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Interface states of quantum lattice models

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Abstract

We review recent results on interface ground states of quantum spin systems.

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1 Introduction

Until recently very little was known about the statistical mechanics of interfaces in quantum models, but in the past few years several interesting results have been obtained. Most of these are for quantum spin systems although some other models such as the Falicov-Kimball model [22, 20, 21, 15, 16, 28, 34, 11], have been discussed, too. Here, we will limit ourselves to quantum spin systems. We will also restrict to ground states, although quite a few interesting results for finite temperatures have been obtained by various authors [7, 8, 5, 10, 11].

This brief review is organized as follows.

- Quantum spin models as infinite dynamical systems.
- The ground state problem.
- Low-lying excitations.
- Recent results in one dimension.
- Recent in higher dimensions.

2 Quantum spin models as infinite dynamical systems

The models are defined by specifying a dynamics on an algebra of quasi-local observables. The local structure is given by the finite subsets of the d−dimensional latttice $\mathbb{Z}^d$. With each site $x \in \mathbb{Z}^d$, there is associated a copy $\mathcal{A}_x$ of the $n \times n$ matrices with complex entries $M_n(\mathbb{C})$. $\mathcal{A}_x$ is the algebra of observables at the site x. For every finite subset $\Lambda \subset \mathbb{Z}^d$, the observables in the volume Λ are given by

$$\mathcal{A}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{A}_x$$

This is a finite-dimensional C^*-algebra, and if $\Lambda_0 \subset \Lambda$, we have the natural embedding

$$\mathcal{A}_{\Lambda_0} = \mathcal{A}_{\Lambda_0} \otimes \mathbb{1}_{\mathcal{A}_{\Lambda \setminus \Lambda_0}} \subset \mathcal{A}_\Lambda$$

The algebra of *local observables* is then defined by

$$\mathcal{A}_{\mathrm{loc}} = \bigcup_{\Lambda \subset \mathbb{Z}^d} \mathcal{A}_\Lambda$$

Its completion is the C^*−algebra of *quasi-local observables*:

$$\mathcal{A} = \overline{\mathcal{A}_{\rm loc}}$$

We will also need the translation automorphsims on $\mathcal{A}$, denoted by $\tau_x, x \in \mathbb{Z}^d$, canonically mapping $\mathcal{A}_\Lambda$ into $\mathcal{A}_{\Lambda+x}$.

The dynamics is determined by a family of *local Hamiltonians*. For simplicity we will only discuss models with translation invariant finite range interactions. I.e., let $h = h^* \in \mathcal{A}_{\Lambda_0}$, for some finite set Λ_0, and define the local Hamiltonians by

$$H_\Lambda = \sum_{x:\Lambda_0+x\subset\Lambda} \tau_x(h)$$

The generator of the dynamics is the unique closed extension of the derivation

$$\delta(A) := \lim_{\Lambda\uparrow\mathbb{Z}^d}[H_\Lambda, A], \qquad \text{for all } A \in \mathcal{A}_{\rm loc} \quad .$$

This generator can be exponentiated to obtain a strongly continuous one-parameter group of C^*-automorphisms $\{\alpha_t\}_{t\in\mathbb{R}}$,

$$\alpha_t(A) := e^{it\delta}(A), \quad A \in \mathcal{A}\,.$$

The standard proof can be found in the books by Bratteli and Robinson [6] or Simon [38]. The construction of quantum spin dynamics has been extended to include long range and multi-body interactions. The best result to date is by Matsui [30].

The most detailed results have been obtained for the ferromagnetic XXZ Heisenberg model. For $x \in \mathbb{Z}^d$, let S^i_x, $i = 1, 2, 3$, be the standard spin-S matrices, generating a $n = 2S + 1$-dimensional irreducible unitary representation of SU(2), with $S = 1/2, 1, 3/2, \ldots$. The local Hamiltonians of the ferromagnetic XXZ Heisenberg model are given by

$$H_\Lambda = -\sum_{\substack{x,y\in\Lambda\\|x-y|=1}} \frac{1}{\Delta}(S^1_xS^1_y + S^2_xS^2_y) + S^3_xS^3_y \tag{2.1}$$

with $\Delta \geq 1$. $\Delta = +\infty$ is the Ising model. $\Delta = 1$ is the isotropic model, also called the XXX model.

3 The ground state problem

A *state* of the quantum spin system is a linear functional ω on $\mathcal{A}$ with the properties:

$$\omega(A^*A) \geq 0, \qquad \text{for all } A \in \mathcal{A}, \quad \omega(\mathbb{1}) = 1$$

The *ground states* of a model are the solutions of the following set of inequalities:

$$\omega(A^*\delta(A)) = \lim_{\Lambda\uparrow\infty} \omega(A^*[H_\Lambda, A]) \geq 0, \qquad \text{for all } A \in \mathcal{A}_{\text{loc}}$$

These inequalities express that all local excitations –created by a local observable A–, raise the energy. This is also called *Local Stability* and we will often refer to this set of inequalities as LS.

