[H_p, H_q] = 0 \; \forall p, q$. This last simply means that we can diagonalize all the modes independently, thus we can operate fixing q. Each H_q is a quadratic form in the creation and annihilation operators. In order to render it more symmetric, we will write (up to a constant term $\cos q + h$)

$$4H_q = \frac{1}{2} \Big((\cos q + h)([a_q^\dagger, a_q] + [a_{-q}^\dagger, a_{-q}]) - i\gamma \sin q ([a_q^\dagger, a_{-q}^\dagger] + [a_q, a_{-q}]) \Big),$$

or in matrix form

$$4H_q = \begin{pmatrix} a_q^\dagger & a_q & a_{-q}^\dagger & a_{-q} \end{pmatrix} \begin{pmatrix} \Gamma_1 & 0 & 0 & -i\Gamma_2 \\ 0 & -\Gamma_1 & -i\Gamma_2 & 0 \\ 0 & i\Gamma_2 & \Gamma_1 & 0 \\ i\Gamma_2 & 0 & 0 & -\Gamma_1 \end{pmatrix} \begin{pmatrix} a_q \\ a_q^\dagger \\ a_{-q} \\ a_{-q}^\dagger \end{pmatrix} \tag{1.12}$$

with $\Gamma_1 = \cos q + h$ and $\Gamma_2 = \gamma \sin q$. This form can be easily diagonalized obtaining the eigenvalues for the energy of the system:

$$E_q^2 = (\cos q + h)^2 + \gamma^2 \sin^2 q. \tag{1.13}$$

This formula gives us informations on the phase diagram of the system. For $\gamma = 0$ we recover the XX model: it exhibits a transition for $h = 1$, since for $h > 1$ it presents a spectral gap (the lowest eigenvalue is greater than zero) and instead for $h < 1$ the spectrum is a continuum interval. For $\gamma \neq 0$ $h = 1$ is always a singular point, since, $\forall \gamma$, we always have continuous spectrum; as well as $h \neq 1$ one again has a spectral gap.

The Bogoliubov-Valatin transformation [**8**][**21**] W that diagonalizes the matrix can be directly verified be the tensor product of (SU(2)×SU(2)) rotations around the y-axis [**15**][**2**]:

$$\begin{aligned} W &= \bigotimes_{q=-\pi}^{\pi} W_q, \\ W_q &= \begin{pmatrix} \mathbb{I}\cos\phi_q & -\sigma^y \sin\phi_q \\ \sigma^y \sin\phi_q & \mathbb{I}\cos\phi_q \end{pmatrix}, \end{aligned} \tag{1.14}$$

that is as to say that the Hamiltonian is diagonal in the new operators

$$\begin{aligned} b_q &= a_q \cos\phi_q + i a_{-q}^\dagger \sin\phi_q \\ b_q^\dagger &= a_q^\dagger \cos\phi_q - i a_{-q} \sin\phi_q, \end{aligned} \tag{1.15}$$

with $\cos 2\phi_q = (\cos q + h)/E_q$, $\sin\phi_q = -\gamma \sin q/E_q$. Sometimes it can be useful to get rid of imaginary unit and make everything real. Let us introduce the unitary matrix

$$T = \begin{pmatrix} e^{i\frac{\pi}{4}} & 0 \\ 0 & e^{-i\frac{\pi}{4}} \end{pmatrix},$$

with $\sigma^y T = T^\dagger \sigma^y$, and $T^\dagger \sigma^y T = (T^\dagger)^2 \sigma^y = -i\sigma^z \sigma^y = -\sigma^x$, and define[3]

$$\tilde{W}_q = \begin{pmatrix} \mathbb{I}\cos\phi_q & -T^\dagger \sigma^y T \sin\phi_q \\ T^\dagger \sigma^y T \sin\phi_q & \mathbb{I}\cos\phi_q \end{pmatrix},$$

as the transformation that diagonalizes our bilinear form with phase adjustment. Thus for the new operator so obtained we have

$$\begin{aligned} \tilde{b}_q &= a_q \cos\phi_q + a_{-q}^\dagger \sin\phi_q \\ \tilde{b}_q^\dagger &= a_q^\dagger \cos\phi_q + a_{-q} \sin\phi_q, \end{aligned} \tag{1.16}$$

Anyway the Hamiltonian in the new variables becomes

$$\begin{aligned} -\sum_q H_q &= -\sum_q \frac{1}{4}\left(E_q [b_q^\dagger, b_q] + E_q [b_{-q}^\dagger, b_{-q}] \right) \\ &= -\frac{1}{2}\sum_q \left(E_q b_q^\dagger b_q + E_q b_{-q}^\dagger b_{-q} \right) \\ &= -\sum_q E_q b_q^\dagger b_q. \end{aligned} \tag{1.17}$$

In the same way it is

$$-\sum_q H_q = -\sum_q E_q \tilde{b}_q^\dagger \tilde{b}_q.$$

It turns useful to explicitly write down the transformation that diagonalized our initial Fermi Hamiltonian in $c, c^\dagger$; denoting by $b \equiv (b_q, b_q^\dagger)$ and $c \equiv (c_j, c_j^\dagger)$ one has

$$b = U^\dagger c U$$

where $U = W \circ FT$ is the composition of a Fourier Transform and our B-V Transformation. Thus the relations defining U (or, better, its matrix element U_{qj}) are

$$\begin{cases} b_q &= \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{iqj} \left(\cos\phi_q c_j + i \sin\phi_q c_j^\dagger \right) \\ b_q^\dagger &= \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-iqj} \left(\cos\phi_q c_j^\dagger - i \sin\phi_q c_j \right), \end{cases} \tag{1.18}$$

[3] It seems to the author more important to write the B-V transform in this form in order to stress its clear rotational nature. Of course, for SU(2) rotations, phase shift, even if meaningless from a physical point of view, can change the transformation.

with the obvious (more useful) inverses:

$$\begin{cases} c_j &= \frac{1}{\sqrt{N}}\sum_q e^{-iqj}\cos\phi_q b_q + ie^{iqj}\sin\phi_q b_q^\dagger, \\ c_j^\dagger &= \frac{1}{\sqrt{N}}\sum_q e^{iqj}\cos\phi_q b_q^\dagger - ie^{-iqj}\sin\phi_q b_q. \end{cases} \tag{1.19}$$

4. Diagonalization in Presence of an Inhomogenous Field

Now we concern of generalizing the previous procedure in the case where the external field is no longer constant. This breaks the translational symmetry, removing the degeneracy of the eigenvalues for $q \to -q$. The obvious consequence is the occurrence of new non conserved observables, and makes more difficult the diagonalization of the Hamiltonian.
We will start, for sake of simplicity, with the simpler case of the XX chain, where the field is acting only in one site, say k. This has been done for the first time in [**2**] (see also [**1**]). Hereafter we will refer to this as the XX *impurity* model.
The Hamiltonian of the model is

$$H_N = \sum_{j=1}^{N-1}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right) + h\sigma_k^z, \tag{1.20}$$

that reads, in terms of fermionic operators, as formula (1.7) with open boundaries, $\gamma = 0$ and $h_j = h\delta_{jk}$, *i.e.*

$$2H_N = -\sum_{j=1}^{N-1}(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger) - hc_k^\dagger c_k. \tag{1.21}$$

Also here we shall perform a Fourier transform of the fermionic operators like (1.8), in order to get

$$H_N = -\sum_q\left[\cos q(a_q^\dagger a_q + a_{-q}^\dagger a_{-q})\right] - \frac{h}{N}\sum_{q,p} e^{i(q-p)k}a_q^\dagger a_p. \tag{1.22}$$

As a consequence of translational symmetry breaking, we have that the last expression can be no longer written as a tensor product of operators acting in independent subspaces for each q. We need further manipulations. Following [**2**], we have to solve the following secular equation in order to diagonalize the Hamiltonian:

$$\sum_{p,q} U_{q\alpha}(\cos q\delta_{qp} + \frac{h}{N}e^{i(q-p)k})U_{p\beta}^\dagger = E_\alpha\delta_{\alpha\beta}.$$

It is easily seen that, for elementary properties of unitary matrices, this equation is equivalent to

$$(E_\alpha - \cos q)U_{q\alpha} = \frac{h}{N}\sum_p e^{-i(q-p)k}U_{p\alpha}, \tag{1.23}$$

in the sense that a matrix with entries satisfying the last equation diagonalizes the Hamiltonian (and viceversa). A first class of eigenvalue are given by $E_\alpha : E_\alpha = \cos q_\alpha$, *i.e.* the unperturbed eigenvalues. In this case we find the transformation according to the relation

$$\sum_p e^{ipm}U_{p\alpha} = 0,$$

meaning that each eigenvector has to be orthogonal to the mode m. If we expand

$$U_{p\alpha} = \frac{1}{N}\sum_k c_k(q_\alpha)e^{ikp} + d_k(q_\alpha)e^{-ikp},$$

since the condition of unitarity is

$$\sum_k c_k^*(q_\alpha)c_k(q_\alpha) + d_k^*(q_\beta)d_k(q_\beta) = \delta_{\alpha\beta}$$

and the condition of orthogonality $c_m(q_\alpha) = -d_{-m}(q_\alpha)$, we can simply choose $c_k(q_\alpha) = -e^{iq_\alpha(k-m)}/\sqrt{2}$ and $d_k(q_\alpha) = e^{iq_\alpha(k+m)}/\sqrt{2}$, such that:

$$U_{p,\alpha} = \frac{1}{\sqrt{2}N}\sum_k^N \left(-e^{ik(q+q_\alpha)}e^{-iq_\alpha m} + e^{-ik(q-q_\alpha)}e^{iq_\alpha m}\right), \tag{1.24}$$

or

$$U_{p,\alpha} = \frac{1}{\sqrt{2}}(\delta_{qq_\alpha}e^{-iq_\alpha m} - \delta_{-qq_\alpha}e^{iq_\alpha m}). \tag{1.25}$$

We notice that

$$U_{q,\alpha} \equiv U_{q,q_\alpha} = U_{q,-q_\alpha},$$

meaning that to the eigenvalue $E_\alpha = \cos q_\alpha$ corresponds only one eigenvector, that is to say that we are considering only the $q_\alpha \geq 0$; therefore there are only $N/2$ solution of this kind (since the perturbation breaks the translation invariance removing the degeneracies). The transformations giving the new operators are then ($b_\alpha = b_{q_\alpha}$)

$$b_\alpha = \frac{1}{\sqrt{2}}\left(e^{iq_\alpha m}a_{q_\alpha} - e^{-iq_\alpha m}a_{-q_\alpha}\right) \tag{1.26}$$

$$b_\alpha^\dagger = \frac{1}{\sqrt{2}}\left(e^{-iq_\alpha m}a_{q_\alpha}^\dagger - e^{iq_\alpha m}a_{-q_\alpha}^\dagger\right), \tag{1.27}$$

together with their inverses

$$a_q = \mathrm{sign}(q)e^{-i|q|m}b_{|q|} \tag{1.28}$$

$$a_q^\dagger = \mathrm{sign}(q)e^{i|q|m}b_{|q|}^\dagger. \tag{1.29}$$

In order to recover the other $N/2$ eigenvalues and eigenvectors, we have to come back to (1.23). If $E_\alpha \neq \cos q_\alpha$ we have, with a little manipulation

$$\sum_q e^{iqm}U_{q\alpha} = \frac{h}{N}\sum_q \frac{1}{E_\alpha - \cos q}\sum_p e^{ipm}U_{p\alpha}$$

i.e. the eigenvalues are given (even in thermodynamic limit) by the zeros of the function

$$F_N(E) = 1 - \frac{h}{N}\sum_q \frac{1}{E_\alpha - \cos q} \underset{N\to\infty}{.} \tag{1.30}$$

Then we look for a transformation unitary matrix of the form

$$U_{p\alpha} = \frac{1}{N}\sum_{k=1}^N c_{k,\alpha}e^{-ipk},$$

that in (1.23) brings to

$$U_{q\alpha} = \frac{h}{N}\frac{e^{-iqm}c_{m\alpha}}{E_\alpha - \cos q},$$

with $c_{m\alpha}$ be determined by the normalization condition to

$$|c_{m\alpha}|^{-2} = \left(\frac{h}{N}\right)^2 \sum_q \frac{1}{(E_\alpha - \cos q)^2}.$$

Definitely one has

$$U_{q\alpha} = \frac{1}{\mathcal{N}_\alpha}\frac{e^{-iqm}}{E_\alpha - \cos q}, \tag{1.31}$$

where $\mathcal{N}_\alpha = |c_{m\alpha}|h/N$. Thus we can give the formulas for the other $N/2$ operators

$$b_\alpha = \sum_q \frac{1}{\mathcal{N}_\alpha}\frac{e^{-iqm}}{E_\alpha - \cos q}a_q \tag{1.32}$$

$$b_\alpha^\dagger = \sum_q \frac{1}{\mathcal{N}_\alpha}\frac{e^{iqm}}{E_\alpha - \cos q}a_q^\dagger, \tag{1.33}$$

and the inverses

$$a_q = \sum_\alpha \frac{1}{\mathscr{N}_\alpha} \frac{e^{iqm}}{E_\alpha - \cos q} b_\alpha \tag{1.34}$$

$$a_q^\dagger = \sum_\alpha \frac{1}{\mathscr{N}_\alpha} \frac{e^{-iqm}}{E_\alpha - \cos q} b_\alpha^\dagger. \tag{1.35}$$

Often it results useful to write down (1.34) and (1.35) in a different form, basically using the residues theorem[4]:

$$a_q = \frac{1}{2\pi i} \oint d\log F_N(E) \frac{1}{\mathscr{N}_\alpha} \frac{e^{iqm}}{E_\alpha - \cos q} b_E \tag{1.36}$$

$$a_q^\dagger = \frac{1}{2\pi i} \oint d\log F_N(E) \frac{1}{\mathscr{N}_\alpha} \frac{e^{-iqm}}{E_\alpha - \cos q} b_E^\dagger. \tag{1.37}$$

Thus we have that, at fixed N, the spectrum of the XX chain with a single impurity is point-wise and it is given in the thermodynamic limit by all the zeros and the poles of the function

$$F(E) = 1 - \frac{h}{\pi} \sum_q \frac{1}{E - \cos q}.$$

Now we can take the thermodynamic limit: we have that the unperturbed eigenvalues fill the interval $[-1,1]$, and since for $|E| > 1$[5]

$$F_N(E) \longrightarrow F(E) = 1 - \frac{h}{\pi} \int_{-\pi}^{\pi} dq \frac{dq}{E - \cos q} = 1 - \frac{h \operatorname{sign}(E)}{\sqrt{E^2 - 1}},$$

we obtain another isolated energy level at $E = \operatorname{sign}(h)\sqrt{1+h^2}$. Therefore we can resume our result in the following

THEOREM 1. *The spectrum of the XX chain with a single impurity at every finite N is point wise, and it is given by all the zeros and the poles of the function $F_N(E)$; in the thermodynamic limit instead it becomes an interval plus an isolated value, namely the set $[-1,1] \cup \{\operatorname{sign}(h)\sqrt{1+h^2}\}$. This represents as well the set of all zeros and poles of the limiting function $F(E)$.*

We notice that the set of eigenvalues can be characterized as the set of all the singularities (the entire interval $[-1,1]$ in this case) and zeros (only one in this case) of $F(E)$, as it is at fixed N.

