Field-induced inhomogeneous ground states of antiferromagnetic ANNNI chains

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Abstract. Finite-size effects are studied in ground states of antiferromagnetic (AF) ANNNI chains in a field. It is shown that the field can induce a variety of inhomogeneous states in finite chains. They are composed of two shifted AF states with the ‘kink’ at their junction and are highly degenerate with respect to the kink position. The phase diagram ‘field–exchange ratio’ for finite chains is presented.

Keywords: phase diagrams (theory), surface effects (theory)
1. Introduction

Finite-size effects in the antiferromagnetic (AF) ground states of short-range Ising chains in a field have some definite peculiarity: the possible perturbations of AF spin order caused by free boundaries cannot be confined to some vicinity of the chain ends but are spread throughout the whole chain. This is the consequence of the AF ground states’ degeneracy in infinite chains (or rings) and, hence, of the infinite correlation length. The origin of degeneracy lies in the translational invariance of infinite systems and rings, generally there can be several ground states shifted along the chain.

Consider the simplest case of a finite chain with nearest-neighbor (NN) AF exchange in a field $H$. If it has an odd number of spins $N$, free boundaries lift the degeneracy, making the state with end spins up (along the field) the unique ground state at $0 < H < 2J$, $J$ is AF exchange. This apparently changes spin order throughout the whole chain. A yet more pronounced effect appears in the case of an even number of spins: while at $0 < H < J$ there is still the usual two-fold degeneracy, at $J < H < 2J$, $N/2$ degenerate ground states appear. Its construction consists in division of the chain into two segments with odd numbers of spins and endowing each segment with the spin structure of an odd chain, i.e. end spins up in both segments, see figure 1(a). Thus each such state has a ‘kink’ composed of two nearby spins up with the usual AF order beyond the kink. It can be readily verified that it has lower energy than perfect AF order at $J < H < 2J$. Such kink states were first found in a macroscopic model of magnetic layers with AF exchange [1]. In the ensemble of nearest-neighbor AF chains the averaging over these states gives the following linearly modulated AF order for average Ising spins [2], see figure 1(b),

$$m_n = \langle s_n \rangle = N^{-1}[1 + (-1)^n (N - 1 - 2n)], \quad n = 0, 1, \ldots, N - 1. \quad (1)$$

Here the number of spins $N$ is even. We may note that ensembles of such AF chains can be realized in dilute crystals with a (quasi) 1d magnetic structure, in solutions of magnetic polymers and in magnetic liquid crystals. The intensity of magnetic neutron diffraction on these objects in such a ‘bow-tie’ phase bears only traces of the underlying AF order exhibiting a broad peak around $k = \pi$ [2].
Ground states of AF ANNNI chains

Figure 1. (a) Kink ground states of a NN AF chain with $N = 8$ at $J < H < 2J$, dotted lines mark kink positions; (b) resulting average magnetization profile for $N = 32$ from equation (1).

Similar field-induced inhomogeneous ground states may exist in more complex Ising models on finite chains and chain-like structures (stripes, tubes) with interactions spreading over several unit cells. In such models it may not be easy to find ground states via the enumeration of possible variants and comparing their energies. Here the regular calculations within transfer-matrix (TM) formalism can be used at low temperatures. In section 2 we consider a simple AF Ising chain with NN exchange to find its ground state within this standard approach. In section 3 we describe TM formalism for the Ising chain with NN and next-nearest-neighbor (NNN) AF exchange (ANNNI model) and apply it in sections 4 and 5 to reveal the appearance of field-induced inhomogeneous ground states in this model.

