

SMEARED SPIN-FLOP TRANSITION IN RANDOM ANTIFERROMAGNETIC ISING CHAIN

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At $T = 0$ and a sufficiently large field, the nearest-neighbor antiferromagnetic Ising chain undergoes a first-order spin-flop transition into the ferromagnetic phase. We consider its smearing under the random-bond disorder such that all independent random bonds are antiferromagnetic (AF). It is shown that the ground-state thermodynamics of this random AF chain can be described exactly for an arbitrary distribution $P(J)$ of AF bonds. Moreover, the site magnetizations of finite chains can be found analytically in this model. We consider a continuous $P(J)$ that is zero above some $-J_1$ and behaves near it as $(-J_1 - J)^\lambda$, $\lambda > -1$. In this case, the ferromagnetic phase emerges continuously in a field $H > H_c = 2J_1$. At $0 > \lambda > -1$, it has the usual second-order anomalies near H_c with the critical indices obeying the scaling relation and depending on λ . At $\lambda > 0$, higher-order transitions occur (third, fourth, etc.), marked by a divergence of the corresponding nonlinear susceptibilities. In the chains with an even number of spins, the intermediate “bow-tie” phase with linearly modulated AF order exists between the AF and ferromagnetic phases at $J_1 < H < H_c$. Its origin can be traced to the infinite correlation length of the degenerate AF phase from which it emerges. This implies the existence of similar inhomogeneous phases with size- and form-dependent order in a number of other systems with infinite correlation length. The possibility to observe the signs of the “bow-tie” phase in low- T neutron diffraction experiments is discussed.

The influence of quenched disorder on first-order phase transitions was first described phenomenologically by Imry and Wortis [1], who have shown that “random-temperature” disorder can diminish or even eliminate jumps of the order parameter and other variables at the transition point. Further studies have revealed a relation of such smeared transitions to the random-field Ising model [2]; it was shown that the smeared transitions can become second-order ones [3–5] and can transform into a phase coexistence region instead of a sharp transition [6].

Yet our understanding of these smearing phenomena is far from exhaustive. We still have no rigorous criteria to decide which of the known outcomes of the smearing — softened jumps, phase coexistence region, or a second-order transition — will be realized and treat this point only qualitatively [7]. For the resulting second-order transition, it is not known definitely whether the critical indices are universal or depend on disorder parameters [3–5]. There is also the unexplored possibility that the phase coexistence region, lacking first- and second-order transition anomalies, contains

higher-order anomalies at some point, appropriate for the higher-order transitions. And we know nothing about the influence of disorder on the athermal and ground-state transitions such as spin-flop transitions in antiferromagnets (AF). At these first-order transitions, some spin sublattice upturns to become (partially) parallel to the external magnetic field at some critical field strength [8]. The AF Ising spin chain provides the simplest example of such a transition from the AF phase to the ferromagnetic one at $T = 0$ and the field $H = 2J$, where J is the absolute value of the AF exchange. In the presence of random J variations, some segments of the chain become ferromagnetic (F) at lower or higher H values, and we can therefore expect some smearing of this first-order transition.

Fortunately, at $T = 0$, the magnetic properties of an AF random-bond chain can be described exactly for an arbitrary distribution of exchanges and even for an arbitrary chain length. Hence, we have a unique possibility to study smeared spin-flop transition in finite samples analytically. Here, we present the results for a continuous distribution of exchanges that makes the first-order jumps completely smeared in the F phase.

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1. DISTRIBUTION FUNCTIONS FOR EFFECTIVE RANDOM FIELDS

We consider the short-range random-bond Ising chain with the Hamiltonian

$$\mathcal{H} = - \sum_{n=0}^{N-1} J_n S_n S_{n+1} - H \sum_{n=0}^{N-1} S_n, \quad (1)$$

where J_n are random nearest-neighbor exchanges with the identical distribution function $P(J)$ such that $P(J) = 0$ for $J \geq 0$.

To date, there are numerous studies of random bond Ising chains both at $T = 0$ and at finite T [9–17]. Their common feature is the existence of a definite thermodynamic limit for the main function describing their properties, that is, for the distribution of effective random fields

$$W_n(F) = \langle \delta(F - F_n) \rangle_J, \quad F_n \equiv \frac{1}{2} \ln \frac{Z_n(+1)}{Z_n(-1)},$$

where $Z_n(S)$ is the partial partition function of the length- n chain (assuming the unit spacing between spins), summed over all spins except the end one S , and the angular brackets denote averaging over the bond distribution function $P(J)$. Recursion relations for $Z_n(S)$,

$$Z_{n+1}(S) = \sum_{S'=\pm 1} \exp \beta S'(JS+H) Z_n(S'), \quad \beta \equiv T^{-1},$$

generate the corresponding relations for F_n ,

$$F_{n+1} = T \operatorname{th}^{-1} [\operatorname{th} \beta J \operatorname{th} \beta (F_n + H)] \equiv U(F_n, J), \quad (2)$$

and for $W_n(F)$,

$$W_{n+1}(F) = \int \langle \delta(F - U(F', J)) \rangle_J W_n(F') dF'. \quad (3)$$

