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On kink states of ferromagnetic chains

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Abstract

We study kink states of quantum, ferromagnetic, easy axis spin $\frac{1}{2}$ chains at zero temperature. These are produced by applying opposite magnetic fields on the two end sites of the chain. For sufficiently strong anisotropy and boundary field, we obtain estimates on the wave function of the lowest energy states in sectors with fixed third component of the total spin. These estimates imply that the magnetization profile has a kink structure with a well-defined location and a finite width. The energies of kink states in different sectors are exponentially close as long as they are not located near the boundaries. The basic tool that we use here is the principle of exponential localization of eigenvectors. We illustrate the method in the simplest case of the Heisenberg XXZ model and then show how it can be generalized to more complicated models. In the particular case of the Heisenberg XXZ model our results are consistent with the exact kink wave functions known for a special value of the boundary magnetic field. © 2000 Elsevier Science B.V. All rights reserved.

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Dedicated to Joel Lebowitz on the occasion of his 70th birthday

1. Introduction

It is well known that the XXZ ferromagnetic anisotropic quantum Heisenberg model[2] with $\Delta > 1$ has two translation invariant ground states with all spins up or all spins down in any dimension $d \geqslant 1$. At low enough temperatures and $d \geqslant 2$ there are two corresponding equilibrium states for any finite amount of anisotropy [1]. Recently, there has been some interest in the study of inhomogeneous equilibrium or ground states of the XXZ model. It was established by Alcaraz et al. [2] that there exist non-translation

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[2] Here we have in mind the lattice $\mathbf{Z}^d$. See Eq. (2.1) for the Hamiltonian in one dimension.

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invariant ground states for all $d \geqslant 1$, describing a kink for $d = 1$ and diagonal interfaces for $d \geqslant 2$. The magnetization profile of these inhomogeneous states varies exponentially fast, from the negative to the positive values of the translation invariant ground states, across a well-defined region of width O(1) with respect to the linear dimensions L of the sample. For $d \geqslant 2$ the interface is planar with normal vector in the $(1, \dots, 1)$ direction. These results are based on exactly known ground state wave functions when the value of the boundary magnetic field is specially tuned. In one dimension the wave function of the kink ground state may be obtained from a Bethe ansatz and it turns out that for a special value of the boundary magnetic field which depends on Δ all kink solutions with different locations have the same ground state energy. This degeneracy is related to a quantum group invariance of the Hamiltonian [3] which then provides a simple alternative way to construct kink wave functions. In more than one dimension there is no known quantum group but, proceeding by analogy, it is possible to guess the exact ground state wave function of $(1, \dots, 1)$ interfaces. These "many-body" wave functions are sufficiently simple to allow for the analysis of various quantities such as the magnetization profile or higher spin correlation functions (see, for example, Ref. [4]). We are not aware of any exact wave function that would describe horizontal interfaces with normal vector $(0, \dots, 0, 1)$. In fact the existence of the latter kind of inhomogeneous state has been established only for $d \geqslant 3$ [5].

It is desirable to develop methods to study inhomogeneous states that do not rely on exact wave functions, since these are rarely known or depend on the fine tuning of some parameter. So far from the rigorous point of view this has been accomplished only in $d \geqslant 3$ for the horizontal interfaces [5]. By using a quantum version of Pirogov–Sinai theory a Gibbs state with a horizontal interface of finite width is constructed for low enough temperatures. Important situations where this method does not work are (i) the ground state diagonal interface in $d = 3$ because of the existence of gapless excitations localized along the interface plane [6], and (ii) the low dimensional cases of the kink $d = 1$ or diagonal and horizontal interfaces for $d = 2$ in the ground state.

In this contribution we give a new proof of the existence of kink states for $d = 1$ and study some of their characteristics by a method that does not make any use of the exact solutions. It turns out that the method has more general validity and can be applied to generalizations of the XXZ model where longer range interactions are included (see Section 4). The basic tool that we use is the principle of exponential localization of eigenvectors [7] which, as we show provides detailed information on the coefficients of the wave function in a suitable basis. This information is then sufficient to estimate the magnetization profile and other quantities. We hope that a combination of the present analysis with other ideas will permit to treat higher dimensional cases as well.