The structure of this theorem permits to be generalized to the case of completely inhomogeneous transverse field.

We can split the field as $h + h_j$, where h is the mean value and h_j, such that $\sum_j h_j = 0$; they can be interpreted as frozen fluctuation of the transverse field around its mean value, in order to maintain the *impurity* point of view.

The Hamiltonian of the XX chain in an inhomogeneous transverse field is

$$H_N = \sum_{j=1}^{N-1} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right) + \sum_{j=1}^{N} (h_j + h) \sigma_j^z, \tag{1.38}$$

or, in terms of fermionic operators (see formula (1.7))

$$2H_N = -\sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger) - 2 \sum_{j=1}^{N} (h_j + h) c_j^\dagger c_j. \tag{1.39}$$

By taking the lattice Fourier Transform we get

$$H_N = -\sum_q \left[(\cos q + h)(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) \right] - \frac{1}{N} \sum_k \sum_{q,p} h_k e^{i(q-p)k} a_q^\dagger a_p. \tag{1.40}$$

[4]It can be easily checked that $F'(E) = \mathscr{N}(E)$ has no poles.

[5]This is the form that condition $E_\alpha \neq \cos q_\alpha$ assumes when $N \to \infty$.

We can follow the same strategy used in the simpler case of only one impurity. At first we write the secular equation:

$$\sum_{p,q} U_{q\alpha}((\cos q + h)\delta_{qp} + \frac{1}{N}\sum_k h_k e^{i(q-p)k})U^\dagger_{p\beta} = E_\alpha \delta_{\alpha\beta}.$$

or equivalently the equations for the eigenvectors

$$(E_\alpha - \cos q)U_{q\alpha} = \frac{1}{N}\sum_{p,k} h_k e^{-i(q-p)k} U_{p\alpha}. \tag{1.41}$$

Again we can look for eigenvalues of the form $E_\alpha = \cos q_\alpha$, with eigenvectors given by the condition

$$\frac{1}{N}\sum_{p,k} h_k e^{-i(q-p)k} U_{p\alpha} = 0.$$

It is easy to imagine that we can generalize the procedure adopted before in the completely inhomogeneous case. Thus we have to sum over all the sites the transformation (1.25), with a suitable normalization, obtaining

$$U_{p,\alpha} = \frac{1}{\sqrt{2h^2}}\sum_{m=1}^{N} h_m(\delta_{qq_\alpha}e^{-iq_\alpha m} - \delta_{-qq_\alpha}e^{iq_\alpha m}). \tag{1.42}$$

with $h^2 = \sum_k h_k^2$. Again we have

$$U_{q,\alpha} \equiv U_{q,q_\alpha} = -U_{q,-q_\alpha},$$

thus the same eigenvector is associated to the eigenvalues corresponding to $\pm q_\alpha$, and we can choose all the q_α positive as well. Therefore we have found $N/2$ eigenvectors and eigenvalues, and the new operators are given by

$$\begin{aligned} b_\alpha &= \frac{1}{\sqrt{2N}}\sum_m \left(e^{-iq_\alpha m}a_{q_\alpha} - e^{iq_\alpha m}a^\dagger_{-q_\alpha}\right) \\ b^\dagger_\alpha &= \frac{1}{\sqrt{2N}}\sum_m \left(e^{iq_\alpha m}a^\dagger_{q_\alpha} - e^{-iq_\alpha m}a^\dagger_{-q_\alpha}\right), \end{aligned} \tag{1.43}$$

with the inverses

$$\begin{aligned} a_q &= \mathrm{sign}(q)\sum_m e^{i|q|m}b_{|q|} \\ a^\dagger_q &= \mathrm{sign}(q)\sum_m e^{-i|q|m}b^\dagger_{|q|}. \end{aligned} \tag{1.44}$$

Starting by (1.41) we can recover the form of the other $N/2$ eigenvalues and eigenvectors. Remembering that $c_{k,\alpha}$ is the k-th Fourier coefficient of $U_{q\alpha}$, *i.e.*

$$U_{q\alpha} = \frac{1}{N}\sum_k c_{k\alpha}e^{-ipk},$$

we have

$$U_{q\alpha} = \frac{\frac{1}{N}\sum_{p,k} h_k e^{-i(q-p)k}U_{p\alpha}}{E_\alpha - (\cos q + h)},$$

and so, multiplying by $\tilde{h}(q)$ (where $\tilde{\cdot}_q$ is the Fourier transform on the lattice calculated in q) and summing over q we get

$$\begin{aligned} \sum_q U_{q\alpha}\tilde{h}(q) &= \frac{1}{N^2}\sum_q\sum_j\sum_k e^{iq(k-j)}h_j c_{k,\alpha} \\ &= \frac{1}{N}\sum_k h_k c_{k,\alpha} \\ &= \sum_q \frac{\tilde{h}(q)}{E_\alpha - (\cos q + h)}\left(\frac{1}{N}\sum_k h_k c_{k,\alpha}e^{-iqk}\right) \end{aligned}$$

The main idea here is that, in analogy with the previous case, $\sum_k h_k c_{k\alpha}$ is a *counter* of the number of impurities in our system. We notice that, as in the single impurity case, the sum has to be pursued on the sites containing impurities: this means that $c_{k\alpha} = 0$ if $h_k = 0$. This is reflected also in the normalization conditions of the eigenvectors:

$$|c_{k\alpha}|^2 = \left(\frac{N}{h_k}\right)^2 \mathcal{N}_\alpha^2 \qquad \text{if } h_k \neq 0,$$

and

$$U_{q\alpha} = \frac{1}{\mathcal{N}_\alpha} \sum_{k:h_k\neq 0} \frac{e^{-iqk}}{E_\alpha - (\cos q + h)}. \tag{1.45}$$

So we can take $c_k = 1/h_k$ if $h_k \neq 0$, zero otherwise, we can define $d_k = 0,1$, as the impurity indicator at the site k, and

$$\begin{aligned} \frac{1}{N}\sum_k h_k c_{k\alpha} &= \frac{1}{N}\sum_k d_k = d_N \in [0,1] \qquad \text{(density of impurities)} \\ \frac{1}{N}\sum_k e^{-iqk} h_k c_{k\alpha} &= \frac{1}{N}\sum_k d_k e^{-iqk} = \tilde{d}_{-q}. \end{aligned}$$

At this point, we can rewrite (1.45) as

$$d_N = \sum_q \frac{\tilde{h}(q)\tilde{d}^*(q)}{E_\alpha - (\cos q + h)} \tag{1.46}$$

and define

$$F_N(E_\alpha) \equiv 1 - \frac{1}{d_N}\sum_q \frac{\tilde{h}(q)\tilde{d}^*(q)}{E_\alpha - (\cos q + h)}, \tag{1.47}$$

the other $N/2$ eigenvectors are given by the zeros of $F_N(E)$. So in analogy with the single impurity system, we have that at fixed N the spectrum is given by the set of zeros and poles of $F_N(E)$ and we can write the transformations formulas:

$$a_q = \sum_{k:h_k\neq 0} \frac{1}{2\pi i} \oint d\log F_N(E) \frac{1}{\mathcal{N}_\alpha(E,h)} \frac{e^{iqk}}{E_\alpha - (\cos q + h)} b_E \tag{1.48}$$

$$a_q^\dagger = \sum_{k:h_k\neq 0} \frac{1}{2\pi i} \oint d\log F_N(E) \frac{1}{\mathcal{N}_\alpha(E,h)} \frac{e^{-iqk}}{E_\alpha - (\cos q + h)} b_E^\dagger. \tag{1.49}$$

For a given sequence of distribution of impurities, provided the existence of a limit distribution for $N \to \infty$ with density d, we can state the following

THEOREM 2. *The spectrum of the XX chain with an arbitrary number of impurities is given in the thermodynamic limit by the set of zeros and the poles of the function* $F(E) \equiv \lim_N F_N(E)$. *At finite size N, it is given by a discrete set, while in the thermodynamic limit it becomes a continuous interval plus isolated points.*

It is easily seen that in the case of a single impurity, $h_k = h\delta_j k$, the equations (1.47), (1.42) and (1.45) reduce to (1.30), (1.25), (1.31).
When we have an inhomogeneous field non vanishing in each site, we see by our formula that the fluctuations automatically compensate each other, and only the mean value determines the spectrum: if $d_j = 1$ always, we have that $F_N(E) = 0$ only if $E_\pm = \pm 1 + h$, that is the lifting of the spectrum one has in presence of a constant magnetic field.

5. Time Evolution I: Generalities

Let us consider a system ruled by a time dependent Hamiltonian H_t. We will concern about the dynamics of certain quadratic Hamiltonian in fermionic operators that reads in the Fourier space as

$$H(t) = \sum_{qp} \alpha_{qp}(t) a_q^\dagger a_p + \beta_{qp}(t) a_q^\dagger a_p^\dagger + \beta_{qp}^*(t) a_q a_p,$$

with, for $t' \neq t''$,

$$[H(t'), H(t'')] \neq 0.$$

Indeed, as previously noticed, in the models of our interest we have that the Hamiltonian has two non commutative parts: the bulk part does not commute with the transverse field. This leads to non trivial dynamics, as well known in quantum mechanics [**10**].
Initially, at $t = t_0$, we can image that the system is at equilibrium, with Hamiltonian H_0 (and $[H_0, H(t)] \neq 0$). Given a generic observable f, its mean will be given by

$$\langle f \rangle_0 = \frac{\mathrm{Tr}(\rho_0 f)}{\mathrm{Tr}\,\rho_0},$$

where $\rho_0 = e^{-\beta H_0}$. Thus we want to evolve the state, *i.e.* the density matrix ρ_t, via quantum dynamics. This is done by the Quantum Liouville Equation:

$$i d_t \rho_t = [H_t, \rho_t],$$

that leads to

$$\rho_t = T\left(e^{i\int_0^t H_{t'}} \rho_0 e^{-i\int_0^t H_{t'}}\right).$$

where T as usual indicates the time ordered product. The time dependent expectation value of an observable is thus given by

$$\langle f \rangle_t = \frac{\mathrm{Tr}(\rho_t f)}{\mathrm{Tr}\,\rho_t}.$$

The Quantum Liouville Equation is generally very difficult to solve, even in our simple class of systems. We must adopt a divers (but of course equivalent) point of view.
In the Heisenberg picture, the time evolution is given by

$$a_q(t) = T\left(e^{i\int_{t_0}^t dt' H(t')} a_q e^{-i\int_{t_0}^t dt' H(t')}\right); \tag{1.50}$$

we will show that the solution of this equation is given by the flux along the trajectories of the 1-parameter semigroup of B-V transformation given by

$$a_q(t) = \sum_p A_{qp}(t) a_p + B_{qp}(t) a_p^\dagger, \tag{1.51}$$

with $A_{qp}(t_0) = \delta_{qp}$ and $B_{qp}(t_0) = 0$. We know that (1.50) solves the Ehrenfest equation

$$i d_t a_q(t) = [a_q, H(t)],$$

and so we look for a solution satisfying

$$i d_t a_q(t) = \sum_p i\dot{A}_{qp}(t) a_p + i\dot{B}_{qp}(t) a_p^\dagger. \tag{1.52}$$

In order to compare the last two formulas, we have to evaluate the commutator in the Ehrenfest equation. This is easily done, noticing that

$$\begin{aligned}
\left[a_p, a^\dagger_{q'} a_{p'}\right] &= \delta_{q'p} a'_p \\
\left[a_p, a^\dagger_{q'} a^\dagger_{p'}\right] &= \delta_{q'p} a^\dagger_{p'} - \delta_{pp'} a^\dagger_{q'} \\
\left[a_p, a_{q'} a_{p'}\right] &= 0 \\
\left[a^\dagger_p, a^\dagger_{q'} a_{p'}\right] &= -\delta_{pp'} a^\dagger_{q'} \\
\left[a^\dagger_p, a^\dagger_{q'} a^\dagger_{p'}\right] &= 0 \\
\left[a^\dagger_p, a_{q'} a_{p'}\right] &= \delta_{pp'} a_{q'} - \delta_{pq'} a_{p'}.
\end{aligned}$$

Hence we have

$$\begin{aligned}
i d_t a_q(t) &= \sum_{q'p'} a_{p'} \left(A_{qq'}(t)\alpha_{q'p'}(t) + B_{qq'}(t)(\beta^*_{q'p'}(t) - \beta^*_{p'q'}(t)) \right) \\
&+ \sum_{q'p'} a^\dagger_{p'} \left(-B_{qq'}(t)\alpha_{q'p'}(t) + A_{qq'}(t)(\beta_{q'p'}(t) - \beta_{p'q'}(t)) \right)
\end{aligned}$$

and comparing the last formula with (1.52), we get

$$i\dot{A}_{qp}(t) = \sum_{q'} A_{qq'}(t)\alpha_{q'p}(t) + B_{qq'}(t)(\beta^*_{q'p}(t) - \beta^*_{pq'}(t)) \tag{1.53}$$

$$i\dot{B}_{qp}(t) = \sum_{q'} -B_{qq'}(t)\alpha_{q'p}(t) + A_{qq'}(t)(\beta_{q'p}(t) - \beta_{pq'}(t)). \tag{1.54}$$

So equations (1.53) and (1.54) represent the evolution equations for the 1-parameter semigroup of B-V transformations that gives quantum dynamics. Of course, all the information for temporal dependance of observables (and thus, the state) is encoded in these equations. Indeed we have that a generic observable $f(\cdot,t)$ has to be of the following form [**19**]:

$$f(S,t) = \sum_{V\subseteq S} f(V,t) \frac{1}{N^{|V|}} \sum_{q_j,p_j,j\in V} :\prod_{j\in V} \eta_{q_j}\xi_{q_j}: e^{\sum_j i(p_j-q_j)j} + h.c.$$

where S is the support of the chain in $\mathbb{Z}$, :: denotes the Wick product [**22**] for the operators

$$\begin{aligned}
\eta_q &= a^\dagger_q + a_{-q} \\
\xi_q &= a^\dagger_{-q} - a_q.
\end{aligned}$$