2. Ground states of NN AF Ising chain

Let us see how TM formalism works for a simple (NN) AF chain and how equation (1) emerges in it. The Hamiltonian of this model

$$\mathcal{H} = J \sum_{n=0}^{N-2} s_n s_{n+1} - H \sum_{n=0}^{N-1} s_n$$

defines the TM

$$U_{s,s'} = \exp \left[ -K(1 + ss') + h(s + s')/2 \right], \quad K = J/T, \quad h = H/T, \quad (2)$$

which is used to find average local spins as

$$m_n \equiv \langle s_n \rangle = \text{Tr}(\hat{V}\hat{U}^n\hat{\sigma}_z\hat{U}^n) / \text{Tr}(\hat{V}\hat{U}^L), \quad L = N - 1, \quad n' = L - n. \quad (3)$$

Here $\hat{\sigma}_z$ is the Pauli matrix,

$$V_{s,s'} = v_s v_{s'}, \quad v_s = \exp [h(s - 1)/2]$$

for free boundaries and $\hat{V} = \hat{I}$—identity matrix for a ring.
At low $T \ll \min(H, J)$ we have
\[
\hat{U} = \begin{pmatrix} \kappa & 1 \\ 1 & 0 \end{pmatrix} = \hat{\sigma}_x + \kappa \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \kappa \equiv \exp(h - 2K).
\]

So at $H < 2J$ $\kappa \to 0$ for $T \to 0$ and the eigenvalues of $\hat{U}$ are
\[
\lambda_\mu \approx \mu + \kappa/2, \quad \mu = \pm 1.
\]

Thus $\kappa$ defines the correlation length $\xi = 1/\ln|\lambda_{+1}/\lambda_{-1}| \approx \kappa^{-1}$ which diverges at $T \to 0$. Using spectral decomposition of $\hat{U}$ [3] we find
\[
\hat{U}_L = \sum_{\mu = \pm 1} \lambda_\mu^L \hat{E}_\mu, \quad \hat{E}_\mu = (\hat{U} - \lambda_\mu \hat{1})/(\lambda_\mu - \lambda_{-\mu}) \approx \frac{1}{2} \left[ \hat{1} + \mu \left( \hat{\sigma}_x + \frac{\kappa}{2} \hat{\sigma}_z \right) \right].
\]

At sufficiently low $T$, $\xi$ becomes much larger than $L$ ($\kappa L \ll 1$) and here we have
\[
\hat{U}_L \approx |\lambda_{+1} \lambda_{-1}|^{1/2} \left[ \hat{E}_{+1} \left( 1 + \frac{\kappa L}{2} \right) + (-1)^L \left( 1 - \frac{\kappa L}{2} \right) \hat{E}_{-1} \right] \\
\approx \nu^+_L \left( \hat{1} + \frac{\kappa L}{2} \hat{\sigma}_x \right) + \nu^-_L \left( \hat{\sigma}_x + \frac{\kappa}{2} \hat{\sigma}_z + \frac{\kappa L}{2} \hat{1} \right),
\]

\[
\nu^\pm_L \equiv \left[ 1 \pm (-1)^L \right]/2.
\]

Thus for $N$ even ($L$ odd) and free boundaries
\[
\text{Tr} \hat{V} \hat{U}_L = 2e^{-h} + \frac{K}{2} \left[ 1 - e^{-2h} + (1 + e^{-2h})L \right] \approx \frac{K}{2} \left( N + 4e^{2(K-h)} \right)
\]

while
\[
\text{Tr} \left( \hat{V} \hat{U}_n \hat{\sigma}_z \hat{U}^n \right) = \frac{K}{2} \left[ 1 + e^{-2h} + (-1)^n(N - 1 - 2n)(1 - e^{-2h}) \right].
\]

So at $0 < H < 2J$ for $N$ even we have approximately at $T \ll \min(H, J)$
\[
m_n = \frac{1 + (-1)^n(N - 1 - 2n)}{N + 4e^{2(K-h)}}
\]

justifying the ground state expression (1) for $m_n$ at $J < H < 2J$. At $0 < H < 2J$ the free energy of even AF chains is (apart from an irrelevant constant)
\[
F = -\frac{T}{N} \ln \left( e^h \text{Tr} \hat{V} \hat{U}_L \right) \approx -\frac{T}{N} \ln \left( 2 + \frac{e^{2(K-h)}N}{2} \right).
\]