One can view the XXZ model as a perturbation of the Ising model by a quantum part, the XX part. Since the Ising model has interface ground states at zero temperature the problem is to determine if these are stable under quantum fluctuations. Here by stable we mean that the width of the interface due to fluctuations is O(1) with respect to the linear dimensions L. It is interesting to compare to the purely classical situation where one studies the stability with respect to small thermal fluctuations. For classical lattice models stable interface states usually exist for $d \geqslant 3$ only. Examples where this has been established are the horizontal interface of the Ising [8] or Widom–Rowlinson [9] models. Note that it is widely believed, but still unproven, that diagonal $(1,1,1)$ interface of the Ising model is unstable. In two dimensions it is known that the Ising model has no inhomogeneous Gibbs states [10]. In particular for Dobrushin boundary conditions the phase separation line has height fluctuations of $O(\sqrt{L})$ so that the magnetization profile is completely washed out for any finite temperature [11]. We wish to stress that even though there is no stable interface it is of interest to uncover the intrinsic local structure of the phase separation line [12,13]. Such questions and more generally surface structures deserve to be studied also in the quantum setting.

Finally, we wish to point out that there are many spin chains where quantum fluctuations destroy the classical kink between two ordered ground states. Variational, perturbative and numerical calculations indicate that this is the case in the Heisenberg antiferromagnet ($\Delta \to -\Delta$), the Majumdar–Ghosh model [14], the Ising and XY models with a transverse field [15]. These are examples where it is found that the magnetization profile is completely delocalized along the whole chain. We are not aware of any rigorous proof of this behavior.

In Section 2 we explain our main results for the XXZ model. The principle of exponential localization and the proof of the results are presented in Section 3. In Section 4 we show how our analysis extends to more general ferromagnetic Hamiltonians.

2. Stability of kinks in the XXZ model

We consider a chain with $2L$ sites labelled by integers $-L \leqslant x \leqslant L-1$. The Hamiltonian of the XXZ model is

$$H_L = -\sum\nolimits_{x=-L}^{L-2}(S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2) - \Delta \sum_{x=-L}^{L-2}\left(S_x^3 S_{x+1}^3 - \frac{1}{4}\right) - h(S_{-L}^3 - S_L^3)\,, \tag{2.1}$$

where we take the anisotropy parameter $\Delta > 1$ and the boundary magnetic field $h \geqslant 0$. We consider the spin $\frac{1}{2}$ case so the Hilbert space is $\mathscr{H}_L = \otimes_{-L\leqslant x\leqslant L-1}\mathbf{C}^2$ with $\mathbf{C}^2 \simeq \alpha|\uparrow\rangle + \beta|\downarrow\rangle$, α and β complex numbers. We decompose $\mathscr{H}_L$ into a direct sum of sectors $\mathscr{H}_L(M)$, $-L \leqslant M \leqslant L$, with the third component of the total spin $S_{\text{tot}}^3 = \sum\nolimits_{x=-L}^{L-1} S_x^3$ equal to M. Since the Hamiltonian commutes with S_{tot}^3 it can be diagonalized separately in each sector $\mathscr{H}_L(M)$.

Removing the first sum in H_L (the XX part) one is left with the Ising model in the presence of a boundary field which has, for $h > \Delta/2$, $2L-2$ degenerate ground states

$$|M\rangle = (\otimes_{-L\leqslant x\leqslant M-1}|\uparrow\rangle) \otimes \left(\otimes_{M\leqslant y\leqslant L-1}|\downarrow\rangle\right)\,, \tag{2.2}$$

where $M = -L+1, \dots, L-1$. The states $|M\rangle$ represent zero width kinks located at site M and belong to the sector $\mathscr{H}_L(M)$ because $S_{\text{tot}}^3|M\rangle = M|M\rangle$.

A convenient orthonormal basis of the sector $\mathscr{H}_L(M)$ may be constructed from $|M\rangle$ by flipping an equal number of spins in both regions $-L \leqslant x \leqslant M-1$ and $M \leqslant y \leqslant L-1$. The states obtained in this way are denoted by $|x_1,\ldots,x_m; y_1,\ldots,y_m\rangle$ where $1 \leqslant m \leqslant L-|M|$ is the number of spins that are flipped in each region and $x_1,\ldots,x_m;\ y_1,\ldots,y_m$ their positions. The positions of the flipped spins will be ordered in the following way: $-L \leqslant x_m < \cdots < x_2 < x_1 \leqslant M-1$ and $M \leqslant y_1 < y_2 < \cdots < y_m \leqslant L-1$. We remark that the basis states considered here should carry a label M but we do not write it explicitely in order to simplify the notation.

The following theorem gives a detailled information about the wave function of a lowest energy state in a given sector $\mathscr{H}_L(M)$.