For translation invariant states, i.e., states satisfying

$$\omega \circ \tau_x = \omega, \qquad \text{for all } x \in \mathbb{Z}^d$$

the ground states are exactly the states that minimize the energy per site:

$$\omega(h) = \inf\{\eta(h) \mid \eta \text{ translation invariant state on } \mathcal{A}\}$$

In general, LS has non-translation invariant solutions, e.g., describing domain walls or interfaces. In this paper, our main interest are these non-translation invariant solutions. In one dimension they are often called kink (and antikink) states, or soliton states. Solutions of LS are commonly contructed as limits as $\Lambda \to \mathbb{Z}^d$, of ground states of the finite-volume Hamiltonians plus boundary terms. See Section 5 for a concrete example.

4 Low-lying excitations

At low temperatures the physical behavior of the systems modelled by quantum spin Hamiltonians is determined by the ground states and the low-lying excitations above it, i.e., states with energy slightly above the ground state energy. The mathematical setting for studying the low-lying excitations is the Gel'fand-Naimark-Segal (GNS) representation, which we now describe.

Let ω be a state satisfying LS, with the generator

$$\delta(A) = \lim_{\Lambda\uparrow\mathbb{Z}^d} [H_\Lambda, A]$$

Then, there is a unique Hilbert space $\mathcal{H}$, a representation π of $\mathcal{A}$ on $\mathcal{H}$, and a vector $\Omega \in \mathcal{H}$, such that,

$$\omega(A) = \langle\Omega, \pi(A)\Omega\rangle, \qquad \text{for all } A \in \mathcal{A}$$
$$\pi(\mathcal{A})\Omega \text{ is dense in } \mathcal{H}$$

This is called the GNS representaton of ω. In the GNS representation the dynamics $\{\alpha_t = e^{it\delta}\}_{t\in\mathbb{R}}$ is generated by a densely defined self-adjoint operator H, the *Hamiltonian* of the infinite system,

$$\begin{aligned}\pi(\alpha_t(A)) &= e^{itH}\pi(A)e^{-itH} \\ &= \lim_{\Lambda\to\mathbb{Z}^d} \pi(e^{itH_\Lambda}Ae^{-itH_\Lambda})\end{aligned}$$

This H depends on the ground state ω, and, in general, so does its spectrum. H can be chosen such that $H \geq 0$, and $H\Omega = 0$. It is the spectrum of this Hamiltonian H that describes the low-lying excitations above the ground state ω. Unlike the spectrum of finite-volume Hamiltonians, it depends only on ω, and only indirectly, i.e., through ω, on the boundary conditions one would impose in finite volume.

The first question one would like to answer about the excitation spectrum is whether there is a gap above the ground state (i.e., 0), or not. I.e., does there exist a $\gamma > 0$ such that

$$\mathrm{spec}(H) \cap (0, \gamma) = \emptyset \quad ? \tag{4.1}$$

The *exact gap* is the supremum of the set of γ's for which (4.1) holds.

5 Recent results in one dimension

One-dimensional quantum spin models, also called spin chains, are of particular interest for several reasons. First of all it is in one dimension that the most detailed rigorous analysis is possible. This was the main motivation for [29]. More recently it has also become possible to realize quantum spin chains experimetally and to compare theory and experiment is surprising detail. It is also interesting that there is a special but not so small class of one-dimensional models for which the exact ground states can be given explicitly [2, 12, 13, 35]. And finally there are the integrable quantum spin chains and the rich mathematical structures they exhibit [19].

None of the works cited above, however, deal with non-periodic ground states. Consequently, the problem of characterizing the complete set of solutions of LS, for any model, was, until recently, never dealt with. See [27] for a discussion of this characterization problem.

In this section we discuss the complete set of ground states, in the sense of LS, and their low-lying excitation spectrum, for the XXZ ferromagnetic chain. This class of models depends on two parameters: the dimension of the spin matrices $(2S+1, S = 1/2, 1, 3/2, \ldots)$, and the anisotropy $\Delta \geq 1$.

Consider finite volumes of the form $\Lambda = [a,b] \subset \mathbb{Z}$, and denote by $\partial\Lambda = [a, a+r] \cup [b-r, b]$, the boundary of Λ, where $r \geq 0$ is a suitably chosen integer.

