On the Dynamics of Quantum Spin Chains with Impurities

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Abstract
We provide a theoretical set up for studying the dynamics in quantum spin chain models with inhomogeneous two-body interaction. We frame in our formalism models that can be mapped into a fermion system with a quadratic Hamiltonian. Local and global existence results of the dynamics are discussed.

1 Introduction and Summary

In this paper we will treat time dependent Hamiltonian in many body quantum mechanics. Since the subject is intrinsically problematic, we will analyse one of the simplest significant class of models available, namely quasi-free Fermi particle systems in one dimension. Nowadays quantum mechanics is a common background to diverse branches of science, and time dependent formalism finds different attitudes in the community. However it arises quite naturally in statistical mechanics in the context of non equilibrium dynamics.

The philosophy in few words is that the action of the environment on our system of interest is described in an effective theory by putting a time dependence in the Hamiltonian. This is fairly a coarse approximation, since it does not take into account the structure of the environment, nor the effect that our system has on it. Nonetheless this picture is very efficacious for many practical proposes, and it deserves certainly to be thoroughly studied. Ultimately, it is indubitably helpful to deepen our comprehension of non equilibrium phenomena.

Spin chains constitute a very appropriate model to study the basic features of many body quantum systems, and indeed there is a sizeable literature on the topic. In particular the dynamical properties of such models are non trivial. For example the global transverse magnetisation of the XY model has been observed to approach a non equilibrium limit when a global transverse field is abruptly switched on. This peculiarity has been the subject of intensive study during the ’70: for exhaustive reviews on the topic we refer to [15] and [3] and references therein.

More recently spin chains have gained increasing interest from different perspectives: e.g. in the statistical mechanics of non equilibrium phenomena they provide a simple quantum model for studying the effect of reservoirs on an extensive system (in the set-up presented for instance in [12] or [4]), along with the properties of the quantum phase transition associated to these models (as for instance in [13]); from the quantum information side one dimensional spin systems are appealing test models for information transfer protocols, also because nowadays we have experimental realisations (with few atoms) of such systems [22].

On the other hand impurities change drastically the scenario, both in equilibrium and in dynamics. They destroy many of the symmetries of the model, so rendering thermodynamics very difficult to analyse. At present a clear picture of the equilibrium features of spin chains with inhomogeneous couplings is actually

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unavailable, and, moreover, it appears to be very far to be achieved, at least from the viewpoint of rigorous statistical mechanics. In particular, it seems to be a priority to shed more light on the Griffith-McCoy smooth phase transition [11] that is expected to be induced by the disorder [10].

Of course, since equilibrium properties of such a class of systems still conserve many aspects not investigated, it is even harder to study the dynamics. The main difficulty is the lack of informations on the structure of the spectrum of the Hamiltonian at a fixed time. But also in the simplest occurrence of one sole impurity (as examined in [1]), the presence of an isolated eigenvalue causes many technical difficulties. We will return on this point in the sequel.

The goal of the paper is to furnish explicit equations for the dynamics of the XY chain in transverse field with inhomogeneous coupling. Dynamics is encoded in an apparently complicate system of integral equations. Since this model is a particular case of quadratic Hamiltonian in the Fermi operators, we will discuss the specific properties of the dynamics in relation to more general results. It turns out that, even though a local existence theorem arises quite naturally for such systems, the extension to global existence is in general much more delicate. This can be thought as a direct consequence of the lack of conservation laws in time dependent theories.

The paper is organised as follows:
In Section 2 we expound the theoretical picture for the dynamics of systems ruled by a quadratic Hamiltonian in annihilation and creation operators for both bosons and fermions.
In Section 3 we will be concerned with states and observables: in particular we will give the explicit form of the time dependent state of the system.
In Section 4 we introduce the standard basic concepts about quantum spin chains and the mapping into fermions.
In Section 5 we will use results in Section 2 in the framework of quantum spin chains. We introduce suitable variables in order to capture the effect given by the presence of impurities and we present the system of integral equations associated to the dynamics.
In Section 6 we will deal with specific cases, displaying explicitly the equations of dynamics for the anisotropic and isotropic XY model in an inhomogeneous transverse field, and we will discuss rather concisely the motion of a single impurity.
Section 7 is left to further discussions and outlooks.
Furthermore, for sake of completeness and readability, we attach an appendix with a succinct survey of the diagonalisation method of the XY Hamiltonian, after the seminal paper of Lieb, Schultz and Mattis [16].

2 Quadratic Hamiltonians: Set Up and Dynamics

Our starting point is a system of $N$ quantum particles on the grid. We do not still specify the statistics of the particles: we describe them by creation and annihilation operators $c, c\dagger$, satisfying the canonical anti-commutation rules (+ sign) or the canonical commutation rules (− sign), respectively if we are dealing with a system of particle obeying to Fermi-Dirac or Bose-Einstein statistics:

$$[c_j, c_k]_\pm = 0, \quad [c_j\dagger, c_k\dagger]_\pm = \delta_{jk}.$$  \hspace{1cm} (1)

We attach a quantum particle to each site, mathematically a Hilbert space $\mathcal{H}_i$, and the states space of the system is the Fock space $\mathcal{F} \equiv \bigoplus_N^{j=1} \mathcal{H}_i$. We are interested in general quadratic time dependent Hamiltonians:

$$H_N(t) = \sum_{j,k \in \mathbb{Z}} J_{jk}(t) c_j\dagger c_k + \frac{1}{2} K_{jk}(t) c_j\dagger c_k + \frac{1}{2} K_{jk}(t) c_j c_k.$$  \hspace{1cm} (2)

Hypotheses on the interaction. We require:

1. stability: $J_{jk}(t) \geq J_0 > -\infty$;
2. $\ell_1$ finiteness: sup$_k$ $\sum_j |J_{jk}(t)|$, sup$_j$ $\sum_k |J_{jk}(t)| < \infty$ and sup$_k$ $\sum_j |K_{jk}(t)|$, sup$_j$ $\sum_k |K_{jk}(t)| < \infty$, $t$-uniformly;

3. boundedness and piecewise continuity in $t \in [t_0, T]$;

The last hypothesis will allow us to use Fourier inverse transform also in $t$ (in the meaning of distributions). Of course $J(t)$ is a Hermitian matrix and $K(t)$ is symmetric or anti-symmetric according to the statistics we are considering.