Since the Hamiltonian is quadratic, the thermal average is evaluated by using the Wick theorem [**22**]:

$$\begin{aligned}
\langle f(S,t)\rangle &= \sum_{V\subseteq S} f(V,t) \frac{1}{N^{|V|}} \sum_{q_j,p_j,j\in V} \left\langle :\prod_{j\in V} \eta_{q_j}\xi_{q_j}: \right\rangle e^{\sum_j i(p_j-q_j)j} + h.c. \\
&= \sum_{V\subseteq S} f(V,t) \frac{1}{N^{|V|}} \sum_{q_j,p_j,j\in V} e^{\sum_j i(p_j-q_j)j} \sum_{\text{all pairings } \Pi_V} (-1)^{\pi'} \prod_{(h,k)\in\Pi_V} \left\langle :\eta_{q_h}\xi_{q_k}: \right\rangle + h.c.
\end{aligned}$$

where π' gives the parity of a given pairing Π_V of the set $\{q_j, p_j : j \in V\}$. In principle the unknown are just the functions $f(V,t)$. We can solve that problem by switching to the Heisenberg picture, and computing

$$\langle f(S,0)\rangle_t = \sum_{V\subseteq S} f(V,0) \frac{1}{N^{|V|}} \sum_{q_j,p_j,j\in V} e^{\sum_j i(p_j-q_j)j} \sum_{\text{all pairings } \Pi_V} (-1)^{\pi'} \prod_{(h,k)\in\Pi_V} \left\langle :\eta_{q_h}(t)\xi_{q_k}(t): \right\rangle + h.c.$$

bearing in mind that now

$$\begin{aligned}\eta_q(t) &= \sum_p \left(A^*_{qp}(t)+B_{-q,p}(t)\right)a^\dagger_p + \left(B^*_{qp}(t)+A_{-q,p}(t)\right)a_p \\ \xi_q(t) &= \sum_p \left(A^*_{-q,p}(t)-B_{q,p}(t)\right)a^\dagger_p + \left(B^*_{-q,p}(t)-A_{q,p}(t)\right)a_p,\end{aligned}$$

and that the averages with respect to the initial density matrix ρ_0 are

$$\begin{aligned}\langle a^\dagger_q a_p\rangle &= \frac{\delta_{qp}}{1+e^{\beta\omega_p}} \\ \langle a^\dagger_q a^\dagger_p\rangle &= 0 \\ \langle a_q a_p\rangle &= 0,\end{aligned}$$

where ω_p are the proper frequencies (or, equivalently in our units, the energies) of the system at initial time. We have that for a given pair $\bar q, \bar p$ the only contributing term is

$$\sigma_{\bar q\bar p}(\beta,t) = \sum_{q'} \frac{A^*_{\bar q q'}(t)B^*_{-\bar p q'}(t) - B_{-\bar q q'}(t)A_{\bar p q'}(t) + B^*_{-\bar q q'}(t)B - \bar p q'(t) - A^*_{\bar q q'}(t)A_{\bar p q'}(t)}{1+e^{\beta\cos q'}}. \tag{1.55}$$

Therefore the time dependence of the state of the system is all in that formula. We have

$$\begin{aligned}\langle f(S,0)\rangle_t &= \sum_{V\in S} f(V,0)\frac{1}{N^{|V|}}\sum_{q_j,p_j,j\in V} e^{\Sigma_j i(p_j-q_j)j} \sum_{\text{all pairings }\Pi_V}(-1)^{\pi'}\prod_{(h,k)\in\Pi_V}\sigma_{\bar q\bar p}(\beta,t)+h.c. \\ &= \sum_{V\in S} f(V,0)\Sigma(V,\beta,t)\end{aligned}$$

with

$$\Sigma(V,\beta,t) = \frac{1}{N^{|V|}}\sum_{q_j,p_j,j\in V} e^{\Sigma_j i(p_j-q_j)j} \sum_{\text{all pairings }\Pi_V}(-1)^{\pi'}\prod_{(h,k)\in\Pi_V}\sigma_{\bar q\bar p}(\beta,t)+h.c. \tag{1.56}$$

is indeed, at least formally, the *state* of the system[6].
Of course, since Heisenberg and Schrödinger pictures are equivalent, it is $\langle f\rangle_t = \langle f(t)\rangle$. So, at least in principle, the problem of evaluating the quantum dynamics for free fermions, *i.e.* quadratic form Hamiltonians, *i.e.* one dimensional integrable spin systems, far or close to equilibrium, is reduced to solve the coupled equations (1.53) and (1.54).

6. Time Evolution II: Spin Chains in a Transverse Field

Let us now check how the formalism developed in the last section works when a transverse field is applied. We will proceed again by steps: at first we will analyze the XX model (with impurities), and then the XY model; as previously seen, the main difference between the two is the need of a B-V transformation in the second one.
In the XX impurity Hamiltonian we have, in the language of the previous section, that:

$$\begin{aligned}\alpha_{qp} &= (\cos q + h)\delta_{qp} + h_{q-p}(t) \\ \beta_{qp} &= 0,\end{aligned}$$

where we let vary with time the magnetic field acting on the impurities, while the coupling remains constant.

[6]We notice that as well as N remains finite, our derivation is exact. The problems could arise when $N\to\infty$, when one should prove that the measures σ and Σ approach to a meaningful limit. This will be done for specific cases.

Since the term β_{qp} vanishes, we have that equations (1.53) and (1.54) decouple (they are in fact the same equation), and the dynamics of the system is simply described only by $A_{qp}(t)$. As will be clearer in the study of the XY model, this is connected to the lack of necessity of performing a B-V transformation in the XX chain. Hence the equation we are interested in is

$$i\dot{A}_{qp}(t) = A_{qp}(\cos p + h) + \sum_{q'} A_{qq'}(t) h_{q'-p}(t). \tag{1.57}$$

Now it results convenient to define the quantity

$$X_q^k(t) = \sum_{q'} A_{qq'}(t) e^{-ik(q'-q)}$$

associated to the k-th impurity. In such a way equation (1.57) becomes

$$i\dot{A}_{qp}(t) = A_{qp}(\cos p + h) + \frac{1}{N}\sum_k h_k(t) X_q^k(t) e^{-ik(q-p)}, \tag{1.58}$$

and can be solved formally by Duhamel principle in an interval $[t_0, t]$:

$$A_{qp}(t) = e^{-i(\cos p+h)(t-t_0)}\delta_{qp} - \frac{i}{N}\sum_k e^{-i(q-p)k}\int_{t_0}^t dt' e^{-i(\cos p+h)(t-t')} h_k(t') X_q^k(t').$$

Now let us call $\omega_p = (\cos p + h)$ the proper frequencies of the system. By direct calculation we get a self consistent recursive equation for the source term:

$$X_q^k(t) = e^{-i\omega_q(t-t_0)} - \frac{i}{N}\sum_j \int_{t_0}^t dt' \left(\sum_p e^{i(q-p)(k-j)} e^{-i(\cos p+h)(t-t')}\right) h_j(t') X_q^j(t'). \tag{1.59}$$

Passing to the limit $N \to \infty$ requires a little care. In primis we have that $X_p(t) \to X(p,t) \in [-\pi, \pi] \times [0, +\infty)$. Then for sake of clearness we are going to distinguish the case of single impurity from the others. In this case we have the evolution equation given by

$$X(q,t) = e^{-i\omega_q(t-t_0)} - i\int_{t_0}^t dt' e^{-ih(t-t')} J_0(t-t') h(t') X(q,t'). \tag{1.60}$$

since

$$\frac{1}{N}\sum_p e^{-i(\cos p+h)(t-t')} \underset{N\to\infty}{\longrightarrow} e^{-ih(t-t')} J_0(t-t').$$

Equation (1.60) is simply generalized in the case of finitely many impurities at finite distance, and reads as

$$X^k(q,t) = e^{-i\omega_q(t-t_0)} - i\sum_j e^{iq(k-j)} \int_{t_0}^t dt' e^{-ih(t-t')} J_{j-k}(t-t') h_j(t') X^j(q,t'), \tag{1.61}$$

and for infinitely many, with a suitable sequence of distributions with a well definite density in the thermodinamic limit, defined $X(k,p,t) : \mathbb{Z} \times [-\pi,\pi] \times [0,+\infty) \to \mathbb{C}$, it is

$$X(k,q,t) = e^{-i\omega_q(t-t_0)} - 2\pi i \sum_{j\in\mathbb{Z}}{}^* e^{iq(k-j)} \int_{t_0}^t dt' e^{-ih(t-t')} J_{j-k}(t-t') h_j(t') X(j,q,t'), \tag{1.62}$$

since

$$\int_{-\pi}^{\pi} dp e^{-ip(k-j)} e^{-i(\cos p+h)(t-t')} = 2\pi e^{-ih(t-t')} J_{j-k}(t-t').$$

With $\sum^*$ we have indicated a suitable measure on $\mathbb{Z}$ defined as follows: we have seen that $h_k = d_k h_k$ where d_k is the indicator of the impurity at k-th site. Thus for a given sequence $f_k^N \to f_k$ defined in invading subsets of $\mathbb{Z}$ (supports of the chain), say S_N, one has [**11**]

$$\frac{1}{N}\sum_{k\in S_N} h_k f_k^N = \sum_{k\in S_N} \frac{d_k}{N} h_k f_k^N = \sum_{k\in S_N}{}^* h_k f_k^N \underset{N\to\infty}{\longrightarrow} \sum_{k\in\mathbb{Z}}{}^* h_k f_k,$$

and it is easily seen that

$$(\min_k h_k)(\min_k f_k) \leq \sum_{k\in\mathbb{Z}}{}^{*} h_k f_k \leq (\max_k h_k)(\max_k f_k).$$

When we have finitely many impurities at a distance growing with N we get another interesting equation. In order to fix the ideas we will analyze the case with only two impurities. Thus equation (1.59) reads

$$\begin{aligned}
X_q^1(t) &= e^{-i\omega_q(t-t_0)} - \frac{i}{N}\int_{t_0}^t dt' \left(\sum_p e^{-i(\cos p+h)(t-t')}\right) h_1(t')X_q^1(t') \\
&- \frac{i}{N}\int_{t_0}^t dt' \left(\sum_p e^{i(q-p)\ell} e^{-i(\cos p+h)(t-t')}\right) h_2(t')X_q^2(t') \\
X_q^2(t) &= e^{-i\omega_q(t-t_0)} - \frac{i}{N}\int_{t_0}^t dt' \left(\sum_p e^{-i(\cos p+h)(t-t')}\right) h_1(t')X_q^1(t') \\
&- \frac{i}{N}\int_{t_0}^t dt' \left(\sum_p e^{-i(q-p)\ell} e^{-i(\cos p+h)(t-t')}\right) h_2(t')X_q^2(t')
\end{aligned}$$

where $\ell : 0 < \lim_N \ell/N < \infty$ is the growing distance between the two impurities. Since $\ell \propto N$, we can choose it such that $e^{i\ell q} = 1$. This renders very simple the limiting form of the previous equations for $N \to \infty$:

$$\begin{aligned}
X_q^1(t) &= e^{-i\omega_q(t-t_0)} - i\int_{t_0}^t dt' J_0(t-t')h_1(t')X_q^1(t') \\
&- \frac{i}{N}\int_{t_0}^t dt' J_0(t-t')h_2(t')X_q^2(t') \\
X_q^2(t) &= e^{-i\omega_q(t-t_0)} - \frac{i}{N}\int_{t_0}^t dt' J_0(t-t')h_1(t')X_q^1(t') \\
&- \frac{i}{N}\int_{t_0}^t dt' J_0(t-t')h_2(t')X_q^2(t')
\end{aligned}$$

so $X_q^1(t) = X_q^2(t) = X_q(t)$, *i.e.* the impurities feel each other in a very weak way, and the perturbation acts as a mean field:

$$X_q(t) = e^{-i\omega_q(t-t_0)} - i\int_{t_0}^t dt' J_0(t-t')\left(h_1(t')+h_2(t')\right)X_q(t'). \tag{1.63}$$

The generalization to an arbitrary (finite) number of far impurities is straightforward.
Let us analyze now the more involved case of XY model with impurities. We have:

$$\begin{aligned}
\alpha_{qp} &= (\cos q + h)\delta_{qp} + h_{q-p}(t) \\
\beta_{qp} &= -i\gamma \sin q \delta_{p,-q}.
\end{aligned}$$

Therefore the evolution equation for the dynamics reads

$$\begin{aligned}
i\dot{A}_{qp}(t) &= A_{qp}(t)(\cos p + h) + i\gamma \sin p B_{q,-p}(t) + \sum_{q'} A_{qq'}(t)h_{q'-p}(t) \\
i\dot{B}_{qp}(t) &= -B_{qp}(t)(\cos p + h) - 2i\gamma \sin p A_{q,-p}(t) - \sum_{q'} B_{qq'}(t)h_{q'-p}(t).
\end{aligned}$$

It is convenient to analyze in primis the unperturbed system ($h = 0$): once we have reduced the system in diagonal form, the analysis is identical to the one of the XX model. That is done with the same B-V transformation used before. It is more handsome to arrange it in the vectorial form

$$i\dot{\mathscr{A}}_{qp}(t) = \Gamma_p \mathscr{A}_{qp}(t_0)$$

with

$$\mathscr{A}_{qp} = \begin{pmatrix} A_{q,p} \\ B_{q,p} \\ A_{q,-p} \\ B_{q,-p} \end{pmatrix}$$

and

$$\Gamma_p = \begin{pmatrix} (\cos p + h) & 0 & 0 & -i\gamma \sin p \\ 0 & -(\cos p + h) & -i\gamma \sin p & 0 \\ 0 & i\gamma \sin p & (\cos p + h) & 0 \\ i\gamma \sin p & 0 & 0 & -(\cos p + h) \end{pmatrix}.$$

We have already diagonalized that matrix in section 3, with the unitary matrix (1.14). Thus the system reads in eigenvariables (we remind: E_p^2 be given by (1.13)) as

$$i\dot{\mathscr{A}}'_{qp}(t) = \begin{pmatrix} E_p & 0 & 0 & 0 \\ 0 & -E_p & 0 & 0 \\ 0 & 0 & E_p & 0 \\ 0 & 0 & 0 & -E_p \end{pmatrix} \mathscr{A}'_{qp}(t_0)$$

solved by

$$\begin{aligned} A'_{qp} &= e^{-iE_p(t-t_0)} A'_{qp}(t_0) \\ B'_{qp} &= e^{iE_p(t-t_0)} B'_{qp}(t_0), \end{aligned}$$

where we again make the choice of equilibrium initial conditions

$$\begin{aligned} A'_{qp}(t_0) &= \delta_{qp} \cos\phi_q \\ B'_{qp}(t_0) &= -i\delta_{q,-p} \sin\phi_q. \end{aligned}$$

In the original variables the solution instead is

$$\begin{aligned} A_{qp}(t) &= \delta_{qp} \left(\cos(E_p(t-t_0)) - i \frac{\cos p + h}{E_p} \sin(E_p(t-t_0)) \right) \\ B_{qp}(t) &= -\gamma \frac{\sin p}{E_p} \delta_{q,-p} \sin(E_p(t-t_0)). \end{aligned}$$

When a perturbative transverse field is added, we can define as before the variables:

$$\begin{aligned} X_q^k(t) &= \sum_{q'} A_{qq'}(t) e^{-ik(q'-q)} \\ V_q^k(t) &= \sum_{q'} B_{qq'}(t) e^{-ik(q'+q)}, \end{aligned}$$

in such a way the evolution equation are

$$\begin{aligned} i\dot{A}_{qp}(t) &= A_{qp}(t)(\cos p + h) + i\gamma \sin p B_{q,-p}(t) + \frac{1}{N} \sum_k h_k(t) X_q^k(t) e^{-ik(q-p)} \\ i\dot{B}_{qp}(t) &= -B_{qp}(t)(\cos p + h) - 2i\gamma \sin p A_{q,-p}(t) - \frac{1}{N} \sum_k h_k(t) V_q^k(t) e^{-ik(q-p)}. \end{aligned}$$