It describes the finite-size effects in the ensemble of even AF chains at low $T$. In particular, the entropy
\[
S = N^{-1} \left[ \ln \left( 2 + \frac{e^{2(K-h)}N}{2} \right) + \frac{2(K-h)N}{N + 4e^{2(K-h)}} \right]
\]

experiences sharp growth from rather low values at $0 < H < J$
\[
S \approx N^{-1} \ln 2 + e^{2(K-h)}(K - h)/2
\]

to greater values at $J < H < 2J$
\[
S \approx N^{-1} \ln (N/2)
\]
reflecting the appearance of $N/2$ ground states. Also the magnetization

$$M = N^{-1} \sum_{n=0}^{N-1} m_n = -\frac{\partial F}{\partial H} = \frac{2}{N + 4e^{2(K-h)}}$$

grows from nearly zero to the constant value $2/N$ when $H$ becomes greater than $J$.

3. AF ANNNI chain

We consider a finite Ising chain with first and second neighbor AF exchange having the Hamiltonian

$$H = J_1 \sum_{n=0}^{N-2} s_n s_{n+1} + J_2 \sum_{n=0}^{N-3} s_n s_{n+2} - H \sum_{n=0}^{N-1} s_n.$$

The ground states of this model on the infinite ring or chain are found in [4] as a function of exchange ratio $\alpha = J_2/J_1$ and $H > 0$. There are four types of order: ordinary AF1 with an (up, down) unit cell, AF2 with an (up, up, down, down) cell, ferrimagnetic (up, up, down) and ferromagnetic [4]. The TM of the model connects the neighboring pairs of spins

$$U_{s,s'} = \exp \left\{-K_1[\alpha (s s'-2)+s_2 s'_1 + (s_1 s_2 + s'_1 s'_2)/2] + h(s_1 + s_2 + s'_1 + s'_2)/2 \right\}$$

and the local magnetization is

$$m_n = \frac{\text{Tr} \left( \hat{V} \hat{U}^L \hat{S}_n \hat{U}^L \right)}{\text{Tr} \left( \hat{V} \hat{U}^L \right)} , \quad L = \left\lfloor \frac{N}{2} \right\rfloor - 1 , \quad l = \left\lfloor \frac{n}{2} \right\rfloor , \quad l' = L - l , \quad (4)$$

$$\left( \hat{S}_n \right)_{s,s'} = \delta_{s,s'} (s_2 \nu_n^+ + s_1 \nu_n^-) = \delta_{s,s'}[s_1 + s_2 + (-1)^{n+1}(s_1 - s_2)]/2. \quad (5)$$

Square brackets in (4) denote the integer part of a number.

The chain with free boundaries and even $N$ has

$$V_{s,s'} = v_s v_{s'} , \quad v_s = \exp \frac{1}{2} \left[ K_1(1-s_1 s_2) + h(s_1 + s_2) \right]$$

while for odd $N$

$$V_{s,s'} = v_s \tilde{v}_{s'} , \quad \tilde{v}_{s'} = v_{s'} \sum_{s=\pm1} \exp s[-K_1(s'_1 + \alpha s'_2) + h]. \quad (7)$$

Adopting the following convention for the relationship between row (column) numbers and configurations $(s_1, s_2)$

$$1 - (++), \quad 2 - (--) , \quad 3 - (+-), \quad 4 - (-+)$$

we can represent $\hat{U}$ at $T \ll \min(J_1, J_2, H)$ as

$$\hat{U} = \begin{pmatrix} c^2 & 1 & c & a \\ 1 & 0 & b & 0 \\ a & 0 & ab & 1 \\ c & b & 1 & ab \end{pmatrix}$$

$$a = \exp(h + K_1 - 2K_2), \quad b = \exp(-h + K_1 - 2K_2), \quad c = \exp(h - K_1 - 2K_2).$$
Apparently, at the low $T$ considered

$$a \gg \max(b, c), \quad bc \ll 1$$

so the approximate equation for eigenvalues $\lambda$ of $\hat{U}$ reads

$$(\lambda^2 - ab\lambda - 1)^2 = \lambda(c\lambda + a)^2. \quad (10)$$

The solutions to equation (10) have four different types of behavior when $T \to 0$ depending on the relations between $a, b$ and $c$. For the eigenvalues with largest moduli we have