These requirements make it possible to pass to Fourier transform: the Hamiltonian becomes

$$H_N(t) = \frac{1}{N^2} \sum_{q,p \in \mathbb{Z}(N)} \alpha_{qp}(t) a_q^\dagger a_p + \frac{1}{2} \beta_{qp}(t) a_q^\dagger a_q^\dagger + \frac{1}{2} \beta^*_{qp}(t) a_q a_p,$$

where

$$\left\{ \begin{array}{l} c_j = \frac{1}{N} \sum_{q \in \mathbb{Z}(N)} e^{-iqj} a_q \\ c_j^* = \frac{1}{N} \sum_{q \in \mathbb{Z}(N)} e^{iqj} a_q \end{array} \right.; \quad \alpha_q(t) = \sum_{j=1}^N e^{iqj} c_j, \quad \beta_q(t) = \sum_{j,k}^N e^{iqj} c_j^*.
$$

and

$$\alpha_{qp}(t) \equiv \sum_{j,k}^N J_{jk} e^{-i(qj-pk)}, \quad \beta_{qp}(t) \equiv \sum_{j,k}^N K_{jk} e^{i(qj+pk)}.$$

The fundamental feature of this Hamiltonian is that for $t' \neq t''$ in general $[H_N(t'), H_N(t'')] \neq 0$. As it is well known, this condition implies a non trivial dynamics. We can regard the time evolution of our system as a dynamical system indexed by $q \in \mathbb{Z}(N)$ with the Heisenberg equations of motion

$d_q a_q(t) = [a_q(t), -iH(t)], \quad q \in \mathbb{Z}(N)$.

These are the equations for the evolution semigroup. We will show that it is actually given by a one-parameter semigroup of Bogoliubov-Valatin transformations [4], namely

$$a_q(t) = \frac{1}{N} \sum_p A_{qp}(t) a_p + B_{qp}(t) a_p^\dagger,$$

with $A_{qp}(t), B_{qp}(t)$ are such that they become $L_2$ function on $[0, 2\pi] \times [0, 2\pi]$ for $N \to \infty$ uniformly in $t$ and $A_{qp}(t_0) = \delta_{qp}$ and $B_{qp}(t_0) = 0$. We seek a solution satisfying

$$id_q a_q(t) = \frac{1}{N} \sum_p iA_{qp}(t) a_p + iB_{qp}(t) a_p^\dagger.$$

We want to evaluate the commutator in the Heisenberg equations and compare it with the last formula. This is easily done: we notice

$$[a_p, a_q^\dagger a_p^\dagger] = \delta_{q'p} a_p^\dagger$$

$$[a_p, a_q^\dagger a_p] = \delta_{q'p} a_p^\dagger \pm \delta_{pp'} a_q^\dagger$$

$$[a_p, a_q^\dagger a_p^\dagger] = 0$$

$$[a_p^\dagger, a_q^\dagger a_p'] = \pm \delta_{pp'} a_q^\dagger$$

$$[a_p^\dagger, a_q^\dagger a_p^\dagger] = 0$$

$$[a_p^\dagger, a_q a_p'] = \delta_{pp'} a_q^\dagger \pm \delta_{pq} a_p$$

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and hence
\[
\begin{align*}
id_t a_q(t) &= \frac{1}{N^2} \sum_{q', p'} a_{p'}^{\dagger} \left( A_{qq'}(t) \alpha_{q'p'}(t) + \frac{1}{2} B_{qq'}(t) \beta_{q'p'}(t) \pm \beta_{q'p'}(t) \right) \\
&\quad + \frac{1}{N^2} \sum_{q', p'} a_{p'}^{\dagger} \left( \pm B_{qq'}(t) \alpha_{q'p'}(t) + \frac{1}{2} A_{qq'}(t) \beta_{q'p'}(t) \pm \beta_{q'p'}(t) \right).
\end{align*}
\]

This leads us to the following first order ODE linear system
\[
\begin{cases}
i A_q(t) &= \frac{1}{N} \sum_{q'} A_{qq'}(t) \alpha_{q'p'}(t) + B_{qq'}(t) \beta_{q'p'}(t) \\
i B_{qp}(t) &= \pm \frac{1}{N} \sum_{q'} B_{qq'}(t) \alpha_{q'p'}(t) + A_{qq'}(t) \beta_{q'p'}(t).
\end{cases}
\]

So the system\(^7\) represents the evolution equations for the one-parameter semigroup of Bogoliubov-Valatin transformations that gives quantum dynamics. It is perhaps remarkable that this structure, quite natural for quadratic Hamiltonians on the grid (see also\([17]\) and \([13]\)), emerges also in other scenarios, as shown for instance in the more involved problem of effective dynamics for mean field interacting particles\([20]\).

As long as \(N\) remains finite, classical theorems on first order ODE linear systems assure local existence and uniqueness of a global solution in an interval of definition \([t_0, T]\). This solves completely the problem of existence of dynamics at finite size. On the other hand, to find an explicit form for the time evolution is a more challenging task. A general approach in literature to cope with this kind of problems is by series expansions of the solution\([4]\).

Of course the thermodynamic limit \(N \to \infty\) requires much more attention. In the limit we are led to consider the integro-differential system
\[
\begin{cases}
i A(q,p; t) &= \int_0^{2\pi} dq' (A(q,q'; t)\alpha(q',p; t) + B(q,q'; t)\beta^*(q',p; t)) \\
\pm i B(q,p; t) &= \int_0^{2\pi} dq' (B(q,q'; t)\alpha(q',p; t) + A(q,q'; t)\beta(q',p; t)) \\
A(q,p; t_0) &= \delta(q-p) \\
B(q,p; t_0) &= 0,
\end{cases}
\]

where \(\alpha(q',p; t), \beta(q',p; t)\) are \(C_q p C_t([0,2\pi]^2 \times [t_0, T])\) functions, obtained as natural limit of \(\alpha_{q'p}(t), \beta_{q'p}(t)\) (that is straightforward by our hypotheses).

It is suggestive here to represent the above system as
\[
\frac{d}{dt} A = \Gamma(t) A(t),
\]

that stands for
\[
\frac{d}{dt} \begin{pmatrix} A(q,p; t) \\ B(q,p; t) \end{pmatrix} = \int_0^{2\pi} dq' \begin{pmatrix} -i\alpha(q',p; t) & -i\beta^*(q',p; t) \\ +i\beta(q',p; t) & +i\alpha(q',p; t) \end{pmatrix} \begin{pmatrix} A(q,q'; t) \\ B(q,q'; t) \end{pmatrix}.
\]

Let us analyse at first the simplest case in which \(\Gamma(t) = \Gamma(t_0)\) is constant in time. It is evidently a compact linear map from \(L_2([0,2\pi]^2)\) into itself. The dynamics exists globally, and the semigroup is given by exponentiation. This is the starting point of the analysis performed in \([17]\).