Solutions of the ground state inequalities can be constructed by adding suitable boundary terms $b_\Lambda \in \mathcal{A}_{\partial\Lambda}$ to the finite-volume Hamiltonians, and taking limits $\Lambda \uparrow \mathbb{Z}$ of finite volume ground states of the form

$$\omega_\Lambda(A) = \frac{\langle \psi_\Lambda, A\psi_\Lambda \rangle}{\langle \psi_\Lambda, \psi_\Lambda \rangle} \quad \text{for all } A \in \mathcal{A}_\Lambda$$

where $\psi_\Lambda \in \bigotimes_{x\in\Lambda} \mathbb{C}^{2S+1}$, is an eigenvector belonging to the smallest eigenvalue of $H_\Lambda + b_\Lambda$.

For the XXZ chains it suffices to take $r = 1$ and boundary terms of the form

$$b_{[a,b]} = B(S^3_{b+1} - S^3_{a-1}) \tag{5.1}$$

Two translation invariant solutions are trivial to find and have been well-known for a long time: the unique states $\omega_\uparrow$ and $\omega_\downarrow$ determined by

$$\begin{aligned} \omega_\uparrow(S^3_x) &= S, && \text{for all } x \in \mathbb{Z} \\ \omega_\downarrow(S^3_x) &= -S, && \text{for all } x \in \mathbb{Z} \end{aligned}$$

By taking $B = \pm S\sqrt{1 - 1/\Delta^2}$, Alcaraz, Salinas, and Wreszinski [4], and independently, Gottstein and Werner [18], found non-translation invariant solutions, e.g., for $S = 1/2$, satisfying

$$\begin{aligned} \omega_{\text{kink}}(S^3_x) &= \frac{1}{2}\tanh(x/\xi) \\ \omega_{\text{antikink}}(S^3_x) &= -\frac{1}{2}\tanh(x/\xi) \end{aligned}$$

where ξ is an explicitly known function of Δ.

The concept of *zero-energy states* plays an important role in the characterization of the complete set of solution of LS. So, we introduce it here, before we continue our discussion of the XXZ model.

Suppose there exists $0 \leq \tilde{h} \in \mathcal{A}_{\Lambda_0}$, such that

$$H_\Lambda + b_\Lambda := \tilde{H}_\Lambda = \sum_{x:\Lambda_0 + x \subset \Lambda} \tau_x(\tilde{h})$$

Then, if a state ω satisfies

$$\omega(\tau_x(\tilde{h})) = 0, \qquad \text{for all } x \in \mathbb{Z},$$

ω is called a *zero-energy state.* It is easy to show that any zero-energy state satisfied LS.

Gottstein and Werner obtained the complete set of zero-energy states of the anisotropic XXZ chain $\Delta > 1$ with the particular boundary terms given in (5.1). They proved that any pure zero-energy state is either one of the two translation invariant ones, or it is a member of a set of mutually equivalent kink states or a set of mutually equivalent antikink states. A state ω is called *pure*, iff for any two states ω_1, ω_2, and $t \in (0,1)$, one has

$$\omega = t\omega_1 + (1-t)\omega_2 \Rightarrow \omega_1 = \omega_2$$

It is obvious that the solution set of LS is convex, and one can prove it is a face. The same holds for the set of zero-energy states of a fixed $\tilde{h}$. Therefore, finding the pure solutions is enough.

To which class ω belongs is determined by the limits $\alpha, \beta \in \{\pm S\}$, i.e., its asymptotic behavior:

$$\alpha := \lim_{x \to -\infty} \omega(S^3_x), \quad \beta := \lim_{x \to +\infty} \omega(S^3_x)$$

The following table summarizes the four types of zero-energy ground states as parametrized by α and β ($\Delta > 1$):

$\alpha\ \beta$	type	dominating configuration
$++$	up	$\|\cdots\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\rangle$
$--$	down	$\|\cdots\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\cdots\rangle$
$-+$	kink	$\|\cdots\downarrow\downarrow\downarrow\downarrow\downarrow\cdots\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\rangle$
$+-$	antikink	$\|\cdots\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\cdots\rangle$

We refer to [4, 3, 18] for more details on the kink and antikink states. The case $\Delta = 1$ will be discussed furtheron.

Let us now return to the question of characterizing *all* solutions of Local Stability. The first result is due to Matsui [31].

Theorem 5.1 (Matsui, 1996) *For the ferromagnetic XXZ chain, with $\Delta > 1$, and $S = 1/2$, the translation invariant states $\omega_\uparrow$ and $\omega_\downarrow$, together with the kink and antikink states described in [18] and discussed above, are the full set of pure solutions of LS.*

Note that this theorem does not say anything about the isotropic model ($\Delta = 1$). The isotropic ferromagnetic chains have an infinite family of translation invariant ground states, given by the state $\omega_\uparrow$ and all rotations of it. As expected, this breaking of the rotation symmetry is accompanied by a gapless excitation spectrum. The proof of the above theorem relies on the existence of gap, and, therefore, does not extend to the isotropic case. Recently, Koma and Nachtergaele obtained a proof of the complete set of ground state for all values of S and $\Delta \geq 1$.