Since the relations linking A, B with X, V are linear, we have

$$\begin{aligned} X_q'^k(t) &= \sum_{q'} A'_{qq'}(t) e^{-ik(q'-q)} \\ V_q'^k(t) &= \sum_{q'} B'_{qq'}(t) e^{-ik(q'+q)}, \end{aligned}$$

and also the following equations for the eigen-variables

$$i\dot{A}'_{qp}(t) = E_p A'_{qp}(t) + \frac{1}{N}\sum_k h_k(t) X'^k_q(t) e^{-ik(q-p)} \quad (1.64)$$

$$i\dot{B}_{qp}(t) = -E_p B'_{qp}(t) - \frac{1}{N}\sum_k h_k(t) V'^k_q(t) e^{-ik(q-p)}. \quad (1.65)$$

now decoupled, and formally identical to (1.58). Thus they have a formal solution by Duhamel principle:

$$A'_{qp}(t) = e^{-iE_p(t-t_0)}\delta_{qp}\cos\phi_q - \frac{i}{N}\sum_k e^{-i(q-p)k}\int_{t_0}^t dt' e^{-iE_p(t-t')} h_k(t') X'^k_q(t') \quad (1.66)$$

$$B'_{qp}(t) = -ie^{-iE_p(t-t_0)}\delta_{q,-p}\sin\phi_q + \frac{i}{N}\sum_k e^{-i(q+p)k}\int_{t_0}^t dt' e^{-iE_p(t-t')} h_k(t') V'^k_q(t') \quad (1.67)$$

As in the previous case (here $\omega_p = E_p$), there are a closed equations for X'^k_q, V'^k_q:

$$X'^k_q(t) = e^{-i\omega_q(t-t_0)}\cos\phi_q - \frac{i}{N}\sum_j \int_{t_0}^t dt' \left(\sum_p e^{i(q-p)(k-j)} e^{-i\omega_p(t-t')}\right) h_j(t') X'^j_q(t') \quad (1.68)$$

and

$$V'^k_q(t) = -ie^{-i\omega_q(t-t_0)} + \frac{i}{N}\sum_j \int_{t_0}^t dt' \left(\sum_p e^{i(q+p)(k-j)} e^{-i\omega_p(t-t')}\right) h_j(t') V'^j_q(t'). \quad (1.69)$$

These equations, although formally identical to the one we got for the XX model, are technically more involved, essentially because of

$$\lim_N \frac{1}{N}\sum_p e^{i(q\pm p)(k-j)} e^{-iE_p(t-t')} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dp e^{i(q\pm p)(k-j)} e^{-iE_p(t-t')}$$

due to the non linear dependance of E_p on $\cos p$, is not a known function. Thus for the XY chain we have a very clear theoretical picture for the dynamics, but we cannot have in general a satisfactory analytical formulation. For this reason we will call the XX chain *solvable*, and later on we will focus mainly on that model. Recalling the content of the previous section, the main object to calculate in order to obtain the time dependent state (at least formally) is

$$\sigma_t(q,p) = -\frac{1}{\pi}\int_0^{\pi} dq' \frac{A^*(q,q',t)A(p,q',t)}{1+e^{\beta\cos p'}}.$$

Of course, the state is in fact uniquely defined by the $X_q(t)$. Indeed once one has computed their exact form, it is always possible to calculate explicitly A_{qp}, by

$$A_{qp}(t) = e^{-i(\cos p+h)(t-t_0)}\delta_{qp} - ie^{-i(q-p)k}\int_{t_0}^t dt' e^{-i(\cos p+h)(t-t')} h_k(t') X_q(t').$$

for one impurity and

$$A_{qp}(t) = e^{-i(\cos p+h)(t-t_0)}\delta_{qp} - i\sum_{k\in\mathbb{Z}}{}^* e^{-i(q-p)k}\int_{t_0}^t dt' e^{-i(\cos p+h)(t-t')} h_k(t') X^k_q(t').$$

for many impurities. An analogous derivation is possible for the XY model, via equations (1.66) and (1.67).

7. Notes

The seminal paper on quantum spin chain is certainly the one by Lieb, Mattis and Schultz [**15**], in which they compute the free energy and correlation function for the XY model and Heisenberg-Ising model by using the fermionic picture and the diagonalization procedure here exposed in Section 3. The fermion technique has revealed a very power tool (and so largely used) for investigating this model: as two remarkable examples, some years later Pfeuty [**18**] studied the quantum Ising model in a transverse magnetic field, and Abraham, Baruch, Gallavotti and Martin-Löf approached the XY model in a transverse magnetic field with a single impurity, finding a representation formula for the spectrum of the Hamiltonian [**1**][**2**]. Actually in this work the last two papers have been particularly inspiring, as can be easily checked by comparison.

Although we will no use it in our work, it is worthwhile to notice that, besides the fermionic picture, there is also a bosonic picture for quantum spin systems, and largely used in general spin waves theory. The mapping is done between spin systems and interacting bosons. The first approach was in a paper by Holstein and Primakoff [**13**], who originally purposed an exact transformation, mapping the Hamiltonian of a 3d quantum spin system in a boson interaction, with the quadratic term corresponding to linear Bloch theory, and the (large) higher order term describing the low-frequency spin waves; then Dyson [**9**] found another not one to one transformation, more suitable for the understanding of the spin waves theory. Now both are largely used as a powerful instrument in the study of quant spin systems, and this bridge is definitely at the base of the fermion-boson correspondence, *i.e.* a mapping between a Clifford and a Heisenberg algebra, widely studied by mathematicians.

Even though the language used is slightly different, the content of section 5 has an overlap with the papers [**16**][**17**]. I have been unaware about those works for long time: I am indebted with Sergio Simonella who provided to me a copy of [**16**], and with Heide Narnhofer, who, more or less at the same time, was very kind to explain to me the content of both the papers, and shipped them to me from Wien.

Quadratic Hamiltonians of Fermi operators are one of the rare cases in which one can exactly recover the evolution equations for a many bodies quantum system. From the non–equilibrium perspective, one can look at the (actual) dynamics of the system and the reservoirs at the same time.

The claimed similarity between two works at more than forty years of distance generates the need for a comment. The problem was dealt and fully solved in the work of Narnhofer, by using a C^*-algebra dynamics approach. If the interaction vanishes exponentially at infinity, it is proven that the time evolution is asymptotically abelian (for the even subalgebra). In order to prove that, the ODEs for the evolution semi-group are derived and solved in [**16**]. Furthermore, in [**17**] is shown that, if the initial state is fully described by the two point function (*quasifree*) the same holds for the asymptotic state given by the dynamics; moreover, the dynamics conserves the KMS property of the state.

The approach here presented brings to the same results (fortunately), but from a different perspective, essentially for two reasons: the dynamics is clearly interpreted with a 1-parameter semi-group of rotations (B-V transformation) on the super-algebra of Fermi operators; the theory is completed with formula (1.55) for the *state* of the system, in which, by using the Wick theorem, we use the hypothesis of integrability of the system. It is worthwhile to stress that in principle the approach works also in the case of non quadratic Hamiltonians, but in this case Wick theorem can no longer be applied, and the formula for a generic observables is not given by an analytic expression (but can be calculated perturbatively [**7**]).

The idea that the dynamics of quantum systems can be represented as a 1-parameter semi-group of B-V transformation is quite natural, and even more for fermionic systems: in this case B-V transformation are SU(2) rotation. It has been exploited in other papers [**12**][**4**], with different techniques, and not in the full generality of integrable models. It is

remarkable that the same idea is central also in recent developments of the (mathematical) theory of boson condensates, yielding new important results in the field [**20**].
It may appear too ambitious the derivation of the explicit equation (1.55) for the state of these systems, although the question is very natural from a non equilibrium statistical mechanics perspective; in fact both in the existing literature [**5**][**3**] both in what follows, what has been done is only calculating some meaningful observables, like the magnetizations or the correlation functions. But the exact calculation of the state is possible, since it has been done with different techniques for example for the XY chain [**12**][**4**], so it represents a future challenge.
However, a direct general formulation of the dynamics of the dynamics of integrable spin chains with transverse field was actually lacking in literature.

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CHAPTER 2

Impurity Oscillations in the XX Chain

In this chapter we will face a classical problem in quantum physics: the magnetic resonances absorption. We will use the formalism of quantum spin chains previously exposed and developed. The classical non equilibrium setting of a single spin, coupled both with a heath bath and with an oscillating transverse field finds a natural mapping in the context of the XX model. This is slightly different to the standard situation, in which the single spin is coupled to two orthogonal fields, one oscillating, the other being fixed. The main idea is that in fact we can interpret the results in this model in analogy to the known achievements about usual resonances absorption. This is as to say that the environment actually behaves as an effective longitudinal field. As well as we know, this is a new perspective in approaching to the topic. Indeed, the theory of linear response apart, all the results here exposed are new.

1. A Spin in an Oscillating Field

The problem of a spin in a periodic magnetic field is a classic topic in quantum mechanics, being the quantum counterpart of the classical motion of a magnetic moment. This section is a short self contained introduction on the subject, with the will to give emphasis to the aspects that will be deepened in the rest of the chapter.
The goal is to know the motion of a spin coupled with a constant magnetic field, say $\vec{B}_0 \equiv (B_0, 0, 0)$, and with another magnetic field orthogonal to the other, periodically varying in time $B_1(t)$. The Hamiltonian reads as[1]

$$H = -\vec{S} \cdot (\vec{B}_0 + \vec{B}_1(t)) = -H_0 - H_1(t). \tag{2.1}$$

One could look at $H_1(t)$ as a time dependent perturbation of H_0. This is particularly interesting because the perturbation does not commute with the unperturbed Hamiltonian, due to the orthogonality of $\vec{B}_0, \vec{B}_1(t)$, yielding a non trivial dynamics.
We will start with a quantum analysis, even tough the problem is treated in the same way of the classical one. Actually, for a generic Hamiltonian $H = \vec{S} \cdot \vec{B}(t)$ we have that the

[1] We will use natural units, with $\hbar = 1$, and also the gyromagnetic ratio will be set to $+1$. This choice implies of course $\vec{m} = \vec{S}$.

Ehrenfest equation

$$i\frac{d}{dt}\vec{S} = [\vec{S}, H]$$

becomes

$$\begin{aligned} i\frac{d}{dt}\vec{S}_i &= -\sum_j [S_i, S_j] B_j(t) \\ &= -\sum_j i\varepsilon_{ijk} S_k B_j(t), \end{aligned}$$

that is equivalent to

$$\frac{d}{dt}\vec{S} = \vec{S} \times \vec{B}(t),$$

and since the field is classical, this last equation implies the corresponding one for the mean values

$$\frac{d}{dt}\left\langle \vec{S} \right\rangle = \left\langle \vec{S} \right\rangle \times \vec{B}(t). \tag{2.2}$$

Equation (2.2) is nothing but the classical equation of motion for a magnetic moment in a magnetic field:

$$\frac{d}{dt}\langle m \rangle = \vec{m} \times \vec{B}(t). \tag{2.3}$$

This reveals the semiclassical nature of the problem: we have a quantum object, namely a spin, interacting with a classical field.

So we can approach the problem in a classical way, by using the rotating coordinates system technique [**17**]. To fix the ideas, let us assume constant magnetic field $\vec{B}(t) = \vec{B}$. Of course if we have a field initially aligned with the magnetic moment nothing happens: this is an equilibrium position. So we will suppose that $\vec{B}$ and $\vec{m}$ are separated by a nonzero angle θ. If we change the frame of coordinates, choosing a rotating one with angular frequency ω, we have that the magnetic moment $\vec{m}$ is related to the one in the rotating frame $\vec{m}'$ by

$$\frac{d}{dt}\vec{m} = \frac{d}{dt}\vec{m}' - \vec{m}' \times \vec{\omega}$$

hence

$$\frac{d}{dt}\vec{m}' = \vec{m}' \times \left(\vec{B} + \vec{\omega}\right) \equiv \vec{m}' \times \vec{B}_e. \tag{2.4}$$

We have defined the effective field $\vec{B}_e = \vec{B} + \vec{\omega}$ such that the equation of motion in the rotating frame is formally identical to the one in the laboratory. We see in particular that if we choose a $\vec{\omega} = -\vec{B}$, then $\vec{B}_e = 0$ and the magnetic moment is a fixed vector. This means that in the laboratory frame it precesses around $\vec{B}$ with angular velocity ω, that is usually called the Larmor frequency of the spin, at the fixed angle θ[2]. It is worthwhile to stress that ω is the energy gap between the eigenstates of the quantum system.

Now we want to decompose $\vec{B} \equiv \vec{B}_0 + \vec{B}_1$, with $\vec{B}_0 \perp \vec{B}_1$, and we want to adopt a frame rotating with velocity ω around $\vec{B}_0$. So in the laboratory frame we will see a constant fixed magnetic field, $\vec{B}_0$, and a rotating one around $\vec{B}_0$ with frequency ω, namely $\vec{B}_1$. For example we can have $\vec{B}_0 \equiv (B_0, 0, 0)$ and $\vec{B}_1 \equiv (0, B_1 \sin\omega t, B_1 \cos\omega t)$. In this case the quantum Hamiltonian is just (2.1).

We have three parameters to take into account: the Larmor frequency of the unperturbed system ω_0, the rotating frequency ω and the Larmor frequency of the perturbation $\vec{\omega}_1 = -\vec{B}_1$. Since we see the rotating field as a perturbation, we will consider $|\omega_1|$ ($|\vec{B}_1|$) small

[2]Obviously the magnitude of $\vec{m}$ is a constant of motion. From (2.4) we get

$$\frac{d}{dt}m^2 = 2\vec{m} \cdot \frac{d}{dt}\vec{m} = 2\vec{m} \cdot \vec{m}' \times \vec{B}_e = 0$$

with respect to $|\omega_0|$ ($|\vec{B}_0|$). The effective field is expressed is terms of these three parameters as

$$|\vec{B}_e| = \sqrt{(\omega - \omega_0)^2 + \omega_1^2}.$$

So if we regard at the motion in the rotating frame, we have a precession of the moment around the effective field $\vec{B}_e$ with a Larmor frequency $\omega_e = -|\vec{B}_e|$. Therefore, in the laboratory frame the total motion will be a composition of this precession and a rotation with angular frequency ω around $\vec{B}_0$. This rotation maintains fixed the angle α between $\vec{B}_0$ and $\vec{B}_e$, given by

$$\sin\alpha = \frac{\omega_1}{|\omega_e|}, \qquad \cos\alpha = \frac{\omega_0 - \omega}{|\omega_e|},$$

and also the angle β between $\vec{m}$ and $\vec{B}_e$ given by

$$\cos\beta = \frac{\vec{m}\cdot\vec{B}_e}{|\vec{m}||\vec{B}_e|},$$

but the angle θ between $\vec{B}_0$ and $\vec{m}$ is time depending, independently on the initial data. For instance, if initially $\vec{m} \parallel \vec{B}_0$, as in the previous equilibrium configuration, we have

$$\cos\theta(t) = \cos^2\alpha + \sin^2\alpha\cos\omega_e t.$$

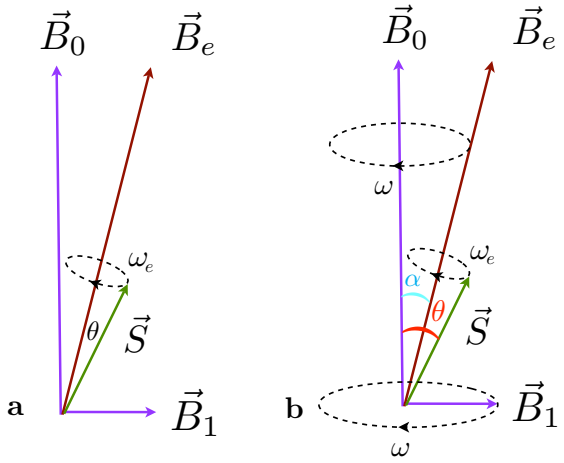

FIGURE 1. **a**) Precession of the spin around the effective field (in bordeaux) given by the sum of $\vec{B}_0$ and $\vec{B}_1$ (both in violet); **b**) Precession of the spin around the effective field rotating with frequency ω. The motion results clearly the composition of two rotation, with angular velocity respectively ω_e and ω.