In dealing with time dependent generators of the dynamics, the easiest occurrence is that as long as \(t\) runs in its interval of definition, \(\Gamma(t)\) remains bounded and the solution keeps lying into its domain. By our hypotheses this is straightforward to verify in every interval \([t', t''] \subset [t_0, T]\) such that the couplings are continuous. In this way \(\Gamma(t)\) is a strongly continuous operator from \(L_2 C_t([0,2\pi]^2 \times [t', t''])\) into itself and one can derive local existence of the dynamics from general theorems (for detailed discussion on the topic see for instance\([15, 21]\):

**Theorem (Local Existence).** Consider a quadratic Hamiltonian as in\([3]\), with summable and stable couplings and piece-wise continuous dependance on time in \(t \in [t_0, T]\), according to Hypotheses 1, 2, 3. Then in each interval \([t', t''] \subset [t_0, T]\) in which the Hamiltonian is continuous in \(t\), the quantum dynamics is defined as a one-parameter continuously \(t\)-differentiable semigroup of Bogoliubov-Valatin transformations.
What is more challenging of course is to extend a local existence result to a global one. As a preliminary observation, we see that \( \Gamma(t) \) represents a family of compact operators in \( L_2([0, 2\pi]^{\times 2}) \) for \( t \in [t_0, T) \), uniformly bounded in \([t_0, T)\). Therefore the spectrum of \( \Gamma(t) \) is uniformly bounded in \( t \); the Hille-Yoshida theorem allows us to conclude that \( \Gamma(t) \) is a family of generators of strongly continuous semigroups of contractions and there is a number \( w \) such that the resolvent set of \( \Gamma(t) \) is contained in \([w, +\infty)\) uniformly in \( t \). Another crucial property we have gratis is that the domain of the generators is the entire space \( L_2([0, 2\pi]^{\times 2}) \) independently of \( t \). Unfortunately, since the family \( \Gamma(t) \) is not by assumptions strongly continuous, this is not enough to ensure existence of the dynamics for all times. Anyway we can recover a similar property by requiring that in each discontinuity point of \( \Gamma(t) \) in \([t_0, T)\) the left and right limit exists. In this way, we can establish a local existence theorem locally around each discontinuity, because each interval containing a discontinuity splits into two intervals in which the previous local theorem holds, and then we can paste together the contributions. We sketch an argument somewhat more explicit: let \( t^* \) be a discontinuity point, we focus on the interval \([t^*-\delta, t^*+\delta]\) for an arbitrary \( \delta > 0 \), such that the unique discontinuity falls at time \( t^* \). We write for every \( t \in [t^*-\delta, t^*+\delta] \)

\[
A(t) = A(t^* - \delta) + \int_{t^* - \delta}^{t} dt' \Gamma(t') A(t') = A(t^* - \delta) + \int_{t^* - \delta}^{t} dt' \chi([t^* - \delta, t]) \Gamma(t') A(t').
\]

Now we can make discrete approximations of \( \Gamma(t) \) in \([t^*-\delta, t^*+\delta]\) (that is possible in virtue to the required regularity): for a given even integer \( N > 0 \) we divide \([t^*-\delta, t^*+\delta]\) in \( N \) intervals of length \( \tau = \frac{2\delta}{N} \) and we have a discretised version of the last formula:

\[
A_h - \tau \sum_{k=1}^{N} \Gamma_{kh} A_k = A(t^* - \delta),
\]

with \( t = h\tau, A_k = A(k\tau) \) and \( \Gamma_{kh} = I(k \leq h)\Gamma(k\tau) \). This is a linear system of equations, where \( \Gamma \) is a diagonal matrix with only the first \( h \) entries non zero; it has a unique solution provided that \( \det(1 - \tau \Gamma) \neq 0 \).

In our setting, due to the freedom in the choice of \( \delta \), it is not hard to verify this condition uniformly in \( N \). Then one can take the limit \( N \to \infty \) to have the existence of the solution for the flux. Thus we have local existence also in presence of (bounded) discontinuities. Hence we can extend the previous theorem to all intervals \([t', t''] \subset [t_0, T)\). In order to recover the whole \([t_0, T]\) we need a compactification condition, namely that the limit \( \lim_{t \to T^-} \Gamma(t) \) exists (it is finite by hypothesis). In this way one obtains existence of the flux for all \( t \in [t_0, T] \) by standard arguments.

We summarise our results in the following

**Theorem (Global Existence).** Consider a quadratic Hamiltonian as in \([\mathbb{Z}]\), with summable and stable couplings and piece-wise continuous dependence on time in \([t_0, T)\), according to Hypotheses 1, 2, 3, with a countable number of discontinuity points \( t^*_i \). Additionally we assume that the left and right limits of the Hamiltonian in each discontinuity point \( t^*_i \) exist, and furthermore the existence of the left limit \( t \to T^- \) as well. Then the dynamics is globally defined in \([t_0, T] \) as a one parameter semigroup of Bogoliubov-Valatin transformations.

The main advantage in this context is that one never deals with unbounded generators. This permits us to profit of piece-wise compactness, and so we need to require just suitable conditions to glue the solutions. The very question of existence of the dynamics therefore relies in our opinion only in the asymptotic behaviour for \( t \to T \). We will discuss this point later on with the aid of a specific example.

### 3 Quadratic Fermion Hamiltonians: States

The derivation presented above is very general in its simplicity, not depending on the particular quantum statistics of the particles. However, being interested in quantum spin, hereafter we will deal exclusively with fermions.
Following the classical reference [19], we introduce a generic time dependent observable as a function $f(t)$ at least in principle it can be set in a diagonal form by a unitary transformation. Thus we write

$$f(t)$$

to have also a possible explicit dependence on time, even if this will play no role in our exposition.

From a subset of the grid $S$ where $\omega$ operators, and compute the thermal average at initial time $t_0$ and the thermal average of an operator $A$ in equilibrium at inverse temperature $\beta$. The partition function reads

$$Z_N(\beta) \equiv \text{Tr} \left[ e^{-\beta H_N(t_0)} \right] ,$$

and the thermal average of an operator $A$ is defined by

$$\langle A \rangle_{\beta,t_0} \equiv \frac{1}{Z_N(\beta)} \text{Tr} \left[ Ae^{-\beta H_N(t_0)} \right] .$$

In particular, due to the fermion statistics, we have

$$\langle a_q^\dagger a_p \rangle_{\beta,t_0} = \frac{\delta_{qp}}{1 + e^{\beta \omega_p}} ,$$

$$\langle a_q a_p^\dagger \rangle_{\beta,t_0} = 0 ,$$

$$\langle a_q a_p \rangle_{\beta,t_0} = 0 ,$$

where $\omega_p$ are the initial eigen-frequencies of the system. Since the Hamiltonian is quadratic we know that at least in principle it can be set in a diagonal form by a unitary transformation.