$$b^{-3} \ll a \quad (h_1 < 2 - 4\alpha), \quad \lambda_\mu \approx ab\left(1 + \frac{\mu}{\sqrt{ab^3}}\right), \quad \mu = \pm 1 \quad (11)$$

$$a \to 0 \quad (h_1 < 2\alpha - 1), \quad \lambda_{\mu,\tau} \approx \mu(1 + \tau\sqrt{ab}/2), \quad \mu, \tau = \pm 1 \quad (12)$$

$$\max(c^3, 1) \ll a \ll b^{-3} \quad (3\left|\frac{1}{2} - \alpha\right| + \frac{1}{2} - \alpha < h_1 < 2 + 2\alpha), \quad \lambda_\mu \approx a^{2/3}e^{i2\pi k/3}, \quad \mu, \tau = \pm 1, \quad k = 0, 1, 2. \quad (13)$$

$$a \ll c^3 \quad (h_1 > 2 + 2\alpha), \quad \lambda \approx c^2. \quad (14)$$

Here $h_1 = H/J_1$.

So in four regions of the $h_1 - \alpha$ plane $\hat{U}$ has different limiting forms at $T \to 0$, which we can obtain leaving in the original TM (8) only those matrix elements which give the eigenvalues listed above, namely,

$$h_1 < 2 - 4\alpha, \quad \hat{U} \approx \begin{pmatrix} 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 \\ a & 0 & ab & 0 \\ 0 & 0 & 1 & ab \end{pmatrix} \quad (15)$$

$$h_1 < 2\alpha - 1, \quad \hat{U} \approx \begin{pmatrix} 0 & 1 & 0 & a \\ 1 & 0 & 0 & 0 \\ a & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (16)$$

$$3\left|\frac{1}{2} - \alpha\right| + \frac{1}{2} - \alpha < h_1 < 2 + 2\alpha, \quad \hat{U} \approx \begin{pmatrix} 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (17)$$

$$h_1 > 2 + 2\alpha, \quad \hat{U} \approx \begin{pmatrix} c^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (18)$$

These different limiting forms of $\hat{U}$ make it evident that we have different ground states in the corresponding regions of the $h_1 - \alpha$ plane. Thus at $h_1 < 2\alpha - 1$ and $T \to 0$, $\hat{U}$ transfers $(++)$ into $(- -)$ then to $(++)$ and so on, while $(- +)$ is transferred to $(- +)$ then
Figure 2. Ground state phase diagram for the finite AF ANNNI chain in a field. Solid lines are phase boundaries for the infinite chains or rings found in [4]. Dotted lines show the boundaries of the inhomogeneous (modulated) phases of finite chains.

to $(+-)$ etc. So here we have $(++--)$ phase $AF2$ in the infinite chain. At $h_1 < 2 - 4\alpha$ the sequence is $(+-) \rightarrow (++) \rightarrow (++) \cdots$ or $(-+) \rightarrow (++) \rightarrow (++)$ etc and it is the ordinary $AF1$ phase.

At $3|\frac{1}{2} - \alpha| + \frac{1}{2} - \alpha < h_1 < 2 + 2\alpha$ the spin structure has period three as matrix elements of $\hat{U}$ generate the sequence $(-+) \rightarrow (+-+) \rightarrow (++)$, that is the ferrimagnetic ground state $(-+ +)$. At $h_1 > 2 + 2\alpha$ only the $(++)$ state survives, so this is the region of ferromagnetic ground state. This phase diagram found in [4] is shown in figure 2.

In the ferrimagnetic phase the finite-size effects are rather trivial, consisting in (partial) lifting the triple degeneracy of the ground states. Nontrivial ground states in finite chains can appear in two AF phases of the present model, so we further consider just these phases.