Theorem 1. *Let $h > \Delta/2$ and $M = -L+1,\ldots,L-1$. Let $|\Psi(M)\rangle$ be a normalized lowest energy state of H_L restricted to the the sector $\mathscr{H}_L(M)$. For $\Delta > 3/2$ we have*

$$|\langle x_1,\ldots,x_m; y_1,\ldots,y_m|\Psi(M)\rangle| \leqslant \left(\frac{3}{2\Delta}\right)^{\sum_{i=1}^m(|x_i-M+1|+|y_i-M|+1)} . \tag{2.3}$$

The probability to find m flipped spins at sites $x_1,\ldots,x_m,\ y_1,\ldots,y_m$ decays exponentially fast with the distance to the site M, which can therefore be interpreted as the location of a kink of width of order $(\ln \Delta)^{-1}$. The kink is clearly apparent in the magnetization profile. Indeed from (2.3) one can easily show that

$$\left|\langle\Psi(M)|S_x^3|\Psi(M)\rangle - \frac{1}{2}\right| \leqslant C_\Delta \left(\frac{3}{2\Delta}\right)^{2|x-M+1|+2}, \quad -L \leqslant x \leqslant M-1 , \tag{2.4}$$

$$\left|\langle\Psi(M)|S_y^3|\Psi(M)\rangle + \frac{1}{2}\right| \leqslant C_\Delta \left(\frac{3}{2\Delta}\right)^{2|y-M|+2}, \quad M \leqslant y \leqslant L-1 , \tag{2.5}$$

where C_Δ is a finite positive constant for all $\Delta > \frac{3}{2}$ and is independent of L and M. An explicit formula for this constant is given in (3.10). We note that estimates (2.3)–(2.5) are invariant under a translation of the position of the kink.

Although our proof works for $\Delta > \frac{3}{2}$ we believe the result is true for all $\Delta > 1$ with the factor $3/2\Delta$ replaced by Δ^{-1}. This expectation comes from a comparison of (2.3) with the exact ASW wave function. If one sets the boundary field to the special value $h(\Delta)=\frac{1}{2}\sqrt{\Delta^2-1}$ the Hamiltonian has a quantum group $SU_q(2)$ invariance where $0<q<1$ is the solution of $\Delta = \frac{1}{2}(q+q^{-1})$ [3]. Exploiting this fact one can generate $2L$ zero energy ground states by applying "creation" or "annihilation" operators to the states with all spins down or up. One finds for $M=-L,\ldots,L$ the degenerate ground states [2]

$$|ASW\rangle_M = |M\rangle + \sum_{m=1}^{L-|M|} \sum_{x_1,\ldots,x_m} \sum_{y_1,\ldots,y_m} q^{\sum_{i=1}^m(|x_i-M+1|+|y_i-M|+1)} |x_1,\ldots,x_m; y_1,\ldots,y_m\rangle , \tag{2.6}$$

where the sums are carried over ordered positions of flipped spins. Since for $\Delta \to \infty$ $q \simeq \Delta^{-1}$ we see that our estimate (2.3) has the correct qualitative behavior for large Δ. We also note that $q < \Delta^{-1} < 3/2\Delta$ for all $\Delta > 1$.

The degeneracy of the ASW states is related to the quantum group symmetry valid for $h = h(\Delta)$. For other values of the magnetic field $h > h(\Delta)$ this symmetry is no more exact and the degeneracy is lifted as shown in Ref. [2] using Bethe ansatz solutions. Here we show directly from (2.3).

Theorem 2. *Let* $0 < \alpha \leqslant 1$. *For* $h > \Delta/2$ *and* L *large enough the ground state energies of the sectors* $\mathscr{H}_L(M)$ *with* $|M| < L - 1 - L^\alpha/2$ *satisfy*

$$|\langle \Psi(M)|H_L|\Psi(M)\rangle - \langle \Psi(0)|H_L|\Psi(0)\rangle| \leqslant (a_\Delta + hb_\Delta)\left(\frac{3}{2\Delta}\right)^{L^\alpha/2}, \tag{2.7}$$

where a_Δ *and* b_Δ *are finite positive constants for all* $\Delta > 3/2$ *and are independent of* L *and* M.

This estimate shows that the different kink energies are exponentially close as long as their distance to the left or right end of the chain is greater than $O(L^\alpha)$, $0 < \alpha \leqslant 1$. In particular for kinks with a location $|M| < L/2$ we can choose $\alpha = 1$, so in the thermodynamic limit the number of kink states which become degenerate is $O(L)$.

3. Proof of main results

The proof of Theorem 1 is an application of the principle of exponential localization which we first state explicitely for the convenience of the reader.