Following the classical reference [19], we introduce a generic time dependent observable as a function $f_N$ from a subset of the grid $S \subseteq \{1, \ldots, N\}$ over the algebra of creation and annihilation operator. We allow this function to have also a possible explicit dependence on time, even if this will play no role in our exposition. Thus we write

$$f_N(S; t) = \sum_{V \subseteq S} f(V; t) \frac{1}{N |V|} \sum_{q_j, p_j \in V} \langle \prod_{j \in V} \eta_{q_j} \xi_{q_j} : e^{\sum_j i(p_j - q_j)j} + h.c. \rangle_{\beta,t_0}$$

and $:$ denotes as usual the Wick product for the operators

$$\eta_q = a_q^\dagger + a_{-q}$$

$$\xi_q = a_q - a_{-q} .$$

For sake of brevity we will skip hereafter the locution $+ h.c.$ to indicate that every operator must be self adjoint. The crucial point here is that the Hamiltonian is quadratic in creation and annihilation operators. Thus the thermal average is evaluated by using the Wick theorem [23]:

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

$$= \sum_{V \subseteq S} f(V; t) \frac{1}{N |V|} \sum_{q_j, p_j \in V} e^{\sum_j i(p_j - q_j)j} \sum_{\text{all pairings } \Pi_V} (-1)^{\pi'} \prod_{(h,k) \in \Pi_V} \langle \eta_{q_h} \xi_{q_k} \rangle_{\beta,t}$$

where $\pi'$ gives the parity of a given pairing $\Pi_V$ of the set $\{q_j, p_j : j \in V\}$. However we can take advantage by switching to the Heisenberg picture: we transfer the time dependence from the thermal average to the operators, and compute the thermal average at initial time $t_0$. Since time evolution is given by a Bogoliubov-Valatin semigroup, we have

$$\eta_q(t) = \sum_p \left( A_{qp}^*(t) + B_{-q,p}(t) \right) a_p^\dagger + \left( B_{qp}^*(t) + A_{-q,p}(t) \right) a_p$$

$$\xi_q(t) = \sum_p \left( A_{-q,p}^*(t) - B_{q,p}(t) \right) a_p^\dagger + \left( B_{-q,p}^*(t) - A_{q,p}(t) \right) a_p$$
and so 
\[
\langle f(S; t) \rangle_t = \sum_{V \subseteq S} f(V; t) \frac{1}{N!|V|} \sum_{q_j, p_j, j \in V} e^{\sum_i (p_j - q_j) i} \sum_{\text{all pairings } \Pi_V} (-1)^{\pi'} \prod_{(h, k) \in \Pi_V} \langle \eta_{q_h(t)} \xi_{q_k(t)} \rangle_{\beta, t_0}
\]

For a given pair \(q, p\) the only contributing term is 
\[
\sigma_{qp}(\beta, t) = \frac{1}{N} \sum_{q'} A_{qq'}^*(t)B_{q'-p}^*(t) - B_{-q}^*(t)A_{q}^*(t) + B_{-q}^*(t)B_{q-p}^*(t) - A_{qq'}^*(t)A_{q'}^*(t).
\]  

(11)

Therefore the time dependence of the state of the system is all in that formula. We have obtained 
\[
\langle f(S; t) \rangle_t = \sum_{V \subseteq S} f(V; t) \frac{1}{N!|V|} \sum_{q_j, p_j, j \in V} e^{\sum_i (p_j - q_j) i} \sum_{\text{all pairings } \Pi_V} (-1)^{\pi'} \prod_{(h, k) \in \Pi_V} \sigma_{qp}(\beta, t)
\]

\[= \sum_{V \subseteq S} f(V; t) \Sigma(V, \beta, t),\]

with 
\[
\Sigma(V, \beta, t) = \frac{1}{N!|V|} \sum_{q_j, p_j, j \in V} e^{\sum_i (p_j - q_j) i} \sum_{\text{all pairings } \Pi_V} (-1)^{\pi'} \prod_{(h, k) \in \Pi_V} \sigma_{qh, pk}(\beta, t),
\]  

(12)

that is indeed the time dependent state of the system. We notice that as long as \(N\) remains finite, the dynamics is well defined and our derivation of the state is exact. The problem arises as \(N \to \infty\): in this case, as we have seen in the previous Section, we need a further assumption on the interaction in order to have existence and uniqueness of the flow.

As a final remark we observe that in the hypotheses of the global existence theorem, the state asymptotically approaches a limit, that is the stationary state of the system. But it is the nature of the time dependent Hamiltonian that determines whether it is an equilibrium state, viz. an ergodic theorem holds, or it is a non equilibrium stationary state. An example of this phenomenon is global versus local transverse perturbations in the XY chains, as it will be further discussed below.

4 Preliminaries on Spin Chains

Now we turn our attention to quantum spin systems, ruled by nearest neighbour two body ferromagnetic interaction on \(\mathbb{Z}\). We will be interested specifically in models admitting a mapping into quasi free fermions analysed before. The most general Hamiltonian for describing such a class of systems is 
\[
H_N = -\sum_{j=1}^{N^*} (J^x_j(t)S^x_j S^x_{j+1} + J^y_j(t)S^y_j S^y_{j+1}) - \sum_{j=1}^{N} h^z_j(t)S^z_j.
\]  

(13)

The space this operator acts on is a tensor product of 1/2-spin vector spaces \(\mathcal{H}_j = \mathbb{C}^2\), each spanned by the vectors \textit{spin up} and \textit{spin down}: \(\mathcal{H}_N = \bigotimes_{j=1}^N \mathcal{H}_j = \mathbb{C}^{2^N}\); the corresponding matrix algebra of \(2 \times 2\) matrices \(GL_2(\mathbb{C})\) is spanned by the Pauli matrices \(\sigma^x, \sigma^y, \sigma^z\) plus the identity \(I\). The Fock space defined as \(\mathcal{F} = \bigoplus_N \mathcal{H}_N\) is as usual the proper space to perform the thermodynamic limit for the system. The spin operators attached to each site \(j\), \(S^x_j, S^y_j, \) and \(S^z_j\), are defined in terms of Pauli matrices as \(S^i_j = \frac{1}{2} \sigma^i_j\), \(i = x, y, z\). 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 mean that \(N + 1 = N\), so periodic boundary conditions are assumed. The following notations is usually adopted: \(A_j \equiv I \otimes I \otimes \ldots \otimes A \otimes I \otimes \ldots \otimes I\), \(i.e.\) the operator \(A_j\) acts as \(A\) on the Hilbert space of the \(j\)-th spin and as the identity on the others. So each observable, for finite \(N\), belongs to the tensor product algebra \(GL_2(\mathbb{C})^{\otimes N}\). Finally we will assume the same space and time regularity for the couplings as in Section 2.
As mentioned above, these spin chains correspond to particular quadratic forms in the Fermi operators, the mapping being given by the Jordan-Wigner transformation, introduced in [14]. We put