With the initial conditions $F_0 = 0$ and, correspondingly, $W_0(F) = \delta(F)$, we can find all $W_n(F)$ and all average thermodynamic variables of our random chain. Thus, for the average magnetization of the site situated at a distance n from one end of the chain with N spins and at the distance $n' = N - n - 1$ from the other end, we have

$$m_{n,N} = \left\langle \frac{\sum_{S=\pm 1} Z_n(S) S e^{\beta HS} Z_{n'}(S)}{\sum_{S=\pm 1} Z_n(S) Z_{n'}(S)} \right\rangle_J = \iint W_n(F) W_{n'}(F') \operatorname{th} \beta (F + F' + H) dF dF'. \quad (4)$$

Usually, it is a tedious task to find all $W_n(F)$ even at $T = 0$, and therefore most of the previous studies rely heavily on the existence of the thermodynamic limit $W_\infty(F)$. In the random AF model with $P(J) = 0$ for $J \geq 0$, the ground-state $W_n(F)$ can be easily found for each n , as we show below. This not only allows studying the finite-size effects analytically but also makes the description of ground-state properties of the chains with an even number of sites N feasible. The “even chains” preserve the two-fold degeneracy of the ground state in sufficiently small H , which results in the infinite correlation length at $T = 0$. Therefore, the boundary effects can spread throughout the whole even chain, which requires considering finite samples. We note that the thermodynamic limit $W_\infty(F)$ can formally be obtained for odd and even n separately, but the results are sensible only for the interior of odd chains, when the correlation length is finite at all H .

At $T = 0$, it is more convenient to consider recursion relations for the integrated probability distributions

$$C_n(F) = \int_{-\infty}^F W_n(F') dF'.$$

Evidently,

$$C_n(-\infty) = 0, \quad C_n(\infty) = 1. \quad (5)$$

Integrating (3), we obtain

$$C_{n+1}(F) = \int \langle \vartheta[F - U(F', J)] \rangle_J \partial_{F'} C_n(F') dF' = \langle \vartheta[F - U(\infty, J)] \rangle_J + \int \langle \delta[F - U(F', J)] \partial_{F'} U(F', J) \rangle_J C_n(F') dF', \quad (6)$$

where $\vartheta(F)$ is the Heaviside step function, $\partial_{F'} \equiv \partial / \partial F'$, and $U(\infty, J) = J$ (cf. (2)). Because $|U(F', J)| \leq |J|$, the average in (6) is confined to the region $J^2 \leq F^2$. In this region, the equation $F = U(F', J)$ has the unique solution

$$F' = -H + \operatorname{th}^{-1} \left(\frac{\operatorname{th} \beta F}{\operatorname{th} \beta J} \right) \equiv V(F, J). \quad (7)$$

Hence, we can represent the delta-function in (6) as

$$\delta[F - U(F', J)] = \vartheta(F^2 - J^2) |\partial_{F'} U(F', J)|^{-1} \times \delta[V(F, J) - F']. \quad (8)$$

Because $\operatorname{sign}[\partial_{F'} U(F', J)] = \operatorname{sign} J$, it follows from Eqs. (6) and (8) that

$$C_{n+1}(F) = Q(F) + \int \langle \operatorname{sign} J \vartheta(F^2 - J^2) C_n[V(F, J)] \rangle_J, \quad (9)$$

$$Q(F) \equiv \langle \vartheta(F - J) \rangle_J = \int_{-\infty}^F P(J) dJ. \quad (10)$$

At $T = 0$, Eq. (9) is greatly simplified because we can then set $V(F, J) = -H + F \text{ sign } J$ (cf. (7)). Hence, at $T = 0$, Eq. (9) becomes

$$C_{n+1}(F) = Q(F) + [1 - Q(|F|)] C_n(F - H) + Q(-|F|) C_n(-F - H). \quad (11)$$

We thus have obtained functional equations for the ground-state C_n , which in many cases can be easily solved for $n \rightarrow \infty$ at least. In particular, for discrete bond distributions when $P(J)$ is a sum of delta-functions, Q is stepwise constant and the same holds for C_n . Then Eqs. (11) become algebraic equations for the jumps of the C_n at some points F_i whose position is dictated by Eq. (11) and by the initial condition $C_0(F) = \vartheta(F)$. In this way, one can easily reproduce many known results for the ground state of various random chains obtained by other methods [9–17]. But we here deal with an even simpler model that has not enjoyed attention previously.