3.1. Principle of exponential localization of eigenvectors [7]

Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$ and suppose that $(A + B)|\psi\rangle = \lambda|\psi\rangle$, $\langle\psi|\psi\rangle = 1$. Let P_ρ be the spectral projection of A corresponding to $[\rho, \infty[$ with $\rho > \lambda$. Suppose that (i) $A > 0$, (ii) $\pm B < \varepsilon A$, $0 < \varepsilon < 1$ and that (iii) for any normalized vector $|\phi\rangle \in P_\rho\mathscr{H}$ we have $\{B(A - \lambda)^{-1}\}^j|\phi\rangle \in P_\rho\mathscr{H}$ for $j = 0, 1, \ldots, n - 1$ with $n \geqslant 1$. Then we have $\langle\phi|\psi\rangle \leqslant \varepsilon^n\rho^n(\rho - \lambda)^{-n}$.

Proof of Theorem 1. For the Hilbert space $\mathscr{H}$ we take a sector $\mathscr{H}_L(M)$ with some $M = -L + 1, \ldots, L - 1$ and we set

$$A = -\Delta \sum_{x=-L}^{L-1} \left(S_x^3 S_{x+1}^3 - \frac{1}{4}\right) - h(S_{-L}^3 - S_L^3) + h\,, \tag{3.1}$$

$$B = -\sum_{x=-L}^{L-1} (S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2)\,. \tag{3.2}$$

When $h > \Delta/2$ the ground states of A are given by (2.2) thus $A \geqslant \Delta/2 - h + h = \Delta/2 > 0$. Using the well-known fact that the isotropic Heisenberg Hamiltonian is non-negative

$$A + \Delta B \geqslant -h(S^3_{-L} - S^3_L) + h \geqslant 0 \,. \tag{3.3}$$

A spin rotation of angle π around the three axis for every even site shows that B is unitarily equivalent to $-B$. Thus we also have $A - \Delta B \geqslant 0$ and therefore we can take $\varepsilon = \Delta^{-1}$ in hypothesis (ii).

For $|\psi\rangle$ we take a ground state $|\Psi(M)\rangle$ of the sector $\mathscr{H}_L(M)$ and applying the variational principle in that sector we have that

$$\lambda \leqslant \langle M|A + B|M\rangle = \langle M|A|M\rangle = \frac{\Delta}{2} \,. \tag{3.4}$$

We set $|\phi\rangle = |x_1,\ldots,x_m; y_1,\ldots,y_m\rangle$, $1 \leqslant m \leqslant L - |M|$. Any such state is an eigenstate of A with eigenenergy at least equal to $\Delta/2 + \Delta = 3\Delta/2$. So $|\phi\rangle \in P_\rho \mathscr{H}_L(M)$ with $\rho = 3\Delta/2$. Now we must determine how many times one may act with $B(A-\lambda)^{-1}$ on this vector without leaving the subspace $P_\rho \mathscr{H}_L(M)$. Since this vector is an eigenvector of A with eigenvalue greater than $3\Delta/2$ and $\lambda \leqslant \Delta/2$, $(A-\lambda)^{-1}|\phi\rangle$ is proportional to $|\phi\rangle$ and belongs to $P_\rho \mathscr{H}_L(M)$. The terms $(S^1_x S^1_{x+1} + S^2_x S^2_{x+1})$ in B exchange the spins at positions x, $x+1$ if they are antiparallel and annihilate the state if they are parallel. Therefore $B(A-\lambda)^{-1}|\phi\rangle$ is a linear combination of states $|x'_1,\ldots,x'_{m'}; y'_1,\ldots,y'_{m'}\rangle$ obtained from $|x_1,\ldots,x_m; y_1,\ldots,y_m\rangle$ by exchanging a single pair of antiparallel spins. The number of pairs of antiparallel spins may increase or decrease at most by one thus $m' = m-1, m, m+1$. If all the new states $|x'_1,\ldots,x'_{m'}; y'_1,\ldots,y'_{m'}\rangle$ in the linear combination are different from $|M\rangle$, in other words $m' \geqslant 1$, they belong to $P_\rho \mathscr{H}_L(M)$ and therefore $B(A-\lambda)^{-1}|\phi\rangle \in P_\rho \mathscr{H}_L(M)$. We repeat this procedure until n is such that $\{B(A-\lambda)^{-1}\}^{n-1}|\phi\rangle$ contains the state $|M-1; M\rangle$ in the expansion on eigenvectors of A. This is because one extra power of $B(A-\lambda)^{-1}$ would generate $|M\rangle$ since $(S^1_{M-1}S^1_M + S^2_M S^2_{M-1})|M-1; M\rangle = |M\rangle$. To generate the state $|M-1; M\rangle$ one must bring $m-1$ down spins among those at positions $x_1,\ldots,x_m$ to position $M-1$ and $m-1$ up spins among those at positions $y_1,\ldots,y_m$ to position M, and each time there is a down spin on site $M-1$ and an up spin on site M one must decrease the number of flipped spins by acting with $(S^1_{M-1}S^1_M + S^2_M S^2_{M-1})$. Finally one must bring the last pair of flipped spins to sites $M-1$ and M. Counting the smallest possible distance that the flipped spins of $|x_1,\ldots,x_m; y_1,\ldots,y_m\rangle$ have to travel we find a lower bound on n