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

and their inverses

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

It is easily seen that the \(c\) operators satisfy fermionic anti-commutation relations:

\[
[c_j, c_k]_+ = 0, \quad [c_j^\dagger, c_k]_+ = \delta_{jk}.
\]

The morphism of algebras naturally induces a morphism of spaces: we have that each \(c_j\) \((c_j^\dagger)\) acts on a two level vector space \(\mathcal{H}_j\) as an annihilation (creation) operator, spanned by the vectors \(|0\rangle\) \((\text{hole})\) and \(|1\rangle\) \((\text{particle})\), as usual in the theory of Fermi systems. It is important to notice that this map does not preserve locality.

Therefore, up to a constant term, the Hamiltonian (13) is transformed in the following quadratic Hamiltonian for a one dimensional Fermi gas:

\[
H_N = -\sum_{j=1}^{N^*} (g + g_j^x(t))(c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) - \sum_{j=1}^{N^*} \gamma_j^x(t)(c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) - \sum_{i=1}^{N} (h + h_j^z(t))c_i c_i^\dagger.
\]

Here we will make a particular choice: we will look at impurities as (time dependent) perturbations of the isotropic XY Hamiltonian in a transverse field. The reason why we opt for perturbing around the isotropic instead of the (somewhat more general) anisotropic model is merely technical and it will be clear in the following. We put

\[
g + g_j = \frac{J_j^x + J_j^y}{2}; \quad \gamma_j = \frac{J_j^x - J_j^y}{2},
\]

and \(\sum_j g_j = \sum_j \gamma_j = \sum_j h_j = 0\). In other words impurities are thought as fluctuations around the XX Hamiltonian. On the other hand in our framework it is more convenient to work in the Fourier space. By putting

\[
\tilde{g}_{q-p} = \sum_{k=1}^{N^*} g_{k,k+1} e^{ik(q-p)}; \quad \tilde{\gamma}_{q+p} = \sum_{k=1}^{N^*} \gamma_{k,k+1} e^{ik(q+p)}; \quad \tilde{h}_{q-p} = \sum_{k=1}^{N^*} h_k e^{ik(q-p)},
\]

the Hamiltonian (15) can be written as

\[
H_N = \frac{1}{N^2} \sum_{q,p \in \mathbb{Z}(N)} \left[(g \cos q + h)\delta_{qp} + h_{q-p}(t) + e^{iq}g_{q-p}(t)(1 + e^{-i(q-p)})\right] a_q^\dagger a_p^\dagger + \left[\gamma_{q+p}(t) \left(\frac{e^{iq} - e^{-ip}}{2}\right)\right] a_q^\dagger a_p^\dagger + h.c.
\]

5 Integral Equations for the Dynamics of Spin Chains

For spin chains we can identify

\[
\alpha_{qp} = (g \cos q + h)\delta_{qp} + h_{q-p}(t) + e^{iq}g_{q-p}(t)(1 + e^{-i(q-p)}),
\]

\[
\beta_{qp} = \gamma_{q+p}(t) \left(\frac{e^{iq} - e^{-ip}}{2}\right).
\]
We would like to apply the theory developed in Section 2 to the last class of Hamiltonians. It turns out however more convenient to deal with the site variables

\[ X_k(t) = \frac{1}{N} \sum_q A_{qq'}(t)e^{-i(k-q)q}, \quad V_k(t) = \frac{1}{N} \sum_q B_{qq'}(t)e^{-i(k+q)q}, \]

rather then the dynamical variables \( A_{qq'}(t), B_{qq'}(t) \). These are in fact conceived to take into account the perturbation in the dynamics due to the impurities. Morally the systems of equations (7) or (8) can be written in terms of these new variables as

\[
\begin{align*}
    i\dot{A} &= \text{Hom}(A, B) + \text{Inhom}(X, V) \\
    i\dot{B} &= \text{Hom}(A, B) + \text{Inhom}(X, V)
\end{align*}
\]

where with Hom (respectively Inhom) we have denoted the part of (7), (8) depending on homogeneous (inhomogeneous) couplings. Here it is important that \( X_k(t), V_k(t) \) enter only in the inhomogeneous part of the last expressions. By Duhamel formula we obtain \( A_{qq'}(t) \) and \( B_{qq'}(t) \) in an integral form

\[
\begin{align*}
    A_{qq'}(t) &= e^{-i\omega_p(t-t_0)} \delta_{qq'} - \frac{i}{N} \sum_k e^{-i(q-p)k} \int_{t_0}^t dt' e^{-i\omega_p(t-t')} \left[ h_k(t') X^k_q(t') \right. \\
    &\quad + g_k(t')(e^{-iqX^k+1_q(t')} + e^{ipX^k+1_q(t')}) + \gamma_k(t')(e^{-iqV^k+1_q(t')} - e^{ipV^k+1_q(t')})] \\
    B_{qq'}(t) &= -ie^{-i\omega_p(t-t_0)} \delta_{qq'} + \frac{i}{N} \sum_k e^{-i(q+p)k} \int_{t_0}^t dt' e^{-i\omega_p(t-t')} \left[ h_k(t') V^k_q(t') \right. \\
    &\quad + g_k(t')(e^{-iqV^k+1_q(t')} + e^{ipV^k+1_q(t')}) + \gamma_k(t')(e^{-iqX^k+1_q(t')} - e^{ipX^k+1_q(t')}).
\end{align*}
\]