So $\theta(t)$ remains small as long as $\omega << \omega_0$; when $|\omega - \omega_0| \simeq |\omega_1|$ the direction of the magnetic moment does deviate appreciably from the direction of $\vec{B}_0$ and when $\omega = \omega_0$, $\vec{m} \perp \vec{B}_0$. Then it returns small when $\omega >> \omega_0$. Huge deviation from the equilibrium position of the unperturbed problem occurs in a certain range of frequencies: precisely for ω in the nearby of the energy gap of the unperturbed system ω_0. This is a resonance phenomenon.

So far we have been dealing only with a circular polarized field (rotating field). One can ask what happen with a linearly polarized one, *i.e.* and oscillating field. The simple but important observation is that such a field can be seen as a sum of two vectors rotating

around the same axes, but in opposite sense, of equal magnitude[3]. In this case it is known that the resonance is shifted; this is due to the effect of the *antirotating* field: if $\omega \simeq \omega_0$ then $-\omega$ is far away the resonance, and the *antirotating* field can be approximated as a constant field very close to $\vec{B}_0$, so affecting the resonance condition.
This was noticed for the first time by Bloch and Siegert, who calculated the shift perturbatively in [**7**], finding the resonance for

$$\omega = |\vec{B}_0| \left(1 + \frac{|\vec{B}_1|^2}{|\vec{B}_0|^2} \right), \tag{2.5}$$

at the first order of the perturbative expansion. However the calculation is lengthy and a bit involved, and we remand to the original paper the interested reader. The same shift has been found also some years later by Autler and Townes in the context of Stark effect [**4**]. Later on, Winter discovered resonances for such a problem also for higher harmonics of the field frequency [**22**]. Moreover, if the field is purely transverse, the even multiple of ω are immaterial: we get higher order resonances near $\omega = \omega_0/(2p+1)$, p a positive integer, and precisely in

$$\omega = |\vec{B}_0| \left(1 + \frac{2p+1}{p(p+1)} \frac{|\vec{B}_1|^2}{|\vec{B}_0|^2} \right), \quad p \geq 1, \tag{2.6}$$

besides the one found by Bloch and Siegert. The probability of finding each of these resonances is decreasing with $\left(\frac{|\vec{B}_1|}{|\vec{B}_0|} \right)^{2p+1}$. These last results are really not surprising from a quantum mechanical point of view: they are just the semiclassical analogue of the multiphoton absorption processes described by quantum field theory.

Our treatment of the motion of an isolated spin is completed. Finally we will briefly review the phenomenological Bloch theory for spin in contact with an heat bath [**6**].
The idea is very simple: when relaxation processes occurs, the solution for the magnetization is the isolated one plus *transient* correction. The main assumptions are the following:

i) A strong field in the longitudinal direction $\vec{B}_0$ is the main term contributing to the Hamiltonian;

ii) The only terms in the Hamiltonian that can affect the spin orientation are the external fields;

iii) The system approaches to the equilibrium value for the longitudinal magnetization under the effect of the thermal perturbation: $\vec{m}_\infty = \chi \vec{B}_0$[4];

iv) The longitudinal and transversal components of the magnetization approaches exponentially fast to the equilibrium values, with different relaxation times T_l and T_t;

So the Bloch equation reads as

$$\frac{d}{dt}\vec{m} = \vec{m} \times \vec{B} - \frac{(\vec{m}_l - \vec{m}_\infty)}{T_l} - \frac{\vec{m}_t}{T_t}. \tag{2.7}$$

[3] A field varying in time as $\cos \omega t$ can be decomposed into two rotating field, varying as $\frac{e^{\pm i\omega t}}{2}$.
[4] χ is the magnetic susceptivity tensor.

The main feature of this equation is that many properties of the isolated equation are inherited; in particular the distribution of resonances. On the other hand it is rather unsatisfactory that Bloch theory fails to be true when assumption *i*) not satisfied, *i.e.* for $|\vec{B}_0| \simeq |\vec{B}_1|$[5]. Nevertheless one may modify assumption *iii*), requiring that relaxation occurs toward a function with the same periodicity of the transverse field

$$\vec{m}_\infty(t) = \chi(\vec{B}_0 + \vec{B}_1(t)).$$

Under this condition, also assumption *iv*) changes, since one can also assume $T_l = T_t \equiv T$, and write the modified Bloch equation as

$$\frac{d}{dt}\vec{m} = \vec{m} \times \vec{B} - \frac{\vec{m} - \chi\vec{B}}{T}. \tag{2.8}$$

2. The Microscopic Model

In the context of spin chains, the microscopic model we choose in order to approach to the problem of magnetic resonances is the XX chain with a single impurity. As studied in the last chapter, in this model we have homogenei couplings between spin, only along the x and y axis, and a transverse magnetic field of component $\vec{B} \equiv (0,0,h\cos(\omega t))$, acting only on a selected spin (say the kth one). So we can interpret the systems as a single spin coupled with a *classical* oscillating field, and also with a one dimensional heat bath, made by all the other spin of the chain. We can write the Hamiltonian accordingly to this decomposition, as

$$H = H_S + H_B + H_I,$$

where

$$\begin{aligned} H_S &= -\vec{B}\cdot\vec{S}_k = -h\cos\omega t S_k^z \\ H_B &= -J\sum_{j=1}^{k-2}(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) - J\sum_{j=k+1}^{N-1}(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) \\ H_I &= -J' S_k^x (S_{k-1}^x + S_{k+1}^x) - J' S_k^y (S_{k-1}^y + S_{k+1}^y). \end{aligned}$$

In what follows, we will prefer to set $J = J' = g$. Of course this is not the most general situation it can occur, since the two interaction could act at a different magnitude scale. This is however a mathematical simplification, supported by physical motivation: indeed the choice of the parameters of major physical interest is when the two interaction are of comparable size $J \simeq J'$[6]; in this regime one can always renormalize the interaction in order to render it uniform on the whole chain. This is finally equivalent to the choice $J = J'$.
In the previous chapter we have seen that the spectrum for such a system is made by a continuous set of eigenvalues in $[-\frac{g}{2}, \frac{g}{2}]$, plus an isolated one $E_h = \text{sign}(h)\frac{g}{2}\sqrt{1+h^2}$. This means that the energy gap is about $\Delta E \simeq gh$.
In order to study the dynamics of such a system, we will adopt the formalism developed in Chapter 1, and in particular our starting point will be formula (1.60). Once we have set $\omega_p = \frac{g}{2}\cos p$, we can rewrite (1.60) for our oscillating field

$$X_p(t,t_0) = e^{-i\omega_p(t-t_0)} - ih\int_{t_0}^{t} dt' J_0\left(\frac{g}{2}(t-t')\right)\cos\omega(t')X_p(t') \tag{2.9}$$

[5] In this regime the Bloch-Siegert shift is non negligible.

[6] It is easy to figure out that when this is not the case, the system behaves as a tensor product of two sub systems: the environment and a magnetic moment under an oscillating field, with $m = \frac{1}{2}$ when $J' << J$, and $m = \frac{3}{2}$ when $J << J'$. In this last case we have that the two adjacent spin will follow in the oscillation the kth one, forming a system of three spin, plus small correction.

with

$$X_p(t_0) = 1.$$

In what follows, it results convenient to adopt the alternative unknown

$$Y(p,t,t_0) \equiv e^{ig\omega_p(t-t_0)} X_p(t),$$

and it is easy to check that we have the following equation for $Y(p,t)$:

$$\begin{aligned} Y(p,t,t_0) &= 1 - ih\int_{t_0}^{t} dt' J_0\left(\frac{g}{2}(t-t')\right) e^{i\omega_p(t-t')} \cos\omega(t') Y(p,t'), \\ Y(p,t_0,t_0) &= 1. \end{aligned} \tag{2.10}$$

Once computed the form of $Y(p,t,t_0)$, we can easily recover the transverse magnetization. Following [**3**] we have

$$\begin{aligned} \langle m(t)\rangle &= \frac{1}{N}\sum_{q,p} e^{ik(q-p)} \left\langle a_q^\dagger(t) a_p(t)\right\rangle \\ &= \frac{1}{N}\sum_{q,p} e^{ik(q-p)} \sum_{q',p'} A^*_{qq'}(t) A_{pp'}(t) \left\langle a^\dagger_{q'} a_{p'}\right\rangle \\ &= \frac{1}{N}\sum_{q'}\sum_{q,p} e^{ik(q-p)} \frac{A^*_{qq'}(t) A_{pq'}(t)}{1+e^{\beta\cos q'}}, \end{aligned} \tag{2.11}$$

and noticing that

$$|X'_q|^2 = \sum_{qp} e^{ik(q-p)} A^*_{qq'}(t) A_{pq'}(t),$$

we get

$$1 + m(t) = \frac{2}{\pi}\int_{-\pi}^{\pi} \frac{dp}{1+e^{\beta\omega_p}} |X_p(t)|^2 = \frac{2}{\pi}\int_{-\pi}^{\pi} \frac{dp}{1+e^{\beta\omega_p}} |Y(p,t)|^2. \tag{2.12}$$

Therefore, in according with the theory developed in the first chapter, the strategy is clear: at first, by equation (2.10) we will calculate the auxiliary function Y_p, then by integrating its square module we will recover the value of the magnetization.

Now we make a fundamental observation: one could expect to find a solution for the magnetization such that it recovers the Bloch equation for a spin in a heat bath. This is in general a very reasonable idea. On the other hand, a crucial assumption in the derivation of the equations by Bloch is the thermalization of the system to an equilibrium state [**6**]; but, as was shown very clearly firstly by Mazur [**15**], the XY chain is not an ergodic system[7]: so the Bloch theory cannot be applied, at least *tout court*[8]. This singular behavior has been confirmed by several other theoretical and numerical studies, *e.g.* [**12**][**5**][**21**][**3**], for for the total magnetization and for the single spin one. So we have to adopt a different picture in order to understand the phenomenology described by our model.

Since the perturbation is time dependent, we will have a time dependent behavior for observables also after a long time. However, it is always possible to separate the asymptotic solution to the finite time corrections, such that we will not be concerned about transient effects. This can be done by a suitable limit $t_0 \to -\infty$ in equation (2.10).

For every fixed $T > t - t_0 > 0$ we can write equation (2.10) as

$$\begin{aligned} Y(p,t,t_0) &= 1 - ih\int_0^T d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau} \cos\omega(t-\tau) Y(p,t-\tau) \\ &+ ih\int_T^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau} \cos\omega(t-\tau) Y(p,t-\tau), \end{aligned}$$

[7] Even tough the proof of Mazur is only for XY chain, there is evidence that it should work for integrable spin chains.

[8] This is not in contradiction with the achievements of Narnhofer (see Notes at the end of the previous chapter). Indeed, the fact that dynamics conserves the KMS condition does not mean that it maps the initial state in the asymptotic one, and in fact Mazur has shown that it is false.

with the elementary change of variables $\tau = t - t'$. We define

$$Y^T(a,t) \equiv 1 - ih\int_0^T d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos\omega(t-\tau)Y(p,t-\tau) \tag{2.13}$$

$$R^T(p,t,t_0) \equiv ih\int_{t-t_0}^T d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos\omega(t-\tau)Y(p,t-\tau), \tag{2.14}$$

such that we have

$$Y(p,t,t_0) = Y^T(a,t) + R^T(p,t,t_0). \tag{2.15}$$

Now we want to show that this equation is meaningful also in the limit $T \to \infty$, and in this limit $R^\infty(p,t,t_0)$ is a vanishing function for $t_0 \to -\infty$, *i.e.* $\lim_{t_0\to-\infty}\lim_{T\to\infty} R^T(p,t,t_0) = 0$. In this way we can study the asymptotic form of the equation:

$$Y^a(p,t) = 1 - ih\int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos\omega(t-\tau)Y^a(p,t-\tau). \tag{2.16}$$

As a common procedure in physics, one can write a solution as a series in the perturbation magnitude

$$Y(p,t,t_0) = \sum_{k\geq 0} h^k Y_k(p,t,t_0), \tag{2.17}$$

and this series is convergent if for example one has the estimate $Y_k(p,t,t_0) \leq C^k$, where C is a finite constant eventually depending on the additional parameters of the theory, *i.e.* ω, g.

PROPOSITION 1. *Whereas* $|Y_k(p,t,t_0)| \leq C(\omega,g,t_0)^k$, *it is* $|R^T(p,t,t_0)| \simeq O\left(\frac{1}{\sqrt{t-t_0}}\right)$ *uniformly in* T.

The rest of this section will be devoted to the proof of the proposition, that is rather technical, and can be eventually skipped by the reader. As a comment on the proof, we notice that the structure of resonances, that will be exposed in the next sections, is a little hidden in this proof, although it is obviously of crucial importance in our problem. Morally this is translated in the fact that, rather than writing down the coupled recursive equations respectively for $Y^T(a,t)$ and $R^T(p,t,t_0)$, and then using the solution for $Y^T(a,t)$ (see section 4) in order to estimate the correction given by $R^T(p,t,t_0)$, we have preferred to use a measure theory argument for giving a global estimate, under the strong hypothesis of bounded moments. This last in fact will be verified a posteriori, once the solution for the asymptotic equation will be written. Such a shortcut has be taken in order to avoid an even longer proof of an obvious fact (the transient part of the solution vanishes after a long time). On the other hand, it is unsatisfactory that in this proof explicitly only the first resonance appears, namely $\omega = |\omega_p \pm \frac{g}{2}|$: it will be however revisited at the light of the results achieved below.

