

QUANTUM INTERFACES

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Abstract. We review recent results on interface states in quantum statistical mechanics.

1. Introduction. When a statistical mechanics model has more than one homogeneous (translation invariant or periodic) Gibbs state, it is interesting to ask whether there are also non-homogeneous phases such as domain wall states. In a domain wall state, also called interface state, different regions are found in a different equilibrium phase (up to small fluctuations) and are separated by a transition region of essentially finite width. That such Gibbs states exist for certain models is well-known since the seminal work of Dobrushin [5] on the interface states of the three-dimensional Ising model.

It is usually quite obvious that the Gibbs state of a finite volume with suitable boundary conditions will have an interface-like structure. The main issue is then whether or not this interface is stable in the thermodynamic limit, e.g., is there a bound on the fluctuations of its position uniform in the volume? For the three-dimensional Ising model, Dobrushin showed that the answer to this question is positive for temperatures below a certain critical value. Subsequently, this has been shown to happen in many more classical spin models. In general one expects the critical temperature for interfaces to be strictly smaller than the critical temperature for the existence of multiple homogeneous phases. The general phenomenon is that with increasing temperatures the thermal fluctuations become stronger and eventually destroy the stability of the interface. This is the so-called roughening transition.

As it is the thermal fluctuations that limit the stability of interfaces in classical models, one may think that in quantum mechanical models the existence of a stable interface is even more precarious as quantum mechanics is an additional source of fluctuations. In many respects quantum fluctuations are not unlike thermal fluctuations, but there

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are some important differences. The first one is that, in contrast to thermal fluctuations, quantum fluctuations may respect local conservation laws. This is important in the study of interfaces at zero temperature (ground states). The second difference is that quantum fluctuations cannot be interpreted independent from the energy. In fact, they have precisely to do with off-diagonal matrix elements of the Hamiltonian. For this reason, their contribution to the entropy is generally not independent from corrections to the energy. This coupling between energy and entropy is what makes the statistical mechanics of quantum models quite a bit more complicated than their classical counterparts. At the same time quantum models show a wider variety of behaviour. E.g., quantum fluctuations may, in certain cases, actually stabilize the interface. This is the main theme of this brief review paper.

Recently, two quantum models with interfaces have been investigated in detail: the XXZ Heisenberg ferromagnet and the Falicov-Kimball model. The first is a quantum spin system on the lattice \mathbb{Z}^d with the following local Hamiltonians:

$$H_\Lambda = - \sum_{\substack{\{x,y\} \subset \Lambda \\ |x-y|=1}} \frac{1}{\Delta} (S_x^1 S_y^1 + S_x^2 S_y^2) + S_x^3 S_y^3, \quad (1)$$

where Λ is any finite subset of \mathbb{Z}^d , $\Delta \geq 1$, and S_x^1, S_x^2, S_x^3 are the standard spin S matrices at the site $x \in \mathbb{Z}^d$. We will give more precise definitions and describe the mathematical setup in the next section.

The Falicov-Kimball model, introduced independently by Falicov and Kimball [11] as an approximation of a two-band Hubbard model, and by Kennedy and Lieb [10] as a simple model of crystallization. The Falicov-Kimball model consists of two subsystems defined on the same lattice \mathbb{Z}^d : “ions”, described by the Ising-type variables $W(x) \in \{0, 1\}$, $x \in \mathbb{Z}^d$, and “electrons”, described by a set of fermion creation and annihilation operators c_x^+, c_x , $x \in \mathbb{Z}^d$. Each have their chemical potential, μ_i and μ_e respectively. The ions and electrons interact via an on-site Coulomb term as in the Hubbard model. The local Hamiltonians are

$$H_\Lambda = - \sum_{\substack{\{x,y\} \subset \Lambda \\ |x-y|=1}} (c_x^+ c_y + c_y^+ c_x) - \mu_e \sum_{x \in \Lambda} c_x^+ c_x - \mu_i \sum_{x \in \Lambda} W(x) + 2U \sum_{x \in \Lambda} W(x) c_x^+ c_x. \quad (2)$$

We will be interested in the half-filled case, i.e., $\mu_i = \mu_e = U$. The models with interaction U and $-U$ are then mathematically equivalent. Therefore, we can assume $U > 0$.