2. GROUND-STATE FIELD DISTRIBUTIONS FOR RANDOM ANTIFERROMAGNETIC CHAINS

If $P(J) = 0$ for $J \geq 0$, then $Q(|F|) = 1$ and Eq. (11) becomes

$$C_{n+1}(F) = Q(F) + Q(-|F|) C_n(-F - H). \quad (12)$$

Changing the variables as $F \rightarrow -F - H$, we obtain another equation,

$$C_{n+1}(-F - H) = Q(-F - H) + Q(-|F + H|) C_n(F). \quad (13)$$

We thus have two equations for two functions, $C_n(F)$ and $\tilde{C}_n(F) = C_n(-F - H)$. In matrix form, they can be written as

$$\mathbf{C}_{n+1} = \hat{R} \mathbf{C}_n + \mathbf{Q}, \quad (14)$$

where

$$\mathbf{C}_n = \begin{pmatrix} C_n(F) \\ \tilde{C}_n(F) \end{pmatrix}, \quad \mathbf{Q}_n = \begin{pmatrix} Q_n(F) \\ \tilde{Q}_n(F) \end{pmatrix}, \quad (15)$$

$$\hat{R} = \begin{pmatrix} 0 & -R(F) \\ -\tilde{R}(F) & 0 \end{pmatrix}, \quad R(F) \equiv Q(-|F|)$$

and the tilde denotes the substitution $F \rightarrow -F - H$. We note that this operation transforms the pair of functions $A(F)$ and $\tilde{A}(F)$ one into another, and this is the

reason for the exact solvability of Eq. (12). Also using the notation $\tilde{A}(F)$ for this substitution we can drop the function arguments in (14) because they are the same (F) for all functions.

Initial conditions for Eq. (14) are

$$\mathbf{C}_0 = \begin{pmatrix} \vartheta(F) \\ \vartheta(-F - H) \end{pmatrix} \quad (16)$$

and the solution for $n \geq 1$ is

$$\mathbf{C}_n = \hat{R}^n \mathbf{C}_0 + \sum_{k=0}^{n-1} \hat{R}^k \mathbf{Q}. \quad (17)$$

The eigenvalues of \hat{R} are

$$r_{\pm} = \pm \sqrt{R\tilde{R}} \equiv \pm \rho \quad (18)$$

and hence in the regions of F where $\rho < 1$, Eq. (17) can be represented as

$$\mathbf{C}_n = \mathbf{C}_{\infty} + \hat{R}^n (\mathbf{C}_0 - \mathbf{C}_{\infty}),$$

$$\mathbf{C}_{\infty} \equiv (\hat{I} - \hat{R})^{-1} \mathbf{Q} = (1 - \rho^2)^{-1} (\hat{I} + \hat{R}) \mathbf{Q}. \quad (19)$$

It is easy to verify that

$$\hat{R}^n = \nu_n^+ \rho^n \hat{I} + \nu_n^- \rho^{n-1} \hat{R}, \quad \nu_n^{\pm} = \frac{1}{2} [1 \pm (-1)^n]. \quad (20)$$

Therefore, \mathbf{C}_n has definite thermodynamic limit \mathbf{C}_{∞} in these regions. But in some regions of F , ρ can be equal to 1 and we then have

$$\hat{R} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \equiv -\hat{\sigma}_x,$$

$$\mathbf{C}_n = \left(\nu_n^+ \hat{I} - \nu_n^- \hat{\sigma}_x \right) \mathbf{C}_0 + \frac{1}{2} \left[n \left(\hat{I} - \hat{\sigma}_x \right) + \nu_n^- \left(I + \hat{\sigma}_x \right) \right] \mathbf{Q}. \quad (21)$$

In what follows, we consider the model with a smooth $P(J)$ such that $P(J) = 0$ for $J > -J_1$. The behavior of Q , \tilde{Q} , R , and \tilde{R} in this case is shown schematically in Fig. 1 for three ranges of H . When $H < 2J_1$ there is the region $-J_1 < F < J_1 - H$ in which $\rho = 1$, while for $2J_1 < H$, we have $\rho < 1$ for all F . This and the form of \mathbf{C}_0 in (16) predetermine the differences of \mathbf{C}_n in three regions of H values.