Here one can see the structure of the interaction. The quantities \( g_k(t), \gamma_k(t) \) are linked respectively to the variable \( X, V \) of the sites \( k, k+1 \), which reflects the nearest neighbour two body inhomogeneous interaction. On the other hand the transverse field is associated to the each single site. The eigen-frequencies of the related homogeneous system \( \omega_p \) depend only on \( g, h \). Of course we could allow \( g, h \) to depend on time as well, simply by substituting every \( \omega_p(t-t_0) \) with \( \int_{t_0}^t dt' \omega_p(t') \). Nevertheless this would just make the theory more complicated, without adding any substantial new feature. Therefore we will suppose that \( g, h \) are fixed. With a further step we can obtain a closed system of integral equations for the site variables, simply by using the definition of \( X_k(t) \) and \( V_k(t) \). We will skip all the calculations and give only the result in the limit \( N \to \infty \):

\[
\begin{align*}
    X^k(q; t) &= e^{-i\omega_0(t-t_0)} - i \sum_j \int_{t_0}^t dt' e^{iq(k-j)-ih(t-t')} \left[ e^{i\phi_{k-j-1}} J_{k-j-1}(t-t') (g_j(t') X^j_q(q; t') - \gamma_j(t') V^j_q(q; t')) \right. \\
    &\quad + e^{i\phi_j} J_{k-j}(t-t') (h_j(t') X^j_q(q; t') + e^{-iq} g_j(t') X^{j+1}_q(q; t')) + e^{i\gamma_j} V^{j+1}_q(q; t')) \\
    V^k(q; t) &= -ie^{-i\omega_0(t-t_0)} + i \sum_j \int_{t_0}^t dt' e^{iq(k-j)-ih(t-t')} \left[ e^{-i\phi_{k-j-1}} J_{k-j-1}^*(t-t') (g_j(t') V^j_q(q; t') - \gamma_j(t') X^j_q(q; t')) \right. \\
    &\quad + e^{-i\phi_j} J_{j-k}^*(t-t') (h_j(t') V^j_q(q; t') + e^{-iq} g_j(t') V^{j+1}_q(q; t')) + e^{-i\gamma_j} X^{j+1}_q(q; t')) \]
\end{align*}
\]

Here we have used (see for instance [9])

\[
\frac{1}{2\pi} \int_0^{2\pi} dp e^{-ipn} e^{-i(g \cos \phi + h)(t-t')} = e^{-ih(t-t')} e^{i\phi_n} J_n(g(t-t')), \]

where \( J_n(t) \) is the Bessel function of first kind and order \( n \) (see [2] for definitions and properties) and \( \phi_n = n\pi/2 \). It is remarkable that we can benefit of this exact representation only by adopting the assumption
γ = 0: in this way the unperturbed spectrum is proportional to cos q; otherwise it assumes a more involved form and, albeit the series still converges to a certain integral as well, it can no longer be identified with a known special function. This essentially concludes our analysis. In the rest of this Section we will point out some further mathematical detail in the theory.

The main feature of our characterisation of the dynamics is to capture the properties of the chain right via the presence of the Bessel functions. They witness indeed the internal structure of the chain that matches the thermodynamic limit they are

\[ J_n(\Omega) = \int_0^{+\infty} d\tau J_n(g\tau) e^{i\Omega \tau} = \chi(\Omega \leq g)e^{i\arcsin(\Omega/g)} + ig^n e^{i\phi_n} \chi(\Omega \geq g)/(\sqrt{\Omega^2 - g^2} + \Omega)^n, \]

that permits us to represent

\[ J(t) = \int_0^{+\infty} d\Omega e^{-i\Omega t} J_n(\Omega). \]

Thus we can decompose the perturbations in frequencies (via Fourier transform) and study the problem of resonances between the three quantities in the play: the proper frequencies of the perturbation, the strength of the perturbation, the proper frequencies of the chain. Such a scheme is particularly evident in the instance of perturbations periodic or quasi periodic in \( t \).

This is just a conceptual picture and to implement it in a concrete example is quite a hard task, even in the simpler cases. We will give a hint of that in the sequel. Nevertheless we believe that it is rather explicative: in general of course the inverse of a continuous function via Fourier transform is not integrable; in our framework this case may arise only because of resonances, manifesting themselves by means of non integrable singularities. Existence of the dynamics will correspond to a proper renormalisation of these resonances.

### 6 Inhomogeneous Transverse Field in the XY Chain

In this last Section we will focus on the explicit form the system of equations takes when the impurities act only at the level of the transverse field. Our treatment will be twofold: at first we will deal with the XY chain, giving a more exhaustive account of the choice \( \gamma = 0 \); then we will turn to the dynamics of the XX chain, that has a considerably simpler form, nonetheless capturing all the main features (encoded in the Bessel functions). We will show explicitly the mechanism behind existence of local and global solutions by briefly discussing the case of oscillation of a single impurity.

For the XY model with impurities in the transverse field we have

\[ \alpha_{qp} = g(\cos q + h)\delta_{qp} + \hat{h}_{q-p}(t), \quad \beta_{qp} = -i \gamma \sin q \delta_{p,-q}. \]

Therefore the evolution equation for the dynamics reads

\[ \begin{align*}
    i\dot{A}_{qp}(t) &= A_{qp}(t)(g \cos p + h) + i\gamma \sin p B_{q,-p}(t) + \frac{1}{N} \sum_{q'} A_{qp'}(t) h_{q'-p}(t) \quad (24) \\
    i\dot{B}_{qp}(t) &= -B_{qp}(t)(g \cos p + h) - 2i\gamma \sin p A_{q,-p}(t) - \frac{1}{N} \sum_{q'} B_{qp'}(t) h_{q'-p}(t). \quad (25)
\end{align*} \]
It is convenient to analyse in primis the unperturbed system \((h = 0)\) and reduce the system in diagonal form. That is done via the same transformation one introduces in order to diagonalise the Hamiltonian (this procedure appeared for the first time in the paper of Lieb, Mattis and Schultz \[16\] and it is reviewed in the Appendix). It is more practical to arrange (24) and (25) in the vectorial form

\[
i \hat{A}_{qp}(t) = \Gamma_p \hat{A}_{qp}(t_0), \quad \text{with} \quad \hat{A}_{qp} = \begin{pmatrix} A_{q,p} \\ B_{q,p} \\ A_{q,-p} \\ B_{q,-p} \end{pmatrix}
\]

and

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

This is in fact the matrix to be diagonalised in order to find the spectrum of the model. This is done by means of the unitary matrix \([12]\), and the eigenvalues for the energy levels are given by \([11]\). Thus the system reads

\[
i \hat{A}'_{qp}(t) = \begin{pmatrix} E_p & 0 & 0 & 0 \\ 0 & -E_p & 0 & 0 \\ 0 & 0 & E_p & 0 \\ 0 & 0 & 0 & -E_p \end{pmatrix} \hat{A}'_{qp}(t_0)
\]

solved by

\[
A'_{qp} = e^{-iE_p(t-t_0)} A'_{qp}(t_0), \quad A'_{qp}(t_0) = \delta_{qp} \cos \phi_q;
\]

\[
B'_{qp} = e^{iE_p(t-t_0)} B'_{qp}(t_0), \quad B'_{qp}(t_0) = -i \delta_q \sin \phi_q.
\]