$$n - 1 \geqslant \sum_{i=1}^{m} (|x_i - M + 1| + |y_i - M|) + (m-1) \,. \tag{3.5}$$

Since $\varepsilon\rho(\rho - \lambda)^{-1} \leqslant 3/2\Delta$ we obtain

$$|\langle x_1,\ldots,x_m; y_1,\ldots,y_m|\Psi(M)\rangle| \leqslant \left(\frac{3}{2\Delta}\right)^{\sum_{i=1}^{m}(|x_i - M+1| + |y_i - M| + 1)} \tag{3.6}$$

which is the desired estimate.

Let us now prove (2.4) and (2.5). The ground state $|\Psi(M)\rangle$ may be expanded on eigenvectors of A

$$|\Psi(M)\rangle = c_0|M\rangle + \sum_{m=1}^{L-|M|} \sum_{x_1,\dots,x_m} \sum_{y_1,\dots,y_m} c_m(x_1,\dots,x_m;y_1,\dots,y_m) \times |x_1,\dots,x_m;y_1,\dots,y_m\rangle . \quad (3.7)$$

In (3.7) the sums are over ordered positions of flipped spins (see after (2.2)). Let $M \leqslant y \leqslant L-1$. Then $(S_y^3 + \frac{1}{2})|x_1,\dots,x_m;y_1,\dots,y_m\rangle$ is non-zero if and only if $y \in (y_1,\dots,y_m)$. Therefore,

$$\left|\langle\Psi(M)|S_y^3|\Psi(M)\rangle + \frac{1}{2}\right| = \sum_{m=1}^{L-|M|} \sum_{x_1,\dots,x_m} \sum_{y\in y_1,\dots,y_m} |c_m(x_1,\dots,x_m;y_1,\dots,y_m)|^2 . \quad (3.8)$$

For the coefficients c_m in (3.8) we can use the upper bound of Theorem 1 and since one can factor out a term $p^{|y-M|+1}$ where $p=(3/2\Delta)^2$ we obtain

$$\left|\langle\Psi(M)|S_y^3|\Psi(M)\rangle + \frac{1}{2}\right| \leqslant p^{|y-M|+1} \sum_{m\geqslant 1} \prod_{j=1}^{m} \left\{ \sum_{x\leqslant M-j} p^{|x-M+1|} \right\} \times \prod_{k=0}^{m-2} \left\{ \sum_{y\geqslant M+k} p^{|y-M|+1} \right\} . \quad (3.9)$$

Performing the geometric sums

$$\left|\langle\Psi(M)|S_y^3|\Psi(M)\rangle + \frac{1}{2}\right| \leqslant p^{|y-M|+1} \sum_{m\geqslant 1} \frac{p^{\sum_{j=1}^{m-1} j}}{(1-p)^m} \frac{p^{\sum_{k=1}^{m-1} k}}{(1-p)^{m-1}} = p^{|y-M|+1} \sum_{m\geqslant 1} \frac{p^{m(m-1)}}{(1-p)^{2m-1}} . \quad (3.10)$$

The last sum in (3.10), which is in fact the constant C_Δ in (2.4), converges for any $p<1$ because of the Gaussian term $p^{m(m-1)}$. Thus we have obtained the desired estimate (2.4) for all $\Delta > \frac{3}{2}$. The discussion for $-L \leqslant x \leqslant M-1$ is similar.