In the following sections we present some recent results on interface states for these two models.

2. Non-translation-invariant ground states of the XXZ models. We will use the *Local Stability* definition of ground state. For a quantum spin system the setting is the following. The algebra of observables of a single spin is $M(2S+1)$, the $2S+1 \times 2S+1$ matrices with complex entries, where $S = 1/2, 1, 3/2, \dots$ (called the *spin*), and $SU(2)$ acts on $M(2S+1)$ through the adjoint representation of its $2S+1$ dimensional unitary irreducible representation. The algebra of local observables of a quantum spin system of spin S on the lattice \mathbb{Z}^d is defined as follows. For every finite subset $\Lambda \subset \mathbb{Z}^d$, the

observables in Λ are given by

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

where, for all $x \in \mathbb{Z}^d$, $\mathcal{A}_{\{x\}} \cong M(2S + 1)$. For $x \in \Lambda$, $\mathcal{A}_{\{x\}}$ is naturally embedded into \mathcal{A}_Λ , by tensoring with identity matrices in the factors $\mathcal{A}_{\{y\}}$, $y \in \Lambda \setminus \{x\}$. In the same way, $\mathcal{A}_\Lambda \subset \mathcal{A}_{\Lambda'}$, if $\Lambda \subset \Lambda'$. The algebra of *local observables*, \mathcal{A}_{loc} , is defined by

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

where the union is over all finite subsets of \mathbb{Z}^d . \mathbb{Z}^d acts on \mathcal{A}_{loc} as translation automorphisms τ_x , $x \in \mathbb{Z}^d$, $\tau_x(\mathcal{A}_\Lambda) = \mathcal{A}_{\Lambda+x}$. A *state* of the quantum spin system is a linear functional ω on \mathcal{A}_{loc} satisfying $\omega(\mathbb{1}) = 1$, $\omega(X^*X) \geq 0$, for all $X \in \mathcal{A}_{\text{loc}}$.

We will limit our discussion to translation invariant models with a nearest-neighbour interaction. This means that the dynamics of the model is determined by a self-adjoint element $h \in M(2S + 1) \times M(2S + 1)$. The local Hamiltonians are given by

$$H_\Lambda = \sum_{\substack{\{x,y\} \subset \Lambda \\ |x-y|=1}} h_{x,y}, \quad \text{for finite subsets } \Lambda \subset \mathbb{Z}^d,$$

where $h_{x,y}$ is a copy of h in $\mathcal{A}_{\{x,y\}}$.

DEFINITION 1 (Local Stability (LS)). A state ω on \mathcal{A}_{loc} is called a *ground state* of the quantum spin system with local Hamiltonians $\{H_\Lambda\}_\Lambda$ iff

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \omega(X^*[H_\Lambda, X]) \geq 0, \quad \text{for all } X \in \mathcal{A}_{\text{loc}} \tag{3}$$

where $[A, B] = AB - BA$, for any $A, B \in \mathcal{A}_{\text{loc}}$.

The inequality (3) expresses the property that any local perturbation of the state ω has greater or equal energy than ω . Clearly, the set of solutions of (3) is convex. One can prove it is a Choquet simplex. Therefore, it is sufficient to determine its extreme points, which are pure states. So, when we say, e.g., that there exactly two ground states, we mean there are two pure ground states.

Our main interest is to determine whether or not there are non-translation invariant solutions to (3). For the one-dimensional ferromagnetic XXZ models we know all solutions of (3). This has recently been proved in [18]. A similar result in higher dimensions is completely lacking at this moment.