4. Ground states in the AF1 phase

Here it is convenient to use the normalized TM $\hat{W} = (ab)^{-1} \hat{U}$ in which we omit the second row and second column with zeros, cf (15),

$$\hat{W} = \begin{pmatrix} 0 & 0 & b^{-1} \\ b^{-1} & 1 & 0 \\ 0 & \varepsilon^2 b^2 & 1 \end{pmatrix}, \quad \varepsilon = \frac{1}{\sqrt{ab^3}}.$$
At $T \to 0$, $\varepsilon$ goes to zero and for $\varepsilon L \ll 1$ we have from the spectral decomposition

$$Z_L = \text{Tr} \left( \hat{V} \hat{W}^L \right) \approx \text{Tr} \left( \hat{V} \hat{G}_+ \right) + L \varepsilon \text{Tr} (\hat{V} \hat{G}_-), \quad \hat{G}_\pm = \hat{E}_+ \pm \hat{E}_-.$$  

Here $\hat{E}_+$ and $\hat{E}_-$ are the idempotent components related to the eigenvalues $1 + \varepsilon$ and $1 - \varepsilon$ correspondingly. Apparently, $2 \varepsilon$ is inverse correlation length. In the lowest order in $\varepsilon$ we have [3]

$$\hat{G}_+ = \begin{pmatrix} 0 & 0 & b^{-1} \\ b^{-1} & 1 & -b^{-2} \\ 0 & 0 & 1 \end{pmatrix}, \quad \varepsilon \hat{G}_- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & b^{-2} \\ 0 & 0 & 0 \end{pmatrix}$$

so for $N$ even

$$Z_L = (2b^2 - 1 + L + 2e^{-2K_2})e^{2K_1}b^{-2} \approx (2b^2 - 1 + L)e^{2K_1}b^{-2}.$$  

Similarly, we get

$$Z_Lm_n \approx \text{Tr} \left( \hat{V} \hat{G}_+ \hat{S}_n \hat{G}_+ \right) + \varepsilon l \text{Tr} \left( \hat{V} \hat{G}_+ \hat{S}_n \hat{G}_- \right) + \varepsilon l' \text{Tr} (\hat{V} \hat{G}_- \hat{S}_n \hat{G}_+).$$

Here $\hat{S}_n$ differs from that in equation (5) by the absence of the second row and the second column.  

For $N$ even ($L$ odd) and $L \geq 3$, $\varepsilon l, l' \geq 1$, $K_2 > 0$ we have

$$m_n = \frac{1 + (-1)^n (l' - l)}{2b^2 - 1 + L}. \quad (20)$$

Thus for $b \to \infty$ ($h_1 < 1 - 2\alpha$) $m_n$ is zero as in the ordinary doubly degenerate AF state but when $b \to 0$ ($1 - 2\alpha < h_1 < 2 - 4\alpha$, F1 region in figure 2) we have a linearly modulated state. Returning to the site numbers in (20), cf equation (4), we get

$$m_n = \frac{1 + (-1)^n (N - 1 - 2n)}{N - 4}, \quad N \geq 6, \quad 2 \leq n \leq N - 3.$$  

The Fourier transform of this $m_n$,

$$\hat{m}_k = \sum_{n=2}^{N-3} e^{ikn} m_n = \frac{e^{i3k/2}}{\cos (k/2)} + \delta(k,0), \quad k = \frac{2\pi r}{N - 4}, \quad r = 0, 1, \ldots, N - 5,$$

depends on $N$ through $k$ values only, so it has a definite thermodynamic limit and can be considered as an order parameter for this inhomogeneous phase. Note that the same $\hat{m}_k$ has the ‘bow-tie’ phase of the NN AF chain (1) for $k = 2\pi r/N$, cf [2]. It defines the intensity of neutron diffraction $I_k \sim |\hat{m}_k|^2$ for a wavevector $k$ expressed in units of the inverse cell parameter.

The calculations for $l = 0$ and $L$ result in $m_0 = m_{N-1} = 1, m_1 = m_{N-2} = -1$ for $K_2 > 0$ and we have the profile shown in figure 3 for $N = 36$. Evidently, here we have $(N - 4)/2$ degenerate ground states formed from the inner $N - 4$ spins by a process similar to that in simple NN AF chain. The couples of the boundary spins stay fixed at the above values as NNN AF exchange forbids two parallel spins at the edges. For $N$ odd $m_n = (-1)^n$ in all AF1 regions.
Figure 3. Magnetization of the linearly modulated state of an ANNNI chain with $N = 36$ at $1 - 2\alpha < h_1 < 2 - 4\alpha$ (F1 region in figure 2).