From Eqs. (16) and (19)–(21), we obtain 1) for $H < J_1$,

$$C_n(F) = \nu_n^- \vartheta(F + H) + \nu_n^+ \vartheta(F),$$

$$W_n(F) = \nu_n^- \delta(F + H) + \nu_n^+ \delta(F), \quad (22)$$

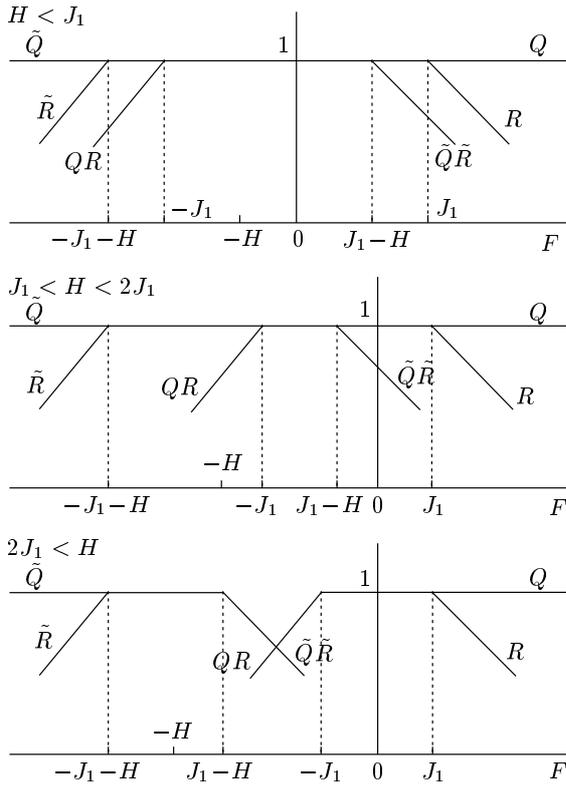


Fig. 1. Schematic behavior of Q , \tilde{Q} , R , and \tilde{R} for a random AF with $P(J) = 0$ for $J > -J_1$

2) for $J_1 < H < 2J_1$,

$$C_n(F) = \nu_n^- \vartheta(F + H) \times [\rho^{n-1}(F)R(F)\vartheta(-J_1 - F) + \vartheta(J_1 + F)] + \nu_n^+ \vartheta(F + H - J_1) [1 - \vartheta(-F)\rho^n(F)], \quad (23)$$

$$W_n(F) = \nu_n^- \vartheta(F + H) \times \partial_F [\rho^{n-1}(F)R(F)\vartheta(-J_1 - F)] - \nu_n^+ \vartheta(F + H - J_1) \partial_F [\vartheta(-F)\rho^n(F)], \quad (24)$$

3) for $2J_1 < H$,

$$C_n(F) = \nu_n^- \{ \vartheta(F + H)\rho^{n+1}(F) + C_\infty(F) [1 - \rho^{n+1}(F)] \} + \nu_n^+ \{ C_\infty(F) [1 - \vartheta(-F)\rho^n(F)] \}, \quad (25)$$

$$W_n(F) = \nu_n^- \{ \partial_F [\vartheta(F + H)\rho^{n+1}(F)] + \partial_F [C_\infty(F) (1 - \rho^{n+1}(F))] \} + \nu_n^+ \{ W_\infty(F) [1 - \rho^n(F)] - C_\infty(F) \partial_F [\vartheta(-F)\rho^n(F)] \}. \quad (26)$$

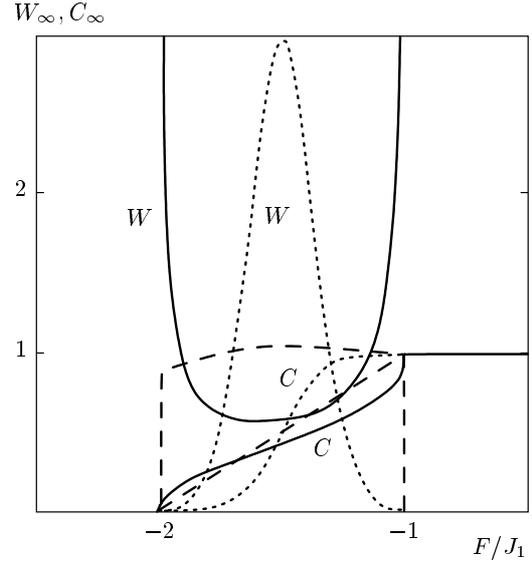


Fig. 2. $C_\infty(F)$ and $W_\infty(F)$ at $2J_1 < H$ for bond distribution (29) with $\lambda = 2$ (dotted lines), $\lambda = 0$ (dashed lines), and $\lambda = -0.5$ (solid lines); $J_0 = 10J_1$ and $H = 3J_1$

In (25) and (26), $C_\infty(F)$ and $W_\infty(F) = \partial_F C_\infty(F)$ are the values of $C_n(F)$ and $W_n(F)$ in the thermodynamic limit $n \rightarrow \infty$:

$$C_\infty(F) = \vartheta(F + J_1) + \vartheta(-F - J_1) \frac{Q(1 - \tilde{Q})}{1 - Q\tilde{Q}}, \quad (27)$$

$$W_\infty(F) = \frac{P(1 - \tilde{Q}) + \tilde{P}Q(1 - Q)}{(1 - Q\tilde{Q})^2} \times \vartheta(F + J_1 - H)\vartheta(-J_1 - F), \quad (28)$$

where $P = P(F)$ and $\tilde{P} = P(-F - H)$. In Fig. 2, $C_\infty(F)$ and $W_\infty(F)$ are shown at $2J_1 < H$ for the bond distribution

$$P(J) = \vartheta(J + J_0)\vartheta(-J_1 - J)(\lambda + 1) \frac{(-J_1 - J)^\lambda}{(J_0 - J_1)^{\lambda+1}} \quad (29)$$

with $J_0 = 10J_1$ and $\lambda > -1$.