Let us note at this point that by similar estimates it is possible to show that the probability P_m to have m flipped spins in the ground state, which is given by a sum over all $|c_m|^2$ with fixed m, has a Gaussian behavior with respect to m

$$P_m \leqslant \frac{p^{m(m-1)}}{(1-p)^{2m}} . \quad (3.11)$$

Proof of Theorem 2. Let D be the smallest integer greater or equal to $\frac{1}{4}L^\alpha$. We will use the auxiliary Hamiltonian associated to the part $M-D \leqslant x \leqslant M+D-1$ of the lattice

$$H_{M,D} = -\sum_{x=M-D}^{M+D-2} (S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2)$$

$$-\Delta \sum_{x=M-D}^{M+D-2} \left(S_x^3 S_{x+1}^3 - \frac{1}{4} \right) - h(S_{M-D}^3 - S_{M+D-1}^3) \,. \tag{3.12}$$

Let $|\Psi_{M,D}\rangle$ be a lowest energy state of $H_{M,D}$ in the sector $\sum_{x=M-D}^{M+D-1} S_x^3 = 0$ of the Hilbert space $\otimes_{M-D\leqslant x\leqslant M+D-1}\mathbf{C^2}$ and consider the state in $\mathscr{H}_L(M)$

$$|\Phi(M)\rangle = (\otimes_{-L\leqslant x\leqslant M-D-1}|\uparrow\rangle) \otimes |\Psi_{M,\,D}\rangle \otimes (\otimes_{M+D\leqslant y\leqslant L-1}|\downarrow\rangle) \,. \tag{3.13}$$

We have

$$\langle \Phi(M)|H_L|\Phi(M)\rangle = \langle \Psi_{M,\,D}|H_{M,\,D}|\Psi_{M,\,D}\rangle + R_1 \,, \tag{3.14}$$

where R_1 is a rest which comes from the terms in H_L associated to the bonds $(M - D - 1, M - D)$ and $(M + D - 1, M + D)$, and the boundary field in (2.1) and (3.12). It is easily seen that

$$R_1 = \left(h - \frac{\Delta}{2} \right) \left\{ \left\langle \Psi_{M,\,D} \left| \left(S_{M-D}^3 - \frac{1}{2} \right) \right| \Psi_{M,\,D} \right\rangle \right.$$

$$\left. - \left\langle \Psi_{M,\,D} \left| \left(S_{M+D-1}^3 + \frac{1}{2} \right) \right| \Psi_{M,\,D} \right\rangle \right\} \,. \tag{3.15}$$

The magnitude of these terms can be estimated by a bound similar to (2.4) and (2.5),

$$|R_1| \leqslant (2h - \Delta) C_\Delta \left(\frac{3}{2\Delta} \right)^{2D} \,. \tag{3.16}$$

By an application of the variational principle to H_L restricted to the sector $\mathscr{H}_L(M)$ we have $\langle \Psi(M)|H_L|\Psi(M)\rangle \leqslant \langle \Phi(M)|H_L|\Phi(M)\rangle$, thus using (3.14), (3.16)

$$\langle \Psi(M)|H_L|\Psi(M)\rangle - \langle \Psi_{M,\,D}|H_{M,\,D}|\Psi_{M,\,D}\rangle \leqslant (2h - \Delta) C_\Delta \left(\frac{3}{2\Delta} \right)^{2D} \,. \tag{3.17}$$

We now prove that the left-hand side of (3.17) is greater than a negative quantity of the same order of magnitude than the right-hand side. To this end we decompose $|\Psi(M)\rangle$ as follows:

$$|\Psi(M)\rangle = |\Psi_0\rangle + |\Psi_1\rangle, \tag{3.18}$$

where $|\Psi_0\rangle$ has no flipped spins outside $M - D, \ldots, M + D - 1$

$$|\Psi_0\rangle = c_0|M\rangle + \sum_{m=1}^{D} \sum_{M-D\leqslant x_m < \cdots < x_1 \leqslant M-1}$$

$$\times \sum_{M\leqslant y_1 < \cdots < y_m \leqslant M+D-1} c_m(x_1, \ldots, x_m; y_1, \ldots, y_m)|x_1, \ldots, x_m; y_1, \ldots, y_m\rangle \tag{3.19}$$

and $|\Psi_1\rangle$ is the sum of terms in (3.7) with at least one flipped spin outside $M-D,\dots,M+D-1$. Using (3.6) one can show that for all $\Delta > \frac{3}{2}$

$$|\langle\Psi_1|\Psi_1\rangle| \leqslant C'_\Delta \left(\frac{3}{2\Delta}\right)^{2D+2}, \tag{3.20}$$

where C'_Δ is a finite positive constant depending only on Δ. The state $|\Psi_0\rangle$ is of the form

$$|\Psi_0\rangle = (\otimes_{-L\leqslant x\leqslant M-D-1}|\uparrow\rangle) \otimes |\tilde{\Psi}_{M,D}\rangle \otimes (\otimes_{M+D\leqslant y\leqslant L-1}|\downarrow\rangle), \tag{3.21}$$