Before we describe the main results on interface ground states of the XXZ model, let us first consider the issue of low-lying excitations. One should expect that the excitation spectrum of local perturbations of an interface ground state differs from the excitation spectrum found starting from a translation invariant ground state of the same model. As we shall see, the XXZ models provide instructive examples of this *gap reduction* phenomenon. In order to define the excitation spectrum with respect to a ground state, one needs to define the dynamics of the model on the C^* -algebra obtained by completing \mathcal{A}_{loc} for the standard norm of bounded linear transformations. Let \mathcal{A} denote this C^* -algebra. By a standard result (see, e.g., [4] or [24]), the following limit exists and defines

a one-parameter group of automorphisms of \mathcal{A} : for all $t \in \mathbb{R}$, $A \in \mathcal{A}_{\text{loc}}$,

$$\alpha_t(A) = \lim_{\Lambda \uparrow \mathbb{Z}^d} e^{itH_\Lambda} A e^{-itH_\Lambda}.$$

Suppose ω is a state satisfying (3). Then, by the GNS construction [4], there exists a Hilbert space \mathcal{H}_ω , a representation $\pi_\omega : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H}_\omega)$, and a vector $\Omega_\omega \in \mathcal{H}_\omega$, such that

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A) \Omega_\omega \rangle, \text{ for all } A \in \mathcal{A}$$

and there is a densely defined self-adjoint operator H_ω , $H_\omega \geq 0$, such that $H_\omega \Omega_\omega = 0$, and

$$\pi_\omega(\alpha_t(A)) = e^{itH_\omega} \pi_\omega(A) e^{-itH_\omega}.$$

This structure is unique up to unitary equivalence. Therefore, we can define, without ambiguity, the excitation spectrum of the model with respect to the ground state ω , to be the spectrum of H_ω . One says that ω has a gap if there exists $\gamma > 0$, such that

$$\text{spec}(H_\omega) \cap (0, \gamma) = \emptyset. \quad (4)$$

The *exact gap* is the supremum of the set of γ 's for which (4) holds. If no $\gamma > 0$ exists for which (4) is true, one says that the excitation spectrum is gapless (or massless). This somewhat imprecise terminology does not mean that no gaps exist higher up in the spectrum.

2.1. Translation invariant ground states. The translation invariant ground states of the ferromagnetic XXZ models are well-known. If $\Delta > 1$, there are exactly two of them, ω_\uparrow and ω_\downarrow , determined by

$$\omega_\uparrow(S_x^3) = S, \quad \omega_\downarrow(S_x^3) = -S, \quad \text{for all } x \in \mathbb{Z}^d$$

The isotropic Heisenberg ferromagnet ($\Delta = 1$), also called the XXX model, has an infinite set of pure translation invariant ground states. They are characterized by the property that their finite-volume restrictions are supported by the maximal spin representation, i.e.,

$$\omega(P_\Lambda^{(S|\Lambda|)}) = 1, \quad \text{for all finite } \Lambda \subset \mathbb{Z}^d$$

where $P_\Lambda^{(J)}$ denotes the orthogonal projection onto the spin- J subspace of

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathbb{C}^{2S+1}.$$

THEOREM 2. *Let ω be a translation invariant ground state of the d -dimensional spin- S XXZ ferromagnet with $\Delta \geq 1$. The exact gap is given by*

$$\gamma = 2Sd \left(1 - \frac{1}{\Delta}\right). \quad (5)$$

The proof of this theorem is easy and well-known. Due to the symmetry of the models one only has to consider the case $\omega = \omega_\uparrow$. One immediately gets a lower bound on the exact gap equal to (5), by considering any local perturbation of ω_\uparrow . That the value given in (5) is also an upper bound follows from a variational bound using spin waves.

2.2. *Kink and antikink states for $d = 1$, $\Delta > 1$.* First, we will describe a spanning set of finite-volume “kink” and “antikink” states and next indicate what the possible thermodynamic limits are. In the case $S = 1/2$ proofs can be found in [7]. The formulas defining the finite-volume states for arbitrary S were first given in [8]. Generalization of the thermodynamic limits to arbitrary S is straightforward.