Equations (22)–(28) suffice for giving the full description of magnetic properties of finite random AF chains at $T = 0$.

3. MAGNETIZATIONS AND PHASE TRANSITIONS AT $T = 0$. ODD N

The average ground-state magnetizations can be obtained by taking the $T = 0$ limit of Eq. (4):

$$m_{n,N} = \iint W_n(F)W_{n'}(F') \times \text{sign}(F + F' + H) dF dF', \quad \text{sign}(0) = 0. \quad (30)$$

This relation can be represented in a more convenient form as

$$m_{n,N} = 1 - 2 \int \tilde{C}_n W_{n'} dF. \quad (31)$$

In (31), expressions (22)–(28) should be used with ϑ -functions defined at zero as $\vartheta(0) = 1/2$ to conform with $\text{sign}(0) = 0$ in (30) and the relation $\text{sign}(x) = \vartheta(x) - \vartheta(-x)$ used in the derivation of (31).

The magnetization for odd and even N can differ drastically. The formal reason for this is that the parity of the distances of a given site from the ends of a chain (n and $n' = N - n - 1$) are the same in the former case and different in the latter.

For odd N , it follows from (22)–(31) that for $H < 2J_1$,

$$m_{n,N} = (-1)^n,$$

and for $H > 2J_1$,

$$m_{n,N} = m_\infty + \int W_\infty \left\{ (\rho^n + \rho^{n'}) \times \left[\tilde{C}_\infty(1 + \rho) - \rho \right] + \rho^{N-1} \left[\rho^2 - \tilde{C}_\infty(1 + \rho^2) \right] \right\} dF + (-1)^n \int W_\infty \left\{ (\rho^n + \rho^{n'}) \left[\tilde{C}_\infty(1 - \rho) + \rho \right] + \rho^{N-1} \left[\tilde{C}_\infty(\rho^2 - 1) - \rho^2 \right] \right\} dF, \quad (32)$$

$$m_\infty = 1 - 2 \int W_\infty \tilde{C}_\infty dF. \quad (33)$$

Integration in (32) and (33) is limited to the interval $J_1 - H < F < -J_1$ in which $W_\infty \neq 0$ (cf. (28)). In this interval, $\rho = \sqrt{Q\tilde{Q}} < 1$, and hence in the thermodynamic limit ($n, n', N \rightarrow \infty$), $m_{n,N} = m_\infty$ and we have phase transition at $H = H_c \equiv 2J_1$ from the AF phase to the F one. From the F-side, this transition is continuous because m_∞ tends to zero as $H \rightarrow H_c + 0$. Indeed, if $P(J)$ vanishes or stays finite at $-J_1$, then $W_\infty \rightarrow \delta(F + H/2)$ (see Fig. 2) and we have

$$m_\infty \approx 1 - 2C_\infty(-H/2) = \frac{1 - Q(-H/2)}{1 + Q(-H/2)} \approx \frac{1}{2} \int_{-H/2}^{-J_1} P(J) dJ.$$

When $P(J)$ diverges at $-J_1$, we can represent m_∞ as

$$m_\infty = 2 \int_{J_1-H}^{-J_1} \frac{Q - \tilde{Q}}{(1 - Q\tilde{Q})^3} (1 - \tilde{Q})^2 P dF \approx \int_{J_1-H}^{-J_1} P dF.$$

With the power-law dependence of $P(J)$ near $-J_1$ as in Eq. (29), we have

$$m_\infty \sim (H - H_c)^{\lambda+1}, \quad \chi \equiv \frac{\partial m_\infty}{\partial H} \sim (H - H_c)^\lambda \quad (34)$$

in both cases. Hence, for $-1 < \lambda < 0$, there is a usual second-order transition with the critical indices

$$\beta = \lambda + 1, \quad \gamma = -\lambda.$$

It follows from the relation $\chi = -\partial^2 E / \partial H^2$ (where E is the average energy) that the index α is equal to γ , and hence the usual scaling relation

$$\alpha + 2\beta + \gamma = 2$$

holds. We can formally obtain the indices ν and η as

$$\nu = (2 - \alpha)/d = 2 + \lambda,$$

$$\eta = 2 - \frac{\gamma}{\nu} = \frac{3\lambda + 4}{\lambda + 2}.$$

These scaling relations imply the following form of the average correlation function near H_c :

$$G_r \equiv \langle S_n S_{n+r} \rangle_{0,J} - \langle \langle S_n \rangle_0 \langle S_{n+r} \rangle_0 \rangle_J = \frac{g(r/\xi)}{r^{2\beta/\nu}}. \quad (35)$$

Here, $\langle \dots \rangle_0$ denotes the average over (J -dependent) ground state(s), $\xi \sim (H - H_c)^{-\nu}$ is the correlation length, and $g(x)$ decreases faster than any power of x as $x \rightarrow \infty$. We cannot verify this prediction because the calculation of G_r in the F phase is a separate task lying beyond the scope of this paper.