5. Ground states in the AF2 phase

According to (16) $\hat{U}$ in this phase ($h_1 < 2\alpha - 1$) can be represented as

$$\hat{U} = \hat{E} + a\hat{G}, \quad \hat{E} = \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}, \quad \hat{G} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$ (21)

As $a \to 0$ for $T \to 0$, we can evaluate the powers of $\hat{U}$ without resorting to spectral decomposition. Thus at $ak \ll 1$

$$\hat{U}^{2k} \approx \hat{I} + ka\hat{D}, \quad \hat{D} = \{\hat{E}, \hat{G}\} = \begin{pmatrix} 0 & \hat{I} \\ \sigma_x & 0 \end{pmatrix}. \quad (21)$$

From this equation it follows that chains with $L$ even do not have inhomogeneous ground states, as in such a case we can neglect the contributions of order $a$ in $m_n$ calculations. However, for $L$ odd (i.e. for $N = 4M$ or $4M + 1$, $M$ is arbitrary positive integer) we have

$$Z_L \approx \text{Tr} \hat{V}\hat{E} + \frac{a}{2} \text{Tr} \hat{V} \left[(L + 1)\hat{G} + (L - 1)\hat{E}\hat{G}\hat{E}\right] \quad (22)$$

and $\text{Tr} \hat{V}\hat{E} = 0$ for $N = 4M$ while for $N = 4M + 1$, $\text{Tr} \hat{V}\hat{E}$ may go to zero as $T \to 0$, see (6) and (7).

Thus further we consider $L$ odd. In such a case

$$Z_L m_n \approx \text{Tr} \hat{V} \left[(-1)^l \left(\hat{I} + a \left[\frac{l}{2}\right] \hat{D}\right)\hat{E}\hat{S}_n \left(\hat{I} + a \left[\frac{l}{2}\right] \hat{D}\right) + a\nu_l^+ \hat{G}\hat{S}_n + a\nu_l^- \hat{S}_n \hat{G}\right]. \quad (23)$$

For $N = 4M$ we get from these equations

$$m_n = \frac{(-1)^{l+n} (L + 1) + 1 - (-1)^l (L - 2l)}{2 (L + 1) + 4e^{2K_1(a-h_1)}}. \quad (24)$$

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Thus at $\alpha < h_1 < 2\alpha - 1$ (F2 region in figure 2) we have

$$m_n = N^{-1}\{1 + (-1)^l[\nu_n^+ (N - 1) - n]\}. \tag{25}$$

Figure 4 shows $m_n$ (25) for $N = 64$. One can see that this is the result of averaging over $N/4 = M$ degenerate ground states which are formed from the AF2 state via flipping an odd number of successive spins in an even or odd sublattice. They are shown in figures 5(b)–(e) for $N = 8$.

The Fourier transform of (25) is

$$\tilde{m}_k = \sum_{n=0}^{N-1} e^{ikn} m_n = \frac{e^{-ik/2} \cos (k/2)}{\cos (k)}, \quad k = \frac{2\pi r}{N} = \frac{\pi r}{2M}, \quad r = 0, 1, \ldots, N - 1.$$

Its singularities at $k = \pi/2$ and $3\pi/2$ reflect the underlying nearly perfect period-four order of the kink states.

According to (24) at $h_1 < \min (2\alpha - 1, \alpha)$, $m_n \to 0$ when $T \to 0$, which means that chain is in doubly degenerate $(++--)$ AF2 ground states. For $N = 8$ one of these states is shown in figure 5(a), its counterpart has all spins reversed.