Theorem 5.2 (Koma and Nachtergaele, 1997, preprint) *For the ferromagnetic XXZ chain, with $\Delta > 1$, and $S \geq 1/2$, the translation invariant states $\omega_\uparrow$ and $\omega_\downarrow$, together with the kink and antikink states generalized to arbitrary S, as in [4] exhaust the set of pure solutions of LS. If $\Delta = 1$, all solutions are translation invariant.*

So, in the isotropic case there are no kink-type ground states. One expects that the same is true for models with a unique translation invariant (or periodic) ground state. This has not yet been proved in general, but Matsui [32] obtained a quite general result in the case of a unique zero-energy state, which we explain next.

Consider an arbitrary spin chain with a translation invariant nearest neighbor interaction, i.e., $h \in \mathcal{A}_{[0,1]}$:

$$H_{[a,b]} = \sum_{x=a}^{b-1} \tau(h)$$

Assume that $h \geq 0$ and that there is a unique translation invariant state ω such that

$$\omega(h_{x,x+1}) = 0, \quad \text{for all } x \in \mathbb{Z}$$

One would expect that in this case ω is the unique solution of LS. Matsui's result, the only result so far, requires an additional assumption on the set of zero-energy states of the the half-infinite chains, i.e., states η on $\mathcal{A}_{[1,+\infty)}$ ($\mathcal{A}_{(-\infty,0]}$, respectively) such that

$$\eta(h_{x,x+1}) = 0, \quad \text{for all } x > 0 \quad (x < 0, \text{ resp.}).$$

Theorem 5.3 (Matsui, preprint) *For a spin chain as described above, if ω is the unique zero-energy ground state and if all zero-energy states of the left and right half-infinite chains are quasi-equivalent, then ω is the unique solution of LS.*

In particular this implies that the AKLT spin 1 chain introduced in [2] has a unique ground state in the sense of LS. The quasi-equivalence of the zero-energy ground states of the half-infinite chains follows, e.g., from the fact that the total spin operators on the half-infinite chain exist as densely defined self-adjoint operators on the GNS Hilbert space of the AKLT ground state. For more information on this issue see [14, 1, 36].

Next, we discuss the low-lying excitation spectrum of the XXZ chains.

For the case $S = 1/2$ the exact gap has been known for some time due to its exact solution by the Bethe Ansatz. However, a rigorous the completeness of the Bethe Ansatz eigenfunctions that is free ¿from any assumptions is not available. It is therefore interesting that one can obtain the exact gap without using the Bethe Ansatz, but solely based on the quantum group symmetry of the model [37].

Theorem 5.4 (Koma and Nachtergaele, [23]) *Let ω be any of the pure zero-energy ground states of the XXZ chain with $S = 1/2$, and $\Delta > 1$. Then, the exact gap above* 0 *in the spectrum of the GNS Hamiltonian is*

$$\gamma = 1 - 1/\Delta$$

If $\omega = \omega_\uparrow$ or $\omega_\downarrow$, 0 is a simple eigenvalue of H. For the kink and antikink states 0 is infinitely degenerate. That γ is the same for all ground states can be understood as a consequence of the quantum group symmetry. Such a symmetry is absent for the XXZ chains with $S \geq 1$, and the the gaps for the translation invariant ground states and the kink and antikink ground states no longer coincide. This is an unpublished result of Koma and Nachtergaele [25]. It is easy to show that the exact gap of the XXZ model in the states $\omega_\uparrow$ and $\omega_\downarrow$ is

$$\gamma = 2Sd(1 - \frac{1}{\Delta})$$

In a non-translation invaraint ground states γ is, in general, smaller (gap reduction).

Theorem 5.5 (Koma and Nachtergaele, in preparation) *For the XXZ chains with $S \geq 1$, and $\Delta > 1$, the exact gap above a kink or antikink ground state satisfies*

$$0 < \gamma < 2S(1 - \frac{1}{\Delta}).$$

6 Recent results in higher dimensions

In higher dimensions there also exist non-translation invariant ground states. In finite volume, this was already noted in [4]. Koma and Nachtergaele proved that ground states with a rigid interface in the diagonal (i.e., $11 \cdots 1$) direction exist in all dimensions. They also proved that the excitation spectrum above the ground state with a 11 interface in two dimensions is gapless [26]. Matsui generalized this to arbitrary dimensions $d \geq 2$ [33].

Theorem 6.1 (Koma and Nachtergaele, unpublished; Matsui, to appear) *If* $d \geq 2, S \geq 1/2, \Delta > 1$, *the XXZ model has pure, non-translation invariant ground states for which the gap vansihes (gapless excitations).*

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