In the original variables the solution is instead given by

\[
A_{qp}(t) = \delta_{qp} \left( \cos(E_p(t-t_0)) - i \frac{g \cos p + h}{E_p} \sin(E_p(t-t_0)) \right)
\]

\[
B_{qp}(t) = - \gamma \frac{\sin p}{E_p} \delta_{q,-p} \sin(E_p(t-t_0)).
\]

When a perturbative transverse field is added, we describe the system in terms of \(X, V\) variables. Since the relations linking \(A, B\) with \(X, V\) are linear, we have

\[
X^r_q(t) = \sum_{q'} A'_{qp}(t)e^{-ik(q'-q)}, \quad V^r_q(t) = \sum_{q'} B'_{qp}(t)e^{-ik(q'+q)},
\]

and also the following equations for the eigen-variables

\[
i \hat{A}'_{qp}(t) = E_p A'_{qp}(t) + \frac{1}{N} \sum_k h_k(t) X^r_{q}(t)e^{-ik(q-p)}
\]

\[
i \hat{B}'_{qp}(t) = -E_p B'_{qp}(t) - \frac{1}{N} \sum_k h_k(t) V^r_{q}(t)e^{-ik(q-p)}.
\]

Now these equations are decoupled and they can be solved separately by Duhamel principle:

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

\[
B'_{qp}(t) = -ie^{-iE_p(t-t_0)} \delta_{q,-p} \sin \phi_q + \frac{i}{N} \sum_k e^{-i(q+p)k} \int_{t_0}^t dt' e^{-iE_p(t-t')} h_k(t') V^r_{q}(t').
\]
As we have already seen (here $\omega_p = E_p$), there are closed equations for $X^{nk}_q, V^{nk}_q$:

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

(31)

and

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

(32)

These equations, although formally identical to the ones we got in the previous Section, are technically more involved, essentially because

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

due to the non linear dependance of $E_p$ on $\cos p$, is not a known function. Thus for the XY chain (i.e. for $\gamma \neq 0$) we still have a clear theoretical picture for the dynamics, but in general we do not have an exact analytical formulation of it.

In the XX Hamiltonian there is a further simplification: it is

$$\alpha_{qp}(t) = (g \cos q + h) \delta_{qp} + h_{q-p}(t), \quad \beta_{qp} = 0. \quad (33)$$

Since the term $\beta_{qp}$ vanishes, equations (11) or (8) decouple (they are in fact the same equation), and the dynamics of the system is plainly described by $A_{qp}(t)$. Hence the equations we are interested in is

$$i \dot{A}_{qp}(t) = A_{qp}(g \cos p + h) + \frac{1}{N} \sum_{q'} A_{qq'}(t) h_{q'-p}(t). \quad (34)$$

In terms of the site variables previously introduced, this translates into a system of equations involving only the $X^{nk}_q(t)$ associated to the $k$-th impurity. At finite $N$ we get the equations

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

(35)

Passing to the limit $N \to \infty$ equations (20), (21) simplify a lot

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

(36)

The simplest, but already quite rich, case to study in this context is the one of a single impurity localised in the site $k$: $h_j(t) = \delta_{jk} h(t)$ and

$$X^{k}(q; t) = e^{-i\omega_q(t-t_0)} - i e^{iq(k-k)} \int_{t_0}^{t} dt' e^{-ih(t-t')} J_{k-k}(g(t-t')) h(t') X^{k}(q; t').$$

(37)

It is immediate to see that the state of the system is completely determined by $X^{k}(q; t) \equiv X(q; t)$. This is defined by

$$X(q; t) = e^{-i\omega_q(t-t_0)} - i \int_{t_0}^{t} dt' J_0(g(t-t')) h(t') X(q; t').$$

(38)

Here we have incorporated in the field its zero mode, and so our unperturbed system has now eigen frequencies $\omega_q = g \cos q$, a choice somewhat natural in this simplified situation.
Equation (38) can be symbolically rewritten as \( X = X_0 + KX \), where \( K \) is an integral operator acting on continuous functions (in \( t \)). Equations of this form are usually approached by seeking a solution like \( X = (1 - K)^{-1}X_0 \) by means of Fredholm theory (for an exhaustive treatment we refer to the original paper by I. Fredholm and the monograph by I. Gohberg, S. Goldberg and M. A. Kaashoek \[8\]). Now we switch on the field, for example continuously, at time \( t_0 \), and let the system evolve up to time \( T > t_0 \). The integral operator has a continuous kernel in each closed interval \([t_0, T]\): this automatically implies existence of the solution and we also have the explicit form of it by Fredholm expansion. This is morally the local existence theorem of Section 2. But as we send \( T \to \infty \) the situation becomes different. Continuity and boundedness of the perturbation are no longer sufficient and necessary conditions in order to ensure existence, and one needs for example a suitable relaxation property at infinity. A possibility is, as already discussed, that the limit \( \lim_{t \to \infty} h(t) = \bar{h} \) exists. In this case the results reported in \[1\] (see also \[3\]) show that the existence of the solution is not affected by the specific time dependence of the perturbation: the system thermalise to an equilibrium state given by the limiting Hamiltonian. It is remarkable that the situation is very different for a perturbation of the same time dependence, but spatially homogenous on the whole chain. In this occurrence the system thermalise as well, but the final state is not an equilibrium state, meaning that the transverse magnetisation does not go to zero in the limit \( h \to 0 \), once the asymptotic limit \( T \to \infty \) has been taken. As already mentioned in the Introduction, this aspect is exhaustively reviewed in \[3\] and in \[15\] it is discussed in relation to more general dynamical properties of simple classical and quantum systems.

More challenging and still unsolved is instead the case of transverse field with an asymptotic oscillating behaviour. Even the occurrence (somehow basic in this context) of time periodic perturbation is hard to manage, although partial results have been achieved: \[1\], \[6\]. These situations indeed do not fall in the hypotheses required by the global existence theorem stated in Section 2. Therefore a proof of the existence of the dynamics for all time will need some new ideas and additional tools.

7 Outlooks

In this paper we have made an attempt to describe with a unified formalism the quantum motion of those spin chain models that can be mapped into free fermions, when the Hamiltonian explicitly depends on time. We have discussed on a general level the problem of existence of dynamics locally and globally in time. Then we have deepened the subject by studying the time evolution for spin chains with a more specific set of integral equations.