At $\lambda > 0$, the higher-order field derivatives of m_∞ diverge, and we can interpret the behavior in (34) as higher-order phase transitions (third order for $0 < \lambda < 1$, fourth order for $1 < \lambda < 2$, and so on). When $P(J)$ tends to zero near $-J_1$ faster than any power of $(-J_1 - J)$, we would have a infinite-order phase transition. But from the AF phase side, there is always a sharp drop of the AF order parameter from 1 to 0, i. e., the first-order transition anomaly. We also note that for $\lambda = 0$, we have only a jump of the linear susceptibility from zero to a finite value at $H = H_c$ as in an

ordinary first-order transition. For integer $\lambda = 1, 2, \dots$, only the corresponding nonlinear susceptibilities experience similar jumps, which have no analogs among the known types of transitions.

In finite samples, there is no sharp transition to the F phase; instead, at $H > H_c$, this phase starts to form gradually in the middle of a chain. When $P(J) \rightarrow 0$ as $J \rightarrow -J_1$, we again use $W_\infty \approx \delta(F + H/2)$ near H_c to obtain

$$m_{n,N} = m_\infty(1 - e^{-\kappa N}) + (-1)^n \left[(1 - m_\infty)(e^{-\kappa n} + e^{-\kappa n'}) - e^{-\kappa N} \right], \quad (36)$$

$$\kappa \equiv -\ln Q(-H/2) \approx 2m_\infty.$$

Hence, the intervals of an order- κ^{-1} length at both ends are still occupied by the (exponentially modulated) AF phase. Therefore, both phases coexist in the finite chain when $N\kappa \geq 2$ ($m_\infty \geq N^{-1}$), the fraction of the AF phase being $2/N\kappa \approx (Nm_\infty)^{-1}$, while when $m_\infty < N^{-1}$, the whole chain is still in the (slightly modulated) AF phase. We also note that $\kappa^{-1} \sim (H - H_c)^{-\beta}$ in general behaves differently from the correlation length $\xi \sim (H - H_c)^{-\nu}$. Similar results hold when $P(J)$ diverges as $J \rightarrow -J_1$ (see Fig. 3).

4. MAGNETIZATION AND PHASE TRANSITIONS AT $T = 0$. EVEN N

For even N , Eqs. (22)–(28), (30), and (31) for $0 < H < J_1$ give

$$m_{n,N} = 0, \quad (37)$$

for $J_1 < H < 2J_1$,

$$m_{n,N} = \left[1 - Q(-H)^{N/2} \right] \mu_{n,N}, \quad (38)$$

$$\mu_{n,N} = N^{-1} \left[1 + (-1)^n (n' - n) \right],$$

and for $2J_1 < H$

$$m_{n,N} = m_\infty + \int W_\infty \left\{ (\rho^n + \rho^{n'}) \times \left[\tilde{C}_\infty(1 + \rho) - \rho \right] + \rho^N (1 - 2\tilde{C}_\infty) \right\} dF + (-1)^n \int W_\infty (\rho^n - \rho^{n'}) \left[\tilde{C}_\infty(1 - \rho) + \rho \right] dF + \mu_{n,N} \left(\int W_\infty \rho^N dF - Q(-H)^{N/2} \right). \quad (39)$$

The vanishing magnetization at $0 < H < J_1$ is a consequence of the ground-state degeneracy of even chains: they have two ground states in such fields, $S_n = (-1)^n$ and $S_n = (-1)^{n+1}$, and $m_{n,N} = 0$ results from averaging over them. Additionally applying a small local