PROOF. In primis we write

$$R^T(p,t,t_0) = \sum_{k\geq 0} h^k R_k(p,t,t_0)$$

with

$$\begin{aligned} R_0^T(p,t,t_0) &= 0, \\ R_k^T(p,t,t_0) &= i\int_{t-t_0}^T d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos(\omega(t-\tau))Y_{k-1}^a(p,t-\tau) \end{aligned} \tag{2.18}$$

The strategy we want to follow will at first prove that

$$0 < |R_1^T| < \frac{D(\omega,g)}{\sqrt{t-t_0}}. \tag{2.19}$$

for a certain function constant in (t,t_0), $D(\omega,g)$, bounded in its arguments. So, noticing that, since $Y_0(p,t,t_0)=1$

$$R_1^T(p,t,t_0) = -i\int_{t-t_0}^{T} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos(\omega(t-\tau)), \tag{2.20}$$

we can regard to this oscillatory integral as the measure of the interval $[t-t_0,T]$ by the signed measure $d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos(\omega(t-\tau))$, absolutely continuous with respect to the Lebesgue measure. Of course this measure is well defined on each interval, because of (2.19) and because it can be easily decomposed in a positive and a negative non singular part [**18**]. So it follows that[9]

$$|R_k^T| < |R_1^T||Y_{k-1}(p,t,t_0)| < C(\omega,g)^k \frac{D(\omega,g)}{\sqrt{t-t_0}}, \tag{2.21}$$

and then

$$|R^T(p,t,t_0)| \leq \frac{D(\omega,g)}{\sqrt{t-t_0}} \sum_{k\geq 0} h^k C(\omega,g)^k. \tag{2.22}$$

So whereas the expansion for the Y converges, namely for $h < C(\omega,g)^{-1}$, we have that $|R^T(p,t,t_0)| \simeq O\left(\frac{1}{\sqrt{t-t_0}}\right)$, and the proposition is proven.
In order to prove (2.19), we notice that the integral is performed over positive values of τ: this allows us to replace $J_0\left(\frac{g}{2}\tau\right)$ with its asymptotic expansion [**13**]. When z is large we have

$$J_0^a(z) = \sum_{j\geq 0} J_0^j(z) \tag{2.23}$$

where

$$J_0^j(z) = \frac{(-1)^{[j/2]}}{2^j\sqrt{\pi}} \frac{\Gamma(j+1/2)}{j!\Gamma(-j+1/2)} \left(\frac{\cos z + (-1)^j \sin z}{z^{j+1/2}}\right). \tag{2.24}$$

Therefore, since $t > t_0$, we can insert (2.23) in (2.20), obtaining

$$\begin{aligned}
R_1^T(p,t,t_0) &= -i\sum_j \int_{t-t_0}^{T} d\tau J_0^j(\tau) e^{i\omega_p\tau}\cos(\omega(t-\tau)) \\
&= \frac{-ie^{i\omega t}}{4} \sum_{j\geq 0} \frac{(-1)^{[j/2]}}{2^j\sqrt{\pi}} \frac{\Gamma(j+1/2)}{j!\Gamma(-j+1/2)} (1-i(-1)^j) I_j^T(\omega_p+\frac{g}{2}-\omega, t-t_0) \\
&+ \frac{-ie^{-i\omega t}}{4} \sum_{j\geq 0} \frac{(-1)^{[j/2]}}{2^j\sqrt{\pi}} \frac{\Gamma(j+1/2)}{j!\Gamma(-j+1/2)} (1-i(-1)^j) I_j^T(\omega_p+\frac{g}{2}+\omega, t-t_0) \\
&+ \frac{-ie^{i\omega t}}{4} \sum_{j\geq 0} \frac{(-1)^{[j/2]}}{2^j\sqrt{\pi}} \frac{\Gamma(j+1/2)}{j!\Gamma(-j+1/2)} (1+i(-1)^j) I_j^T(\omega_p-\frac{g}{2}-\omega, t-t_0) \\
&+ \frac{-ie^{-i\omega t}}{4} \sum_{j\geq 0} \frac{(-1)^{[j/2]}}{2^j\sqrt{\pi}} \frac{\Gamma(j+1/2)}{j!\Gamma(-j+1/2)} (1+i(-1)^j) I_j^T(\omega_p-\frac{g}{2}+\omega, t-t_0),
\end{aligned}$$

where we have defined

$$I_j^T(\Omega, t-t_0) \equiv \int_{t-t_0}^{T} d\tau \frac{e^{i\tau\Omega}}{\tau^{j+\frac{1}{2}}}. \tag{2.25}$$

What is left is just to evaluate these integrals. It is convenient to discuss imprimis the case $j \geq 1$, where one can use the summability of the denominator (we recall that we are far away from the origin):

$$|I_j^T(\Omega, t-t_0)| \leq \int_{t-t_0}^{+\infty} d\tau \frac{1}{\tau^{j+\frac{1}{2}}} = \frac{2}{2j-1} \frac{1}{(t-t_0)^{j-\frac{1}{2}}}, \qquad j \geq 1. \tag{2.26}$$

[9] It is as to say $\langle x \rangle \leq \langle |x| \rangle$.

For the $j=0$ term the things are slightly different, since we the integral is divergent for $\Omega=0$. However, since the condition $\Omega=0$ is translated in our case to $\omega=|\omega_p \pm g|$, this is automatically excluded by the hypothesis of boundedness of $|Y_1|$[10]. So for $\Omega \neq 0$ we have

$$|I_0^T(\Omega, t-t_0)| \leq \frac{1}{\sqrt{t-t_0}} \left| \int_{t-t_0}^{+T} d\tau e^{i\tau\Omega} \right| \leq \frac{2}{\Omega\sqrt{t-t_0}}. \tag{2.27}$$

Once we are allowed to take the limit $T \to \infty$ we can explicitly perform this integral, obtaining precisely

$$I_0(\Omega, t-t_0) = \sqrt{\frac{\pi}{2\Omega}}(1+i) - \sqrt{\frac{2\pi}{\Omega}} \left(C(\sqrt{\Omega(t-t_0)}) + iS(\sqrt{\Omega(t-t_0)}) \right) \tag{2.28}$$

where $C(x)$ and $S(x)$ are the Fresnel integrals. Recollecting all these estimates, and summing over j, we easily get the upper bound of (2.19).
The lower bound is equivalent to the condition

$$\begin{aligned} \left| \int_{t-t_0}^{T} d\tau J_0\left(\frac{g}{2}\tau\right) \sin\omega_p\tau\cos\omega\tau \right|^2 &> 0 \\ \left| \int_{t-t_0}^{T} d\tau J_0\left(\frac{g}{2}\tau\right) \cos\omega_p\tau\cos\omega\tau \right|^2 &> 0. \end{aligned}$$

We notice that, fixed t_0, T, for every $t \in]t_0, T+t_0[$ these two integrals can never vanish at the same time for every $\omega_p \neq 0$. If $p = \pm\frac{\pi}{2}$, or $p = \pm\pi$, we have that respectively only the first (second) one survives: it is zero for a countable set of values of $t \in]t_0, T+t_0[$, and finite as long as $T < \infty$. This is enough to ensure (2.21) *a.e.* in t.

□

3. Linear Response Theory

As a first step, we want to find the linear response of the magnetization to the oscillating field. This will be of the form

$$m_{LR}(t) = h(\chi_r(\omega)\cos\omega t + \chi_i(\omega)\sin\omega t), \tag{2.29}$$

where χ_r, χ_i are respectively the real and imaginary magnetic susceptivity tensor, in the linear approximation supposed to be a scalar [**1**].
We will focus hereafter only on the asymptotic behavior. With a glance to our equation, it is clear that we need to calculate the auxiliary function $Y^a(p,t)$ only at the first order in h. Indeed

$$|Y^a(p,t)| = 1 + 2h\Re(Y_1^a(p,t)) + O\left(h^2\right).$$

and so, since we have of course

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \frac{dp}{1+e^{\beta\omega_p}} = 1,$$

the linear response for the magnetization reads as

$$m_{LR}(t) = \frac{4h}{\pi}\int_{-\pi}^{\pi} \frac{dp}{1+e^{\beta\omega_p}} \Re(Y_1^a(p,t)).$$

Therefore we have to calculate explicitly $Y_1^a(p,t)$. It is useful to recall the following formula [**13**]:

$$f(\Omega) \equiv \int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\Omega\tau} = \frac{\chi(|\Omega| \leq \frac{g}{2}) + i\chi(|\Omega| \geq \frac{g}{2})}{\sqrt{|\Omega^2 - \left(\frac{g}{2}\right)^2|}}. \tag{2.30}$$

[10] This is related to the distribution of the resonances, that will be discussed in the next sections.

that will be crucially used in many calculations hereafter. So we have

$$\begin{aligned} Y_1^a(p,t) &= \frac{-i}{2}\int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau}\cos\omega(t-\tau) \\ &= \frac{-i}{2}\left(e^{i\omega t}\int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i(\omega_p-\omega)\tau} + e^{-i\omega t}\int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i(\omega_p+\omega)\tau}\right) \\ &= \frac{-i}{2}\left(e^{i\omega t} f(\omega_p-\omega) + e^{-i\omega t} f(\omega_p+\omega)\right). \end{aligned} \tag{2.31}$$

where, according to (2.30), it is

$$f(\omega_p-\omega) \equiv \frac{\chi\left(\omega_p > \omega-\frac{g}{2}\right) + i\chi\left(\omega_p < \omega-\frac{g}{2}\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega_p-\omega)^2\right|}}, \tag{2.32}$$

$$f(\omega_p+\omega) \equiv \frac{\chi\left(\omega_p < \frac{g}{2}-\omega\right) + i\chi\left(\omega_p > \frac{g}{2}-\omega\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega_p+\omega)^2\right|}}. \tag{2.33}$$

The form of $Y_1^a(p,t)$ is such that it is divergent for $\omega = \omega_p \pm \frac{g}{2}$ [11]. So, for every $p \in [-\pi,\pi]$, we have divergences for different values of ω. This is anyhow immaterial, since the $Y^a(p,t)$ is only an auxiliary function. This point will be better discussed in the next section.
Now we can write the real part of $Y_1^a(p,t)$ as

$$\Re(Y_1^a(p,t)) = \Im\left[f(\omega_p-\omega)+f(\omega_p+\omega)\right]\cos\omega t + \Re\left[f(\omega_p-\omega)-f(\omega_p+\omega)\right]\sin\omega t,$$

and so the linear response of the transverse magnetization has the form (2.29) with

$$\chi_r(\omega) = \frac{4}{\pi}\int_{-\pi}^{\pi}\frac{dp}{1+e^{\beta\omega_p}}\Im(f(\omega_p-\omega)+f(\omega_p+\omega)), \tag{2.34}$$

$$\chi_i(\omega) = \frac{4}{\pi}\int_{-\pi}^{\pi}\frac{dp}{1+e^{\beta\omega_p}}\Re\left(f(\omega_p-\omega)-f(\omega_p+\omega)\right). \tag{2.35}$$

It is worthwhile to notice that $\chi_r(\omega,g)$ is an even function of ω, while $\chi_i(\omega)$ is odd: the linear response, as expected, is an even function of ω (or of t), as it is the oscillating external field.
Now we will proceed to an exact calculation of these two integrals. At first we notice that, since the integrating functions depend on p only through $\omega_p \propto \cos p$, we can replace

$$\int_{-\pi}^{\pi} \to 2\int_0^{\pi};$$

then we can write the integral in $d\omega_p$:

$$\int_0^{\pi} dp \to \int_{-\frac{g}{2}}^{\frac{g}{2}}\frac{d\omega_p}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}}.$$

[11] We see that we can distinguish two cases: if $\omega > g$ then $\omega_p < |\omega - g/2|\ \forall p$ (and so we never have $\omega_p > |\omega - g/2|$) and

$$Y_1^a(p,t) = \frac{1}{2}\left(\frac{e^{i\omega t}}{\sqrt{(\omega_p-\omega)^2-\left(\frac{g}{2}\right)^2}} + \frac{e^{-i\omega t}}{\sqrt{(\omega_p+\omega)^2-\left(\frac{g}{2}\right)^2}}\right);$$

otherwise for $\omega < g$ we have to keep all the terms.

Thus we have for example for $\chi_r(\omega)$

$$\begin{aligned}\chi_r(\omega) &= \frac{8}{\pi}\int_{-\frac{g}{2}}^{\frac{g}{2}} \frac{d\omega_p}{1+e^{\beta\omega_p}} \frac{1}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}} \frac{\chi\left(\omega_p<\omega-\frac{g}{2}\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega-\omega_p)^2\right|}} \\ &+ \frac{8}{\pi}\int_{-\frac{g}{2}}^{\frac{g}{2}} \frac{d\omega_p}{1+e^{\beta\omega_p}} \frac{1}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}} \frac{\chi\left(\omega_p>\frac{g}{2}-\omega\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega+\omega_p)^2\right|}} \\ &= \frac{8}{\pi}\int_{-\frac{g}{2}}^{\omega-\frac{g}{2}} \frac{d\omega_p}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}} \frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega-\omega_p)^2\right|}}, \end{aligned} \tag{2.36}$$

where we have sent $\omega_p \to -\omega_p$ in the second addendum, noticing that

$$\frac{1}{1+e^{\beta\omega_p}} + \frac{1}{1+e^{-\beta\omega_p}} = 1.$$

It is worthwhile to stress that $\chi_r(\omega)$ does not depend on β; moreover, it is divergent for $\omega = g$. In this limit indeed the integral is taken in $\left[-\frac{g}{2}, \omega-\frac{g}{2}\right] \to \left[-\frac{g}{2}, \frac{g}{2}\right]$, and, once we have decomposed

$$\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega-\omega_p)^2\right|} = \sqrt{\left|\frac{g}{2}-\omega_p\right|}\sqrt{\left|\frac{g}{2}+\omega_p\right|}\sqrt{\left|\omega+\frac{g}{2}-\omega_p\right|}\sqrt{\left|\omega-\frac{g}{2}-\omega_p\right|},$$

it is clear that when $\omega \to g$ we get in the integral a denominator

$$\frac{1}{\sqrt{\left|\frac{g}{2}-\omega_p\right|}} \frac{1}{\sqrt{\left|\omega-\frac{g}{2}-\omega_p\right|}} \to \frac{1}{\frac{g}{2}-\omega_p},$$

and so a logarithmic divergence arises for $\omega \to g$. There is also an explicit expression in terms of special functions [**13**], due to the independence on the temperature:

$$\chi_r(\omega) = \begin{cases} \frac{g}{\pi\omega} K\left(\frac{\omega}{g}\right) & \text{for} \quad \omega < g \\ \frac{\omega}{g\pi} K\left(\frac{g}{\omega}\right) & \text{for} \quad \omega > g, \end{cases} \tag{2.37}$$

where $K(\cdot)$ is the complete elliptic integral of first kind. It is also important to note that $\chi_r(\omega)$ is regular for $\omega \to 0$[12].
In the same way we get for $\chi_i(\omega)$

$$\begin{aligned}\chi_i(\omega) &= \frac{8}{\pi}\int_{-\frac{g}{2}}^{\frac{g}{2}} \frac{d\omega_p}{1+e^{\beta\omega_p}} \frac{1}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}} \frac{\chi\left(\omega_p>\omega-\frac{g}{2}\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega-\omega_p)^2\right|}} \\ &+ \frac{8}{\pi}\int_{-\frac{g}{2}}^{\frac{g}{2}} \frac{d\omega_p}{1+e^{\beta\omega_p}} \frac{1}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}} \frac{\chi\left(\omega_p<\frac{g}{2}-\omega\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega+\omega_p)^2\right|}} \\ &= \frac{8}{\pi}\int_{\omega-\frac{g}{2}}^{\frac{g}{2}} \frac{d\omega_p}{\sqrt{\left(\frac{g}{2}\right)^2-\omega_p^2}} \frac{\tanh\left(\frac{\beta\omega_p}{2}\right)}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega-\omega_p)^2\right|}}, \end{aligned} \tag{2.38}$$

since

$$\frac{1}{1+e^{\beta\omega_p}} - \frac{1}{1+e^{-\beta\omega_p}} = \tanh\left(\frac{\beta\omega_p}{2}\right).$$

[12] It has

$$\lim_{\varepsilon\to 0}\int_{-1}^{-1+\varepsilon} \frac{dy}{\sqrt{1+y}} \frac{1}{\sqrt{\varepsilon-1-y}} = \pi.$$

We notice that this term is always finite, and presents a jump in $\omega = g$: for $\omega < g$, since $\tanh(\cdot) \leq 1$ uniformly (so the bound is uniform in β) it is always dominated by its zero temperature value, that is (see [**13**] 3.147 4 pg 242)

$$\chi_i(\omega) \leq \frac{8}{\pi} \int_{\omega - \frac{g}{2}}^{\frac{g}{2}} \frac{d\omega_p}{\sqrt{\left(\frac{g}{2}\right)^2 - \omega_p^2}} \frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2 - (\omega - \omega_p)^2\right|}} = \frac{8}{\pi} K\left(\sqrt{1 - \frac{\omega^2}{g^2}}\right)$$

that is always a bounded function for $\omega < g$ (in particular, for $\omega \to g^-$, $K(0) = \pi/2$); instead for $\omega > g$ it is easily seen that it vanishes. This means that for high frequencies the linear response exhibits only a cosine oscillation.