The central feature emerging by our analysis is that we can a priori distinguish two cases: on one hand time dependent perturbation approaching a determined limit in the extrema of the definition interval in time; in this scenario one has global existence of time evolution and the system approaches a final state. Therefore investigations are focused on the properties of such a state, which are far to be trivial in general (they are eventually connected to the quantum phase transition of the model). On the other hand we have the case of temporal dependence with asymptotic oscillations. We can single out this last situation as the more challenging one to deal with, because the possible global existence of the dynamics requires a more delicate study.

Anyhow this is inscribed in a well known and vastly ranging topic in theoretical physics, namely semiclassical interaction between light and matter. In our framework we figure out the non autonomous spin systems as feeling the presence of an oscillating classical external field. As we have discussed, a rigorous mathematical approach to this question is hard to pursue and we can point out at least two (probably not independent) hard aspects of the problem: the global existence of the time evolution is ultimately related to the preservation of the infinite dimensional analogous of the KAM tori in presence of a perturbation; the analysis of the final state has possibly to take into account an infinite number of crossing of the critical point of the model.

However, our investigation of the problem is not limited to this paper, and we plan to report soon further developments.
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Appendix. Diagonalisation of the XY Chain

This appendix is devoted to review the procedure of diagonalisation developed in [16] (see also [3]). After a Fourier transform of the Fermi operators, the Hamiltonian of the XY model becomes (up to the irrelevant addendum \( \sum_q e^{iq} = 1 \))

\[
2H_N(\gamma, h) = -\sum_q (2g \cos q + 2h)a_q^\dagger a_q + e^{-iq}a_q^\dagger a_{-q}^\dagger - e^{iq}a_qa_{-q}
\]

\[
= -\sum_q \left[ (g \cos q + h)(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - i\gamma \sin q(a_q^\dagger a_{-q}^\dagger + a_qa_{-q}) \right]
\]

\[
= -\sum_q H_q(g, \gamma, h), \quad \text{(39)}
\]

bearing in mind that

\[
\sum_q g(q)\alpha_q\alpha_{-q} = \frac{1}{2}\sum_q (g(q) - g(-q))\alpha_q\alpha_{-q}
\]

\[
\sum_q g(q)\alpha_q\beta_{-q} = \frac{1}{2}\sum_q g(q)\alpha_q\beta_q + g(-q)\alpha_{-q}\beta_{-q}
\]

\[
\alpha_q\beta_{-q} = \frac{1}{2}[(\alpha_q, \beta_q) + \delta_{qp}\delta_{\alpha\beta}],
\]

for every couple of Fermi operators such that \([\alpha_q, \beta_p]_+ = \delta_{qp}\). We notice that all the \(H_q\) acts in independent subspaces, that is

\[
2H_q = I \otimes \ldots \otimes \left[ (g \cos q + h)(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - i\gamma \sin q(a_q^\dagger a_{-q}^\dagger + a_qa_{-q}) \right] \otimes \ldots \otimes I
\]

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

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

or in matrix form

\[
4H_q = \begin{pmatrix}
    a_q & a_q^\dagger & a_{-q} & a_{-q}^\dagger
\end{pmatrix}
\begin{pmatrix}
    \Gamma_1 & 0 & 0 & -i\Gamma_2 \\
    0 & -\Gamma_1 & -i\Gamma_2 & 0 \\
    0 & i\Gamma_2 & \Gamma_1 & 0 \\
    i\Gamma_2 & 0 & 0 & -\Gamma_1
\end{pmatrix}
\begin{pmatrix}
    a_q \\
    a_q^\dagger \\
    a_{-q} \\
    a_{-q}^\dagger
\end{pmatrix}, \quad \text{(40)}
\]

with \(\Gamma_1 = g \cos q + h\) and \(\Gamma_2 = \gamma \sin q\). This matrix can be easily diagonalised, thereby obtaining the eigenvalues for the energy of the system:

\[
E_q^2 = (g \cos q + h)^2 + \gamma^2 \sin^2 q. \quad \text{(41)}
\]
The Bogoliubov-Valatin transformation $W$ that diagonalises the matrix can be directly verified to be the tensor product of $(\text{SU}(2) \times \text{SU}(2))$ rotations around the $y$-axis:

$$W = \prod_{q=-\pi}^{\pi} W_q,$$

$$W_q = \left( \begin{array}{cc} \mathbb{1} \cos \phi_q & -\sigma^y \sin \phi_q \\ \sigma^y \sin \phi_q & \mathbb{1} \cos \phi_q \end{array} \right),$$

(42)

that is the Hamiltonian is diagonal in the new operators

$$b_q = a_q \cos \phi_q + i a_{\perp q}^\dagger \sin \phi_q \quad b_q^\dagger = a_{\perp q}^\dagger \cos \phi_q - i a_q \sin \phi_q,$$

(43)

with $\cos 2\phi_q = (g \cos q + h)/E_q$, $\sin \phi_q = -\gamma \sin q/E_q$. 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

$$\hat{W}_q = \left( \begin{array}{cc} \mathbb{1} \cos \phi_q & -T^\dagger \sigma^y T \sin \phi_q \\ T^\dagger \sigma^y T \sin \phi_q & \mathbb{1} \cos \phi_q \end{array} \right),$$

as the transformation that diagonalises our bilinear form with phase adjustment. Thus for the new operator obtained in this way we have

$$\hat{b}_q = a_q \cos \phi_q + a_{\perp q}^\dagger \sin \phi_q \quad \hat{b}_q^\dagger = a_{\perp q}^\dagger \cos \phi_q + a_q \sin \phi_q,$$

(44)

The Hamiltonian in the new variables becomes

$$- \sum_q H_q = - \sum_q \frac{1}{4} \left( E_q [b_q^\dagger b_q] + E_q [b_{\perp q}^\dagger b_{\perp q}] \right)$$

$$= - \frac{1}{2} \sum_q \left( E_q \hat{b}_q^\dagger \hat{b}_q + E_q \hat{b}_{\perp q}^\dagger \hat{b}_{\perp q} \right)$$

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

(45)

Analogously we find

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

It turns useful to specify the transformation that diagonalises 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 $U = W \circ F T$ is the composition of a Fourier transform and our Bogoliubov-Valatin transformation. Thus the relations defining the matrix elements $U_{qj}$ are

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

(46)

with the obvious (more useful) inverses:

$$\left\{ \begin{array}{l} c_j = \frac{1}{\sqrt{N}} \sum_q e^{-iqj} \cos \phi_q b_q + ie^{iqj} \sin \phi_q b_q^\dagger \quad \text{and} \\ c_j^\dagger = \frac{1}{\sqrt{N}} \sum_q e^{iqj} \cos \phi_q b_q^\dagger - ie^{-iqj} \sin \phi_q b_q \end{array} \right..$$

(47)
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