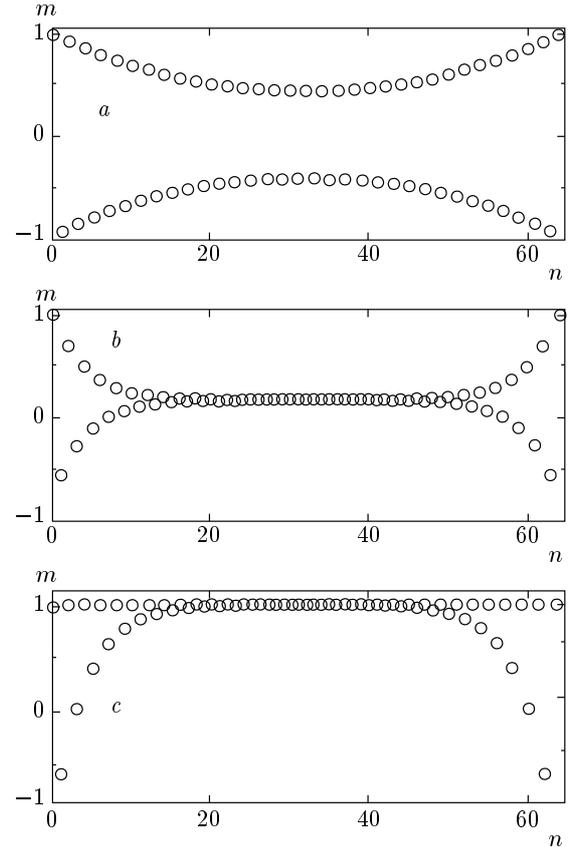


Fig. 3. Average ground-state magnetizations of odd chains with $N = 65$ and $P(J)$ from Eq. (29) with $J_0 = 10J_1$: (a) $H = 3J_1$, $\lambda = 0.1$; (b) $H = 3J_1$, $\lambda = -0.5$; (c) $H = 6J_1$, $\lambda = -0.5$

field $\delta H > 0$ to one of the spins, e.g., S_k , we can lift this degeneracy, thus recovering the straight AF order with the unique ground state having $S_k > 0$. This also means that this phase has an infinite correlation length because a small local field changes the average magnetization throughout the whole sample. It shows up in the correlation function

$$G_r = \langle S_n S_{n+r} \rangle_0 - \langle S_n \rangle_0 \langle S_{n+r} \rangle_0 = (-1)^r,$$

where $\langle \dots \rangle_0$ denotes the average over two ground states unaffected by disorder. The amplitude of G_r does not fall at large r , indicating a infinite correlation length. While G_r describes the response of the system to infinitesimal local perturbations, it cannot quantitatively describe the effect of strong perturbations such as a local spin upturn (see below). But we can naturally expect that the variations of magnetization caused by a strong local perturbation would also spread throughout the system.

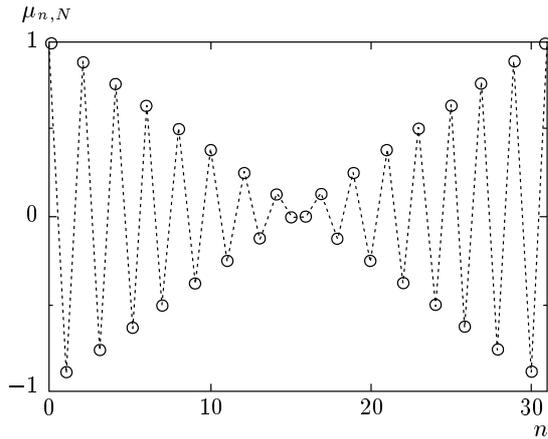


Fig. 4. Linearly modulated AF profile $\mu_{n,N}$ of a chain with $N = 32$. The dotted line is a guide to the eye

The specific phase appearing at $J_1 < H < 2J_1$ with a linearly modulated AF order (see Fig. 4) is also a consequence of the ground-state degeneracy. It also exists in the ordinary (nonrandom) AF chain with the exchange $-J$ and an even number of spins when $J < H < 2J$.

The mechanism of its appearance is quite simple. In normal AF states, even chains always have one of the end spins, e.g., S_0 , pointing opposite to the field. At $H > J$, it would upturn to point along the field, thus diminishing the energy by $2(H - J)$. But the simultaneous upturn of three spins at this end, S_0, S_1 , and S_2 , gives the same energy gain and generally the same effect results from the upturn of any odd number of spins S_0, S_1, \dots, S_{2k} . Thus we have $N/2$ ground states, each having a “kink” — one pair of neighboring spins pointing along the field (see Fig. 5). Averaging over them gives the “bow-tie” profile shown in Fig. 4. Indeed,

$$\begin{aligned}
 m_{n,N} &= \frac{2}{N} \sum_{k=1}^{N/2} \left[(-1)^n \vartheta \left(2k - n - \frac{3}{2} \right) + \right. \\
 &\quad \left. + (-1)^{n+1} \vartheta \left(n - 2k + \frac{3}{2} \right) \right] = \\
 &= (-1)^n \frac{2}{N} \left\{ \frac{N}{2} - 2 \left[\frac{n+1}{2} \right] \right\} = \mu_{n,N}.
 \end{aligned}$$

In the last expression, $[(n + 1)/2]$ is the integer part of $(n + 1)/2$.