For $N = 4M + 1$ and $|1 - \alpha| < h_1 < \min (2\alpha - 1, \alpha + 1)$ we get from (7), (22) and (23)

$$m_n = \frac{2\nu_n^- [1 + (-1)^l (l'/2) - (l/2)] + \nu_n^+ (-1)^l (L + 1) + 4\nu_n^+ e^{2K_1(1-h_1)} \nu_n^- + e^{2K_1(\alpha-h_1)} (-1)^l}{(L + 1) (1 + 2e^{2K_1(1-h_1)}) + 4e^{2K_1(\alpha-h_1)}}. \tag{26}$$

Calculating $m_n$ for the other regions of the $h_1-\alpha$ plane where the AF2 phase exists we finally get for $N = 4M + 1$:

$\alpha < h_1 < 2\alpha - 1$, F2 region in figure 2,

$$m_n = \nu_n^+ (-1)^l + \frac{2\nu_n^-}{L + 1} \left\{1 + (-1)^l \left(\left\lfloor\frac{l'}{2}\right\rfloor - \left\lfloor\frac{l}{2}\right\rfloor\right)\right\}; \tag{26}$$

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Figure 5. Procedure of ground state formation at $\alpha < h_1 < 2\alpha - 1$ for $N = 8$. (a) The parent state. The ground states are obtained via flipping in it one spin ((b), (c)) or three spins ((d), (e)). Flipped spins are marked by the dots.

$\alpha < 1, \quad h_1 < 2\alpha - 1, \quad$ F3 region in figure 2,

$$m_n = \frac{2\nu_n^+\nu_n^-}{L+1} = \frac{1}{M} \sum_{r=1}^{M} \delta(n, 4r - 2);$$  \hspace{1cm} (27)

max$(1, h_1) < \alpha, \quad$ the rest of the AF2 phase in figure 2, \quad $m_n = \nu_n^+(-1)^l$. \hspace{1cm} (28)

The profile (26) for $\alpha < h_1 < 2\alpha - 1$ (F2 region) is shown in figure 6 for $N = 65$. We see that an even sublattice has AF order with up spins at the edges but the odd sublattice is formed via averaging over $(N - 1)/4 = M$ kink states. In contrast, at max$(1, h_1) < \alpha$ the AF order in the odd sublattice stays intact up to a global reversal so spins in it have zero average value, see equation (28).

The Fourier transform of (26) is

$$\tilde{m}_k = \sum_{n=0}^{N-1} e^{i kn} m_n = 1 + 1/\cos(k), \quad k = 2\pi r/N = \pi r/2M, \quad r = 0, 1, \ldots, N - 1.$$  

It also shows independence of its form on $N$ and singularities at $k = \pi/2$ and $3\pi/2$.

The profile (27) at $\alpha < 1, h_1 < 2\alpha - 1$ (F3 region) is the result of the averaging over $(N - 1)/2 = 2M$ ground states. The procedure of their formation is shown in figure 7 for $N = 9$. It makes the number of satisfied NN bonds larger at the expense of the NNN bonds. This provides the energy gain as $\alpha < 1$. Note that this phase exists even at $H = 0,$

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Figure 6. Magnetization profile at $\alpha < h_1 < 2\alpha - 1$ (F2 region) for $N = 65$.

Figure 7. Procedure of ground state formation at $\alpha < 1, h_1 < 2\alpha - 1$ (F3 region) for $N = 9$. (a) Two parent states, below there are ground states obtained from them via flipping of one spin (b) and three spins (c). Flipped spins are marked by the dots.

purely due to finite-size effects. The zero-field kink states similar to those in figures 7(b) and (c) were first found in the layered ANNI model (which is equivalent to the present one at $T = H = 0$) for $1/2 < \alpha < 1$ [5].

6. Discussion and conclusions

The above results are summarized on the phase diagram in figure 2. The F1 phase exists in even chains and is quite similar to that in an ordinary NN AF chain. In the F2 region the chains with $N = 4M$ and $4M + 1$ have modulated phases. The F3 phase of the $N = 4M + 1$
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The mechanism of appearance of field-induced inhomogeneous ground states in finite AF chains lies in the degeneracy of their (infinite) AF ground states in a field. In the above examples the kink states are formed via the conjunction of two shifted AF states, which results in the appearance of a nonzero magnetic moment along the field. The energy gain from this may overcome the energy needed for kink formation at large enough $H$. One may be interested if this mechanism can work in higher dimensions, non-Ising systems or quantum models having degenerate ground states. At present there is no definite answer to this, yet it seems worthwhile to study the finite-size effects in such systems.

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