It is convenient to define $q \in (0, 1]$ such that $\Delta = (q + q^{-1})/2$. For all $x \in \mathbb{R}$, define $\phi(x) \in \mathbb{C}^{2S+1}$ by

$$\phi(x) = \sum_{m=-S}^S q^{x(S-m)} \sqrt{\frac{(2S)!}{(S-m)!S+m!}} |m\rangle \tag{6}$$

where $\{|m\rangle \mid -S \leq m \leq S\}$ is an orthonormal basis of eigenvectors of S^3 satisfying

$$S^\pm |m\rangle = \sqrt{(S \mp m)(S \pm m + 1)} |m \pm 1\rangle$$

where $S^\pm = S^1 \pm iS^2$. Consider $\Lambda = [-L, L]$. For any $x_0 \in \mathbb{R}$ we define $\psi(L, x_0) \in (\mathbb{C}^{2S+1})^{\otimes 2L+1}$ by

$$\psi(L, x_0) = \bigotimes_{x=-L}^L \phi(x - x_0). \tag{7}$$

It is not hard to show that the set of vectors $\{\psi(L, x_0) \mid x_0 \in \mathbb{R}\}$ spans the kernel of the following modification of the local Hamiltonian

$$H_L^{\text{kink}} = - \sum_{x=-L}^{L-1} \frac{1}{\Delta} (S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2) + (S_x^3 S_{x+1}^3 - S^2) + S \sqrt{1 - \Delta^{-2}} (S_{x+1}^3 - S_x^3). \tag{8}$$

Note that the last term in the interaction yields a boundary term when summed over an interval. Therefore,

$$\lim_{\Lambda \uparrow \mathbb{Z}} [H_\Lambda, X] = \lim_{L \rightarrow \infty} [H_L^{\text{kink}}, X], \quad \text{for all } X \in \mathcal{A}_{\text{loc}}$$

and the set of ground states, i.e., solutions of (3), is not affected by the presence of these terms.

Next, we describe the set of thermodynamic limits of these finite volume states. First of all, as is easy to see, the two translation invariant ground states, ω_\uparrow and ω_\downarrow , can be obtained as weak limits of the finite-volume kink states:

$$\begin{aligned} \omega_\uparrow(A) &= \lim_{L \rightarrow \infty} \frac{\langle \psi(L, -L), A\psi(L, -L) \rangle}{\|\psi(L, -L)\|^2} \\ \omega_\downarrow(A) &= \lim_{L \rightarrow \infty} \frac{\langle \psi(L, L), A\psi(L, -L) \rangle}{\|\psi(L, L)\|^2} \end{aligned}$$

ω_\uparrow and ω_\downarrow are pure and mutually disjoint. Any other pure states are mutually equivalent and disjoint from the two translation invariant states. They can be represented as vector states in the GNS Hilbert space of any one of them, which we call $\mathcal{H}_{\text{kink}}$. A weak limit of the kink states is disjoint from ω_\uparrow and ω_\downarrow iff

$$\lim_{x \rightarrow -\infty} \omega(S_x^3) = -S, \quad \text{and} \quad \lim_{x \rightarrow +\infty} \omega(S_x^3) = +S.$$

All weak limits that are disjoint from the translation invariant states are normal, i.e., they are represented by a density matrix on $\mathcal{H}_{\text{kink}}$. Complete proofs of these statements are given by Gottstein and Werner in [7] for the case $S = 1/2$. Generalization to arbitrary S is straightforward.

THEOREM 3 ([13, 18]). **(i)** *All the ground states in the sense of (3) of the isotropic ferromagnetic Heisenberg chain ($\Delta = 1$), for any $S \geq 1/2$, are translation invariant.*

(ii) *The set of translations invariant states, kink and antikink states described above, is the complete set of ground states in the sense (3) of the anisotropic ferromagnetic XXZ chains (any $S \geq 1/2$, $\Delta > 1$).*

The case $S = 1/2$, $\Delta > 1$, was proved by Matsui [13], the other cases, including the isotropic models which are gapless, are in [18].