4. Magnetic Resonances I

In this section we develop the general theory of equations (2.16).
Indeed, as already stressed many times, the first goal of our approach would be to write down, at least formally, a *solution* for the $Y^a(p,t)$ and then compute the observables. As we will see it is not trivial to show that the formal solution we are going to try is in fact a regular solution of (2.16), and in general it is not true. The reason is that $Y^a(p,t)$ is not really expected to be a function, but rather a distribution, and in principle (integrable) singularities are allowed to appear, since we will always evaluate it under an integral over p.
However, it is instructive to perform also a second order calculation of $Y^a(p,t)$, in order to better understand the structure of the formal solution we are going to present. The key instrument is the recursive form of (2.16). We remind we want to write a solution like

$$Y^a(p,t) = \sum_{k \geq 0} h^k Y_k^a(p,t)$$

with

$$\begin{aligned} Y_0^a(p,t) &= 1 \\ Y_k^a(p,t) &= 1 - ih \int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p \tau} \cos(\omega(t-\tau)) Y_{k-1}^a(p,t-\tau). \end{aligned} \tag{2.39}$$

Bearing in mind the form of the first order solution (2.31), for the second order we have to evaluate the integral

$$Y_2^a(p,t) = \frac{(-i)^2}{2} \int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p \tau} \cos\omega(t-\tau) \left(e^{i\omega(t-\tau)} f(\omega_p - \omega) + e^{-i\omega(t-\tau)} f(\omega_p + \omega)\right),$$

that is easily done simply by writing $\cos\omega(t-\tau) = (e^{i\omega(t-\tau)} + e^{-i\omega(t-\tau)})/2$ and then by using (2.30)[13]. We see that we have a constant term, and oscillations with frequencies $\pm 2\omega$. Namely:

$$\begin{aligned} Y_2^a(p,t) &= \left(\frac{-i}{2}\right)^2 \Big(\frac{f(\omega_p + \omega) + f(\omega_p - \omega)}{g|\sin p|} \\ &+ e^{i2\omega t} f(\omega_p - \omega) f(\omega_p - 2\omega) + e^{-i2\omega t} f(\omega_p + \omega) f(\omega_p + 2\omega) \Big), \end{aligned} \tag{2.40}$$

where

$$f(\omega_p) = \frac{2}{g|\sin p|}.$$

Let us spend some word about the coefficients. We can distinguish now three cases:

[13] It is suggestive that this is exactly the decomposition of a polarized field into two opposite rotating fields discussed in Section 1.

(1) $\omega > g$;

(2) $\frac{g}{2} < \omega < g$;

(3) $0 < \omega < \frac{g}{2}$.

We see that for $\omega > g$ the solution is simpler. In this case again we have no restriction on the p, and we get

$$\begin{aligned} Y_2^a(p,t) &= \left(\frac{-i}{2}\right)^2 \Big[\left(\frac{i}{\sqrt{(\omega+\omega_p)^2 - \left(\frac{g}{2}\right)^2}} + \frac{i}{\sqrt{(\omega-\omega_p)^2 - \left(\frac{g}{2}\right)^2}} \right) \frac{1}{g|\sin p|} \\ &- \frac{e^{i2\omega t}}{\sqrt{\left((\omega_p-\omega)^2 - \left(\frac{g}{2}\right)^2\right| \sqrt{(\omega_p-2\omega)^2 - \left(\frac{g}{2}\right)^2}}} \\ &- \frac{e^{-i2\omega t}}{\sqrt{\left((\omega_p+\omega)^2 - \left(\frac{g}{2}\right)^2\right| \sqrt{(\omega_p+2\omega)^2 - \left(\frac{g}{2}\right)^2}}} \Big], \end{aligned} \tag{2.41}$$

and the only divergence we have is $\omega = g$ and $\omega_p = \pm\frac{g}{2}$.
For $g/2 < \omega < g$ we have only the constrain arising from the first order calculation, since $\omega - g/2 < 2\omega - \frac{g}{2}$, so we do not see the divergence coming from $\sqrt{(\omega_p \pm 2\omega)^2 - 1}$ (apart the case $\omega = \frac{g}{2}$, $\omega_p = \pm\frac{g}{2}$), but only $\omega_p = \pm 1, \pm|\omega - \frac{g}{2}|$.
Lastly, for $0 < \omega < \frac{g}{2}$ we can evaluate the coefficient of $e^{\pm i\omega t}$. It is

$$\begin{aligned} f(\omega_p-\omega)f(\omega_p-2\omega) &= \frac{\chi\left(\omega_p < \omega - \frac{g}{2}\right) - \chi(\omega_p > 2\omega - \frac{g}{2}) + i\chi(\omega - \frac{g}{2} < \omega_p < 2\omega - \frac{g}{2})}{\sqrt{\left|(\omega_p-\omega)^2 - \frac{g}{2}\right|}\sqrt{\left|(\omega_p-2\omega)^2 - \left(\frac{g}{2}\right)^2\right|}} \\ f(\omega_p+\omega)f(\omega_p+2\omega) &= \frac{-\chi\left(\omega_p > \frac{g}{2} - \omega\right) + \chi(\omega_p > \frac{g}{2} - 2\omega) + i\chi(\frac{g}{2} - 2\omega < \omega_p < \frac{g}{2} - \omega)}{\sqrt{\left|(\omega_p+\omega)^2 - \frac{g}{2}\right|}\sqrt{\left|(\omega_p+2\omega)^2 - \left(\frac{g}{2}\right)^2\right|}}; \end{aligned}$$

here we have divergences in $\omega_p = \pm\frac{g}{2}, \pm|\omega - \frac{g}{2}|, \pm|2\omega - \frac{g}{2}|$.
Of course the same can be repeated to the other orders. The task is pursued as follows: by using (2.30) in (2.39), we have that we must calculate only integrals of the form

$$\begin{aligned} \int_0^{+\infty} d\tau J_0\left(\frac{g}{2}\tau\right) e^{i\omega_p\tau} \cos\omega(t-\tau) e^{ik\omega(t-\tau)} &= \frac{e^{i\omega(1+k)t}}{2} f(\omega_p - \omega(1+k)) \\ &+ \frac{e^{-i\omega(1-k)t}}{2} f(\omega_p + \omega(1-k)) \end{aligned} \tag{2.42}$$

for integer k. So we will expect $Y_k^a(p,t)$ be a superposition of harmonics of the frequency ω up to the k-th one, with some coefficients. In particular, the distribution of the harmonics is the following: for a natural number $k \geq 0$, that will label the order of the expansion in powers of ε, we define recursively the set

$$\begin{aligned} I_0 &\equiv \{0\}, \\ I_k &\equiv \{h \in \mathbb{Z} : h = i-1 \text{ or } h = i+1 \text{ with } i \in I_{k-1}\}, \end{aligned} \tag{2.43}$$

such that $I_1 = \{-1, 1\}$, $I_2 = \{-2, 0, 2\}$, et cetera. We have that to the order k, the harmonics appearing in $Y_k^a(p,t)$ are exactly given by $h\omega$ with $h \in I_k$. We also define for a given $z \in \mathbb{Z}$ the subset of I_k:

$$\bar{I}_k(z) \equiv \{h \in I_k : h+1 = z \text{ or } h-1 = z\}.$$

Of course it is $|\bar{I}_k(z)| = 2$ if $z \neq \pm k$, $|\bar{I}_k(z)| = 1$ otherwise. A sequence of $k+1$ numbers $(h_0, ..., h_k)$, $h_j \in I_j$, $0 \leq j \leq k$ is a *path of length* k if $h_{j-1} \in \bar{I}_{j-1}(h_j)$ for $1 \leq j \leq k$ (see fig.

3), meaning that $h_j = h_{j-1} \pm 1$. We denote the set of all paths of length k as P_k, and write

$$Y_k^a(p,t) = \left(\frac{-i}{2}\right)^k \sum_{h\in I_k} e^{ih\omega t} \sum_{(h_0,\dots,h_k=h)\in P_k} \prod_{j=1}^{k} f(\omega_p - h_j\omega). \tag{2.44}$$

Now we have to discuss the coefficients. It easily seen that we can have several cases, as we choose ω. In all of them a singularity arises every time we have a term containing $h=0$ for $\omega_p = \pm\frac{g}{2}$. If $\omega > g$, we have that again only one singularity arises when $\omega_p = \pm\frac{g}{2}$ for $\omega \to g$. For $\omega < g$ for every k we have to divide the set $(-g/2, g/2)$ (where ω_p runs) in at most $2k+1$ intervals, each internal extremum $\pm|j\omega - \frac{g}{2}|$, $j = 1,..,k$ be a singularity. Of course it is possible that not all of these points fall in $(-g/2, g/2)$, so we have to distinguish several cases: $\omega > g$, $g/2 < \omega < g$, $g/3 < \omega < g/2$, ..., $g/j < \omega < g/(j-1)$, $j = 1,...,k$. So, already at this stage, we see clearly the disposition of resonances: up to the order k, we have resonant frequencies $\omega = g/j$, $j = 1,...,k$, each having an effect of size h^j, according to the theory of Winter [**22**].

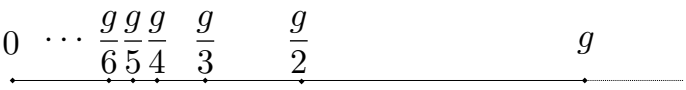

FIGURE 2. Disposition of resonances on the real line.

All that may appear a little muddled: for sake of clearness we will rewrite everything with an equivalent graphical language, namely the trees formalism. This is a very well known method, used in many field of theoretical and mathematical physics. We will adopt the approach developed in [**10**][**11**].
Since our problem is linear, we will deal with linear trees, or chains. Given k points, $k \in \mathbb{N}$, we define a chain of order k as an ordered collection of k nodes (v). We will denote it with δ_k, and we can represent drawing the nodes, in according to their order, from left to right, and linking them with straight lines (ℓ). An additional line entering the first node can be added: we will name it the root. To each chain we can assign the following functions:

$$\begin{cases} \sigma_v & = & \pm 1 & \text{node function;} \\ \mu_\ell & \equiv & \sum_{v\prec\ell} \sigma_v & \text{the moment carried by a line;} \\ f(\mu_\ell, \omega_p) & \equiv & f(\omega_p - \mu_\ell\omega) & \text{line propagator;} \end{cases}$$

the notation $v \prec \ell$ usually means *all the nodes v on the right of the line* ℓ. Thus we can define a *value function* for a given chain

$$\mathrm{Val}(\delta) = \prod_{\ell\in\delta} f(\mu_\ell, \omega_p). \tag{2.45}$$

We will denote by Δ_k the set of all chains of order k, for each positive integer k (of course $|\Delta_k| = 2^k$). Moreover, a chain with k nodes has k lines: $k-1$ internal lines and the root. The moment carried by the root is the total moment of the chain, and we will denote it simply by μ. It is very easy to check that, at order k, μ takes values in I_k. So it is convenient to define $\Delta_{k,\mu}$ as the set of chains of order k with total moment μ, such that we can definitely write

$$Y_k^a(p,t) = \left(\frac{-i}{2}\right)^k \sum_{\mu\in I_k} e^{i\mu\omega t} \sum_{\delta\in\Delta_{k,\mu}} \mathrm{Val}(\delta),$$

and

$$Y^a(p,t) = \sum_{k\geq 0} \left(\frac{-ih}{2}\right)^k \sum_{\mu\in I_k} e^{i\mu\omega t} \sum_{\delta\in\Delta_{k,\mu}} \mathrm{Val}(\delta). \tag{2.46}$$

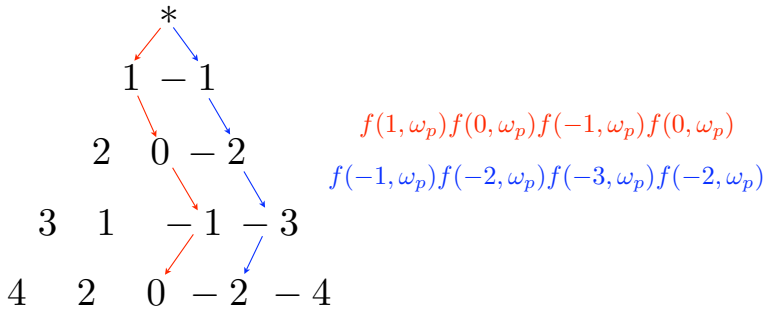

FIGURE 3. Two examples of *path* defining the value function. Each row of the triangle represents a set I_k, $k = 1,2,3,4$ from above.

It is useful to point out also the form of the complex conjugate[14]

$$Y^{*a}(p,t) = \sum_{k\geq 0}\left(\frac{ih}{2}\right)^k \sum_{\mu\in I_k} e^{-i\mu\omega t} \sum_{\delta\in\Delta_{k,\mu}} \mathrm{Val}^*(\delta). \tag{2.47}$$

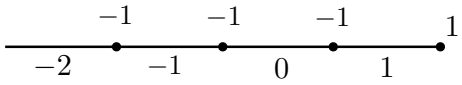

FIGURE 4. An example of chain $\delta \in \Delta_{4,-2}$ with four nodes and total momentum -2. On each node there is a dichotomic variable, and under each line there is the momentum it carries. The value function for this chain is $f(1,\omega_p)f(0,\omega_p)f(-1,\omega_p)f(-2,\omega_p)$.

It is worthwhile to stress that $\mathrm{Val}^* = \prod f^*$ is related with Val by meaningful symmetries, as specified in the following

PROPOSITION 2. *For each value of $\omega > 0$ we have*

(1) $f(\mu,\omega_p) = f(-\mu,-\omega_p)$;

(2) $f^*(\mu,\omega_p) = f(\mu,\omega_p)s_\mu(\omega_p)$.

with $s_\mu(\omega_p) = \mathrm{sign}\left(\frac{g}{2} - |\mu|\omega + \mathrm{sign}(\mu)\omega_p\right)$.

Before the proof let us notice some consequences of our results: in primis we have that for $f(-\mu,\omega_p) = f(\mu,-\omega_p)$, so switching from a chain to the conjugate one is like sending $\omega_p \to -\omega_p$; then we have

$$f^*(-\mu,\omega_p) = f^*(\mu,-\omega_p) = f(\mu,-\omega_p)s_\mu(-\omega_p) = f(-\mu,\omega_p)s_{-\mu}(\omega_p);$$

furthermore, since the functions f turns out to be either real or purely imaginary, we get immediately the following

COROLLARY 1. *Fixed an $\omega \in B_n$ we have that for all $\mu : |\mu| \geq n+1$, $f(\mu,\omega_p)$ is purely imaginary.*

Now we can proceed with the

[14] It may appear strange the minus sign in the oscillatory exponential in the r.h.t. of this equation, since both μ and $-\mu$ are in I_k. This convention anyhow renders more clear the rest of the exposition.