where $|\tilde{\Psi}_{M,D}\rangle$ belongs to the sector with $\sum_{x=M-D}^{M+D-1} S_x^3 = 0$. Proceeding similarly than in (3.14)–(3.16) we get

$$\langle\Psi_0|H_L|\Psi_0\rangle = \langle\tilde{\Psi}_{M,D}|H_{M,D}|\tilde{\Psi}_{M,D}\rangle + R_2 \tag{3.22}$$

with

$$|R_2| \leqslant (2h-\Delta)C_\Delta \left(\frac{3}{2\Delta}\right)^{2D}. \tag{3.23}$$

Since $|\Psi_{M,D}\rangle$ is the ground state of $H_{M,D}$ the variational principle together with (3.22) and (3.23) imply

$$\langle\Psi_0|H_L|\Psi_0\rangle \geqslant \langle\Psi_{M,D}|H_{M,D}|\Psi_{M,D}\rangle - (2h-\Delta)C_\Delta \left(\frac{3}{2\Delta}\right)^{2D}. \tag{3.24}$$

Now

$$\begin{aligned}\langle\Psi(M)|H_L|\Psi(M)\rangle &= \langle\Psi_0|H_L|\Psi_0\rangle + \langle\Psi_0|H_L|\Psi_1\rangle + \langle\Psi_1|H_L|\Psi_0\rangle + \langle\Psi_1|H_L|\Psi_1\rangle \\ &\geqslant \langle\Psi_0|H_L|\Psi_0\rangle - 3\parallel H_L \parallel\parallel \Psi_1 \parallel,\end{aligned} \tag{3.25}$$

where the norm of H_L is estimated by taking the norm of each term in (2.1) $\parallel H_L \parallel \leqslant h+(\Delta/2+1/2)2L$ and $\parallel \Psi_1 \parallel$ is estimated by (3.20). Therefore from (3.25) and (3.24) we obtain the inequality

$$\begin{aligned}&\langle\Psi(M)|H_L|\Psi(M)\rangle - \langle\Psi_{M,D}|H_{M,D}|\Psi_{M,D}\rangle \\ &\quad \geqslant -((2h-\Delta)C_\Delta + (h+(\Delta+1)L){C'_\Delta}^{1/2})\left(\frac{3}{2\Delta}\right)^{2D}.\end{aligned} \tag{3.26}$$

We note that by relabeling the sites of the auxiliary Hamiltonian (3.12)

$$\langle\Psi_{M,D}|H_{M,D}|\Psi_{M,D}\rangle = \langle\Psi_{M=0,D}|H_{M=0,D}|\Psi_{M=0,D}\rangle, \tag{3.27}$$

so if we take $|M| < L-1-\frac{1}{2}L^\alpha$, $0<\alpha\leqslant 1$, and D the smallest integer $\geqslant L^\alpha/4$ we obtain from (3.17), (3.26)

$$|\langle\Psi(M)|H_L|\Psi(M)\rangle - \langle\Psi_{M=0,D}|H_{M=0,D}|\Psi_{M=0,D}\rangle| \leqslant \frac{1}{2}(a_\Delta + hb_\Delta)\left(\frac{3}{2\Delta}\right)^{L^\alpha/2}, \tag{3.28}$$

where a_Δ and b_Δ are two positive finite constants independent of L and M. In particular this implies estimate (2.7) of Theorem 2.

4. Extension to other ferromagnetic chains

In this section we sketch a generalization of the main results in Section 3 to spin chains containing longer range interactions. We consider the spin $\frac{1}{2}$ Hamiltonian

$$H = -\sum_{r=1}^{R} J_r \left\{ \sum_{x=-L}^{L-r-1} (S_x^1 S_{x+r}^1 + S_x^2 S_{x+r}^2) + \Delta_r \sum_{x=-L}^{L-r-1} \left(S_x^3 S_{x+r}^3 - \frac{1}{4} \right) \right\} \\ -h(S_{-L}^3 - S_L^3) \tag{4.1}$$

with $J_1 = 1$, $\Delta_1 = \Delta$, $J_r \geqslant 0$, $\Delta_r \geqslant \Delta$ for $r \geqslant 2$.