THEOREM 4 ([17],[19]). *For $d = 1$, any $S \geq 1/2$, and any $\Delta > 1$, the XXZ model has a gap in any of its pure kink and antikink ground states. In the case of $S = 1/2$ the exact gap is given by*

$$\gamma = 1 - \frac{1}{\Delta}$$

which is identical to the gap in the translation invariant states. If $S \geq 1$ the gap in a kink or an antikink state is strictly less than in the translation invariant states.

2.3. Diagonal interfaces in higher dimensions. One can show that in any dimension $d \geq 1$ the anisotropic XXZ ferromagnet has ground states with a rigid interface in the $11 \cdots 1$ direction [19]. If $d \geq 2$ these interfaces have gapless excitations. This was first shown by Koma and Nachtergaele in $d = 2$ and later generalized by Matsui to all dimensions $d \geq 2$ [14].

2.4. Other interfaces in higher dimensions. In three and more dimensions the existence of ground states (and equilibrium states at sufficiently low temperatures) with interfaces in the 100 direction can be obtained for sufficiently large Δ by the expansion technique of Borgs, Chayes and Fröhlich [1, 2].

3. Interface Gibbs states of the Falicov-Kimball model. We will limit the discussion to the three-dimensional model. In analogy with the situation for the Ising model we do not expect that interface equilibrium states exist in one or two dimensions. In dimensions greater than three, on the other hand, there is little doubt that interface states exist and that their existence can be proved by the same methods as in three dimensions. Therefore, we now discuss only the three-dimensional model.

Our analysis starts from the Ising-type Hamiltonian that one obtains by, following [16], integrating out the fermionic variables of the Falicov-Kimball model (2) in their equilibrium state for a fixed configuration $\{W(x)\}$. This can be done unambiguously as the equilibrium state for the spinless free fermions in a potential is unique. After performing the transformation

$$s_x = (-1)^{|x|}(2W(x) - 1)$$

this leads to an effective Hamiltonian for the variables $\{s_x\}$ with a ferromagnetic nearest neighbor interaction and a host of other terms that involve multispin interactions of arbitrary order:

$$H_{\Lambda}^{\text{eff}}(\{s_x\}) = -J(U) \sum_{\substack{\{x,y\} \cap \Lambda \neq \emptyset \\ |x-y|=1}} s_x s_y + \sum_{\substack{B \cap \Lambda \neq \emptyset \\ |B| \geq 2}} R_B(U) \tag{9}$$

where $J(U) = 1/4U + \text{h.o.} > 0$, where h.o. meaning terms of higher order in U^{-1} starting with U^{-3} . R_B is translation invariant and can be shown to satisfy a bound of the form

$$\sum_{B \ni 0} |R_B| e^{rn(B)} < \infty \tag{10}$$

for some $r > 0$, and where $n(B)$ is the length of the shortest closed path in the lattice visiting all sites in B at least once.

3.1. A. The 100 interface. The 100 interface, by which we mean any flat interface oriented perpendicular to one of the three coordinate directions in the lattice, is essentially the same as the well-known Dobrushin interfaces. One only has to show that the higher-order terms in the Hamiltonian (9) do not destroy it. Given the summability property (10) it is not surprising that this can be done.

THEOREM 5 ([6]). *There exist constants U_0, C , and D , such that for all $U > U_0$, and $\beta > DU$ there exists a Gibbs state ω_{100} of the half-filled three-dimensional Falicov-Kimball model with the properties*

$$\begin{aligned} \omega_{100}(\sigma_x) &\geq m_{\beta} - Ce^{-\beta/2U} && \text{if } x_1 \geq 1 \\ \omega_{100}(\sigma_x) &\leq -m_{\beta} + Ce^{-\beta/2U} && \text{if } x_1 \leq -1 \end{aligned}$$

where $m_{\beta} > 0$ is the magnetization in the homogeneous phases at inverse temperature β .

3.2. B. The 111 interface. The standard Ising model does not have a 111 interface due to the degeneracy of the ground states of the finite-volume Hamiltonians with the boundary conditions that could be expected to produce it, are of order e^{cL^2} . This leads to fluctuations in its position of order $\sqrt{\log L}$, [22]. In the case of the Falicov-Kimball model the 111 interface is stable at sufficiently low temperatures and in this the terms of order U^{-3} in the effective Hamiltonian (9) play a crucial role.