PROOF. We write

$$f(\mu,\omega_p)=\begin{cases}\frac{1}{\sqrt{\frac{g}{2}-(\omega_p-\mu\omega)^2}} & \text{if} \quad |\omega_p-\mu\omega|<\frac{g}{2}\\ \frac{1}{\sqrt{(\omega_p-\mu\omega)^2-\frac{g}{2}}} & \text{if} \quad |\omega_p-\mu\omega|>\frac{g}{2}.\end{cases}$$

It is evident that changing the sign of both μ and ω_p the form of f does not change. So (1) is proven. Moreover, let us fix $\mu=|\mu|$, ω_p, and we notice that for

$$\begin{array}{lll}\omega_p & > & -\frac{g}{2}+|\mu|\omega \quad \text{f is real}\\ \omega_p & < & -\frac{g}{2}+|\mu|\omega \quad \text{f is imaginary.}\end{array}$$

On the other hand, for $\mu=-|\mu|$ we can repeat the same replacing $\mu\to-\mu$ and $\omega_p\to-\omega_p$:

$$\begin{array}{lll}(-\omega_p) & > & -\frac{g}{2}+|\mu|\omega \quad \text{f is real}\\ (-\omega_p) & < & -\frac{g}{2}+|\mu|\omega \quad \text{f is imaginary.}\end{array}$$

Definitely we get

$$\begin{array}{ll}f(\mu,\omega_p)=f^*(\mu,\omega_p) & \text{if} \quad \text{sign}(\mu)\omega_p+\frac{g}{2}-|\mu|\omega>0\\ f(\mu,\omega_p)=-f^*(\mu,\omega_p) & \text{if} \quad \text{sign}(\mu)\omega_p+\frac{g}{2}-|\mu|\omega<0,\end{array}$$

so

$$f(\mu,\omega_p)=\text{sign}(\text{sign}(\mu)\omega_p+\frac{g}{2}-|\mu|\omega)f^*(\mu,\omega_p),$$

and (2) is proven. □

Of course at this stage the series defining $Y^a(p,t)$ is purely formal, since both the finiteness of each order, both the total convergence have not been proven. As we have just noticed, these are in general properties that, in principle, even a meaningful solution of (2.16) has not to satisfy. Actually two different aspects occur: the first is that finiteness of the moments is not necessary, being essentially $Y^a(p,t)$ a distribution: one can relax this requirement simply asking that it has integrable moments; but also this last is too strong (and it turns actually to be false), because of the effect of the cancellations occurring in the combination of $Y^a(p,t)$ and $Y^{*a}(p,t)$ in the computation of observables, as we will see for the transverse magnetization.
As a clear example of that, let us treat a case in which one can control the series (2.46), point-wise in p, but the estimate on $Y^a(p,t)$ (that, even though not proven to be optimal, is quite natural) is not enough in order to prove an analogue results for the transverse magnetization.
When we choose a frequency ω far away the resonance, obviously the propagator simplifies a lot, and we can easily deal with the series. This means that we can focus our attention on the intervals $B_n\equiv(\frac{g}{n+1},\frac{g}{n})$, $n\in\mathbb{Z}^+$ (see fig. 2)[15].

PROPOSITION 3. *Fixed $\omega\in B_n$ for a given integer $n\geq 0$, there is a costant dependig on the parameters of the theory $C_n(\omega,g)$, and a function of p $D_n(p)$, such that the series (2.46) is absolutely convergent for all but a finite countable set of values of $p\in[-\pi,\pi]$ and $0<h<\sqrt{D_n(p)C_n(\omega,g)}$, and it defines the unique solution of equation (2.16).*

PROOF. Let us fix $\omega\in B_n$. We have that each function $f(\mu,\omega_p)$ has divergences for $\omega_p=\left(\mu\omega\pm\frac{g}{2}\right)$ or $\omega=\frac{g}{2}\left(\frac{\frac{2\omega_p}{g}\pm1}{\mu}\right)$. This latter implies that, since $\omega>\frac{g}{n+1}$, it must be $\mu<\frac{1+\cos p}{2}(n+1)<(n+1)$, *i.e.* all the divergences at the left of B_n are protected. Therefore if $\omega\in B_n$ divergences may occur in $f(\mu,\omega_p)$ for $\mu\leq n$.

[15]To $n=0$ it corresponds the open set $(g,+\infty)$.

We can estimate all the (possibly) divergent propagators with the highest one: this will be determined by p. Indeed the denominator appearig in $f(\mu,\omega_p)$

$$\frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega_p-n\omega)^2\right|}}$$

is divergent for

$$\cos^2 p=\left(\frac{2\omega\mu}{g}\pm 1\right)^2.$$

Now for $\mu\geq 0$, we have that $\frac{2\omega\mu}{g}+1\geq 1$, so the above relation is never satisfied, unless $\mu=0$; in the same way it is for $\mu\leq 0$ $\frac{2\omega\mu}{g}+1<-1$ unless $\mu=0$. So we can discard these two cases, since they are of course included also in the opposite choice of signs. In order to fix the ideas let us take $\mu>0$. We have that $\frac{2\omega\mu}{g}-1$ is in general in $[-1,1]$, since $\omega\mu\leq g$. So there is a p such that

$$\cos^2 p=\left(\frac{2\omega\mu}{g}-1\right)^2,$$

and the last relation selects two specific values of μ_p (correspondingo to the *minus* and *plus* solution)

$$\begin{aligned}\mu_p' &= \frac{g}{\omega}\cos^2\frac{p}{2}\\ \mu_p'' &= \frac{g}{\omega}\sin^2\frac{p}{2}.\end{aligned}$$

For a given $p\in[-\pi,\pi]$, the functions $f(\pm\mu_p',\omega_p)$ and $f(\pm\mu_p'',\omega_p)$ are singular. But we notice that

$$\mu_p'+\mu_p''=\frac{g}{\omega}$$

and, since $\omega\in B_n$, $\frac{g}{\omega}$ cannot be an integer number: thus only one of μ_p' and μ_p'' is an integer; we will name this number simply μ_p. But μ_p can assume the values $\{0,1,...,n\}$: hence, in order to assure the boundedness of the propagators, we have to invert the previous relation, by excluding a countable set of values of p:

$$p_\mu^+=\pm 2\arccos\sqrt{\frac{|\mu|\omega}{g}}\quad\text{or}\quad p_\mu^-=\pm 2\arcsin\sqrt{\frac{|\mu|\omega}{g}},\quad |\mu|=0,1,...,n.$$

So we have that, for a fixed p, divergences arises only in $f(\pm\mu_p,\omega_p)$. They exhibit a behavior like

$$\frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega_p-\mu\omega)^2\right|}}=\frac{1}{\frac{g}{2}\sqrt{\left|(\cos p_\mu^+-\cos p)(\cos p_\mu^--\cos p)\right|}}.$$

It is handsome to define the following function of p:

$$D_n^{-1}(p)\equiv\sup_{0\leq\mu\leq n}\frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2-(\omega_p-\mu\omega)^2\right|}}.$$

Let us say that at order k, we have at most $\frac{k}{2}$ terms like this last[16]. The other $\frac{k}{2}$ terms are given by propagators of other momenta. We notice that the maximum among them is reached for propagator bringing $n+1$ or $n+2$: at fixed order k only one among these

[16]For $k\leq n$ it is easily seen that we have only diverging temrs, while for $k>n$ lines bringing propagators with other momenta appears; however, p by p, only one among them will be dominant, namely $D_n(p)$.

momenta is allowed, since if $n+1 \in I_k$ then $n+2 \in I_{k+1}$, and $I_k \cap I_{k+1} = \emptyset$. Thus for the other lines we use the estimate

$$\frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2 - (\omega_p - (n+1)\omega)^2\right|}} \leq \frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2 - \left(\frac{g}{2} - (n+1)\omega\right)^2\right|}}$$

and we set

$$C_n^{-1}(\omega, g) \equiv \max\left[\frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2 - \left(\frac{g}{2} - (n+1)\omega\right)^2\right|}}, \frac{1}{\sqrt{\left|\left(\frac{g}{2}\right)^2 - \left(\frac{g}{2} - (n+2)\omega\right)^2\right|}}\right].$$

Definitely, the value function can be bounded by

$$\mathrm{Val}(\delta_k) \leq \left(\frac{1}{D_n(p)C_n(\omega, g)}\right)^{\frac{k}{2}}.$$

So

$$\begin{aligned} |Y^a(p,t,\omega)| &\leq \sum_{k\geq 0}\left(\frac{h}{\sqrt{D_n(p)C_n(\omega,g)}}\right)^k \\ &= \frac{1}{1-\frac{h}{\sqrt{D_n(p)C_n(\omega)}}}, \end{aligned}$$

that is well defined of course only if

$$0 < h < \sqrt{D_n(p)C_n(\omega, g)}.$$

that is

$$0 < h^2 < 2\frac{\omega}{g} D_n(p) \min\left[(n+1)^2\left(\frac{g}{n+1} - \omega\right), (n+2)^2\left(\omega - \frac{g}{n+2}\right)\right]. \tag{2.48}$$

□

In order to extend the same task to the magnetization, we need a different approach, essentially for the following reason: if we write

$$m = \sum_{k\geq 1} h^k \sum_{k_1+k_2=k} \frac{2}{\pi}\int_0^\pi dp Y_{k_1}^* Y_{k_2}$$

and we use the rough estimates

$$|Y_k| \leq \left(\frac{1}{D_n(p)C_n(\omega, g)}\right)^{\frac{k}{2}},$$

we get

$$|m| \leq \frac{2}{\pi}\sum_{k\geq 1}\left(\frac{h}{\sqrt{C_n(\omega, g)}}\right)^k \int_0^\pi \frac{dp}{D_n(p)^{k/2}} \tag{2.49}$$

where the integral is in general divergent for every ω. This approach is therefore too naif: cancellations occur in order to eliminate all that terms that have divergences.
Anyway from condition (2.48) we have an important information: uniformly in p, by the bound $D_n(p) \leq 1$, the perturbative scheme breaks down for

$$\omega = \frac{g}{n+1}\left(1 + \left(\frac{h}{g}\right)^2\right) + O\left(\frac{h}{g}\right)^3.$$

For $n = 0$ we recover exactly the Bloch-Siegert relation (2.5). For higher harmonics we have a results similar to the one by Winter (2.6), but we see that the form of the shift is different and we have not yet excluded the even harmonics. This aspects are linked each

other, and definitely they are related to the rough estimate of the line propagator via the definition of $C_n(\omega, g)$, that can be improved in order to get a better control. However it is important to stress once again that the achievements of Winter have been obtained by studying a particular observable, *i.e.* the transverse magnetization: we will try to recover them in what follows.

5. Notes

As general textbook references on magnetic resonances it has been used [**1**][**20**].
The theory of the motion of an isolated spin has been reviewed also by Bloch, in the paper where he derives the Bloch equations [**6**]. The rotating coordinate method has been introduced (a least in a systematic way) by Rabi, Schwinger and Ramsey [**17**], and then generalized in a geometric interpretation for every oscillating two state system (*maser*) by Feynman, Vernon and Hellwarth [**9**]. The difference occurring between oscillating and rotating fields is subtle, and not deepened by all the authors addressing this kind of problem, even after the paper by Bloch and Siegert [**7**]. A clear study can be found in the work of Autler and Townes [**4**]: they insert in a more clear picture (namely, Floquet theory) the results by Bloch and Siegert, and studying them in the context of Stark effect (the perturbation is a electric field) rather than Zeeman effect (the perturbation is a magnetic field). The key work for our purpose is instead the thesis of Winter [**22**], in which he find and discuss the new effects given by oscillating fields, in particular the occurrence of resonances for higher harmonics of the frequency. His theory has been reinterpreted in a more general framework, again by using Floquet theory, by Shirley [**19**].
The theory of Bloch equation was firstly presented in [**6**], and it is widely treated also in [**1**][**20**]. An almost contemporary and even fundamental works on the absorption of magnetic resonances are [**16**] and [**8**]: in these paper the authors present both a theoretical and experimental approaches.
The problem of validity of Bloch equation for quantum spin chains has obtained a very little attention in the literature. Tjon in [**21**] discussed it in a model very close to the one here exposed, namely the XX chain with an impurity on the border. Tjon conclusion is that the Bloch theory is not valid for describing the model.
On the other hand, more or less at the same time, some results were achieved indicating that the magnetization in quantum spin chain is in general a non ergodic observable. Mazur [**15**], formulated a general criterion in order to determine the non ergodic behaviour of an observable X in a classical physical system. Mazur condition is espressed in terms of an inequality for the autocorrelation function of a given observable

$$R(X) = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \, \langle X(0)X(t)\rangle \,,$$

and a quantity $Q(X)$ that is a certain modified mean value of X with respct to a given ensemble depending on the structure of the model. If

$$R(X) < Q(X),$$

X is not ergodic. Then this result has been applied to the total magnetization of the quantum XY model, finding that it satisfies this condition, *i.e.* violates ergodicity. Anyway the extension to the quantum regime is not very deepened in the beautiful paper of Mazur, as it has been also noticed in [**5**]. A rigorous derivation of Mazur inequality in the quantum case is still lacking in literature. On the other hand, other works on XY chain confirmed Mazur's achievement for the total magnetization, for instance [**12**][**5**].
An attempt to extend these results to local observables was done by Tjon [**21**] and Abraham, Barouch, Gallavotti and Martin-Löf [**2**][**3**]. They both studied (with different approaches) the magnetization of an impurity of the XX chain, finding that it does not approach to its equilibrium value at infinite time. In particular our microscopic model for magnetic resonance absorption, by using the XX impurity chain, was firstly studied in [**3**].

In this paper the authors introduced the scheme we have adopted, finding the form of the magnetization for divers kind of time dependence of the external field. In the last part they analyzed the case of a cosine oscillating field and calculated the linear response of the system for high temperature, perturbatively in the strength of the field. A resonance phenomenon is observed, via the lack of analyticity of the linear response for a certain value of the frequency (in the paper it is $\omega = 2$, corresponding to $\omega = g$ in our notations).
A strong conceptual analogy exists with the famous work by Kubo and Tomita [**14**] in which the authors analyzed the analogue problem of magnetic resonances absorption for one spin coupled with a strong ferromagnetic hamiltonian and a small oscillating field, the two terms being non commuting. In this context they presented the general method of relaxation tensor in order to calculate the linear response for the magnetization. It is worthwhile to observe that, while in the problem faced by Kubo and Tomita the arising of resonances is a natural phenomenon, in the XX impurity problem studied in [**3**] the interpretation of the divergences as magnetic resonances is not direct. In this sense the work by Abraham, Barouch, Gallavotti and Martin-Löf, by finding and analyzing the resonance in the linear response, suggests for the first time a bridge between the two models.
All the other results discussed in this chapter are new, and they have been obtained in collaboration with Livia Corsi.

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