This model is rotation invariant about the three axis so we can again diagonalize the Hamiltonian separately in each sector. For simplicity we discuss the stability of the kink in the sector $\mathscr{H}_L(M=0)$. The state $|0\rangle$ in (2.2) has an energy $\sum_{r=1}^{R} \frac{r}{2} J_r \Delta_r - h$ and is a ground state of the classical part of the Hamiltonian when the boundary magnetic field $h > \sum_{r=1}^{R} \frac{r}{2} J_r \Delta_r \equiv e_0$. All basis states $|x_1,\dots,x_m; y_1,\dots,y_m\rangle$ with $m \geqslant 1$ are eigenstates of the classical part with eigenenergy at least equal to $e_0 + \Delta$. To apply the principle of exponential localization we set

$$A = -\sum_{r=1}^{R} J_r \Delta_r \sum_{x=-L}^{L-r-1} \left(S_x^3 S_{x+r}^3 - \frac{1}{4} \right) - h(S_{-L}^3 - S_L^3) + h \tag{4.2}$$

and

$$B = -\sum_{r=1}^{R} J_r \sum_{x=-L}^{L-r-1} (S_x^1 S_{x+r}^1 + S_x^2 S_{x+r}^2) \,. \tag{4.3}$$

For $h > e_0$ we have $A \geqslant e_0 > 0$. Moreover since for $\Delta_r \geqslant \Delta$

$$\pm \Delta (S_x^1 S_{x+r}^1 + S_x^2 S_{x+r}^2) + \Delta_r (S_x^3 S_{x+r}^3 - \tfrac{1}{4}) \geqslant 0 \tag{4.4}$$

summing over x and r we get that $\pm \Delta B + A \geqslant 0$ and therefore hypothesis (ii) is satisfied with $\varepsilon = \Delta^{-1}$. We can apply the variational principle as in (3.4) to get that the energy of the ground state $|\Psi(0)\rangle$ satisfies $\lambda \leqslant \langle 0|A|0\rangle = e_0$. Any state $|x_1,\dots,x_m; y_1,\dots,y_m\rangle$ belongs to the subspace $P_\rho \mathscr{H}_L(M=0)$ with $\rho \geqslant e_0 + \Delta$. We must now determine how many times one can act with $B(A-\lambda)^{-1}$ on basis states before leaving the subspace $P_\rho \mathscr{H}_L(M=0)$. We have to stop when a state of the form $|x_1; y_1\rangle$ with $-R \leqslant x_1 \leqslant -1$ and $0 \leqslant y_1 \leqslant R-1$ is generated. Then for states with $x_m < \cdots < x_2 < x_1 \leqslant -R$ and $R-1 \leqslant y_1 < y_2 < \cdots < y_m$ we have

$$n \geqslant \sum_{i=1}^{m} \left(\left[\left| \frac{x_i}{R} + 1 \right| \right] + \left[\left| \frac{y_i}{R} \right| \right] + 1 \right) , \tag{4.5}$$

where $[a]$ is the integer part of a. Therefore, the projection of the ground state on basis states containing flipped spins only outside the region $-R,\dots,R$ satisfies

$$|\langle x_1,\dots,x_m; y_1,\dots,y_m|\Psi(0)\rangle| \leqslant \left(\frac{1}{\Delta} \left(1 + \frac{e_0}{\Delta} \right) \right)^{\sum_{i=1}^{m} ([|x_i/R+1|]+[|y_i/R|]+1)} . \tag{4.6}$$

Of course, this inequality is valid only if

$$1+\frac{e_0}{\Delta}=1+\sum_{r=1}^{R}\frac{r}{2}J_r\frac{\Delta_r}{\Delta}<\Delta\,. \tag{4.7}$$

We recall that we must also have $J_1=1$, $\Delta_1=\Delta$, $J_r\geqslant 0$, $\Delta_r\geqslant\Delta$, $r\geqslant 2$. We do not believe that these conditions on the coupling constants are optimal, but some conditions are certainly needed. Note that a limitation on the magnitude of Δ_r for $r\geqslant 2$ is natural. Indeed if we take $\Delta_2\to\infty$ then an alternating spin configuration has the same energy than a totally ferromagnetic one already at the level of the classical part. On the other hand if the anisotropy parameters are too weak (for example if $\Delta_r=0$ for $r\geqslant 2$) the quantum fluctuations induced by the XX parts of the Hamiltonian might destroy the kink. Assuming that typically J_r are much smaller than 1 we see that the kink is stable as long as Δ_r is less than $O(\Delta^2)$ for Δ large enough. In this case the width of the kink will be of the order of $R+(\ln\Delta)^{-1}$.

From (4.6) one can deduce estimates similar to (2.4)–(2.5) for the magnetization profile and also (2.7) for the energy differences of ground states in different sectors.

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