The leading coefficients of the relevant terms of order U^{-3} are such that stepped interfaces are favored over flat ones as can be seen from the following expressions

$$\begin{aligned} h_p \begin{pmatrix} + & + \\ + & - \end{pmatrix} &= -16U^{-3} + \text{h.o} \\ h_p \begin{pmatrix} + & - \\ + & - \end{pmatrix} &= -12U^{-3} + \text{h.o} \\ h_p \begin{pmatrix} + & - \\ - & + \end{pmatrix} &= 0 + \text{h.o} \\ h_{\{x,z\}} \begin{pmatrix} + & - & + \end{pmatrix} &= 0 + \text{h.o} \\ h_{\{x,z\}} \begin{pmatrix} + & - & - \end{pmatrix} &= -2U^{-3} + \text{h.o} \end{aligned}$$

Here, h.o denotes U^{-5} and higher powers of U^{-1} . The subscript p denotes a plaquette, and the reflections and rotations of the spin configurations indicated have the same energy. The pairs $\{x, z\}$ are such that $|x - z| = 2$ and again there are identical terms for reflected and spin-flipped configurations. That the signs of these terms are such that a 111 interface is indeed stable, is a consequence of the fermion commutation relations. A Falicov-Kimball model with hard core bosons would not have a stable 111 interface.

THEOREM 6 ([6]). *There exist constants U_0, C , and D , such that for all $U > U_0$, and $\beta > DU^3$ there exists a Gibbs state ω_{111} of the half-filled three-dimensional Falicov-Kimball model with the properties*

$$\begin{aligned}\omega_{111}(\sigma_x) &\geq m_\beta - Ce^{-3\beta/2U^3} && \text{if } x_1 + x_2 + x_3 \geq 1 \\ \omega_{111}(\sigma_x) &\leq -m_\beta + Ce^{-3\beta/2U^3} && \text{if } x_1 + x_2 + x_3 \leq -1\end{aligned}$$

where $m_\beta > 0$ is the magnetization in the homogeneous phases at inverse temperature β .

We expect that the Falicov-Kimball model has stable interfaces in other directions as well, but even higher order terms in the Hamiltonian will play a role, and, consequently their stability will require even lower temperatures. E.g., we expect that the 112 interface is stabilized by terms of order U^{-5} . One can expect that the Falicov-Kimball model has infinite number of interface phase transitions.

4. Outlook. The next step in the study of interfaces in the XXZ models would be the case of (sufficiently small) positive temperatures. In dimensions 3 and up we expect that Gibbs states with a domain wall exist for the anisotropic model. The situation of the isotropic model is less clear. In fact, for the isotropic ferromagnetic Heisenberg model a proof of the existence of translation invariant ordered phases has not yet been found. For the XXZ model at finite temperatures we do not have definite results on 111 interface states at this moment. The results for the simpler, but to some extent similar, Falicov-Kimball model described in the previous section can be considered as a first step and work on the XXZ model is now in progress. The existence of 100 interfaces at sufficiently low temperatures for the anisotropic XXZ ferromagnet in dimensions ≥ 3 follows from the general results of Borgs, Chayes, and Fröhlich [1, 2], which are obtained by a perturbation expansion.

Quantum interfaces should exhibit new properties also out of equilibrium. Although we are just starting to understand how to construct examples of dynamical semigroups for quantum spin systems, we believe that interfaces could be a good testing ground for studying these dynamics. The issue of metastable states raises a set of particularly interesting questions. For the Ising model the theory of metastable states is quite advanced and very detailed results have recently been obtained by Schonmann and Shlosman [23]. The technical difficulties one is faced with in the quantum case seem quite forbidding, but interesting progress has been made by Majewski, Olkiewicz and Zegarliński [20, 21]. It would be interesting to investigate the dynamics of domain walls and droplets using the dynamical semigroups constructed by these authors.

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