This ordering can also be viewed as a boundary effect caused by the end-spin upturn and propagating through the whole sample due to the infinite correlation length of the degenerate AF phase in which it orig-

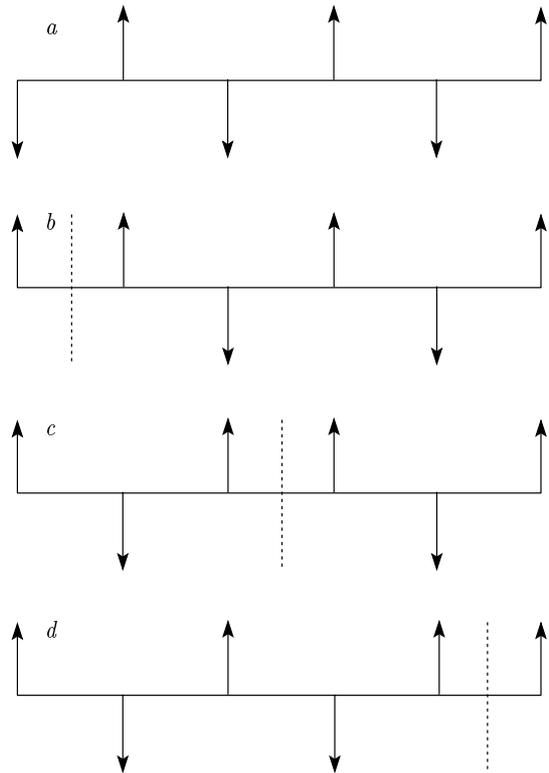


Fig. 5. The kink states (b)–(d) originated from the AF order (a) via upturn of the spins to the left of the dashed lines

inated. We can therefore expect that such inhomogeneous phases with ordering dependent on the form and size of a sample would also exist in many other systems with an infinite correlation length. Among them are Heisenberg magnets that in the ordered phase have an infinite transverse correlation length and a number of frustrated magnets in which the ground-state degeneracy also results in a divergence of the correlation length at $T = 0$.

It seems that the studies of statistical mechanics of the one-dimensional Ising model somehow overlooked the existence of this “bow-tie” phase and the “kink” states in Fig. 5 were first found in the framework of macroscopic Mill’s model for a finite-layered AF [18] (see also [19]). This model becomes the AF Ising chain in the limit of infinite anisotropy, but, being macroscopic, it does not require averaging over all kink states. The authors of Refs. [18, 19] therefore just noted that the system with an even number of layers can exist in one such state chosen from the set of $N/2$ degenerate ones. But in statistical mechanics dealing with statistical ensembles, averaging over degenerate states is an inherent procedure. In this framework, taking the

limit $T \rightarrow 0$ in the standard expressions for the AF chain [20], we would obtain $m_{n,N} = \mu_{n,N}$ for even N and $J < H < 2J$. Unfortunately, this is a rather difficult task that requires calculating the limits of cumbersome expressions (cf. Ref. [20]). This probably explains why this has not been done before.

Our expression for $m_{n,N}$ at $J_1 < H < 2J_1$ in (38) differs from that in the nonrandom case by the factor $1 - Q(-H)^{N/2}$ only. $Q(-H)$ is the probability to find a “strong” AF bond with $|J| > H$, and there are $N/2$ bond positions around which a kink can appear if the bond is “weak”, with $|J| < H$ (cf. Fig. 5). Hence, $Q(-H)^{N/2}$ is the probability that all these positions are occupied by strong bonds and pure AF states are preferable, while $1 - Q(-H)^{N/2}$ is the probability that there is at least one weak bond in the allowed locations and a kink with parallel spins can be created.

One may question the physical observability of the “bow-tie” phase because it requires an ensemble of chains with equal lengths. As a physical realization of random AF chain ensembles, the quasi-1d AF and magnetic polymer solutions with vacancies and impurities can be mentioned, but they would have a large diversity of chain lengths. However, this diversity cannot hinder the observation of the “bow-tie” phase with neutron diffraction experiments if we have a number of parallel chains having different lengths. The reason for this is that the form of neutron scattering intensity $I(k)$ does not change qualitatively with the chain size. Indeed,

$$I(k) \sim |m_{k,N}|^2,$$

where $m_{k,N}$ is a Fourier transform of $m_{n,N}$ with a discrete transferred wave vector

$$k = \frac{2\pi l}{N}, \quad l = 0, 1, \dots, N - 1.$$

In the linearly modulated AF phase under consideration we have

$$I(k) \sim |\mu_{k,N}|^2 = \left| \frac{2(1 - \delta_{k,\pi})}{e^{ik} + 1} + \delta_{k,0} \right|^2 = \frac{1 - \delta_{k,\pi}}{\cos^2(k/2)} + 3\delta_{k,0} \quad (40)$$

for an arbitrary N . Hence, $I(k)$ has the same profile for all N , the only difference being in the set of transferred wave vectors, which do not interfere but rather supplement each other as Fig. 6 shows. This makes the observation of the signs of the linearly modulated AF phase feasible in low-temperature neutron diffraction experiments.

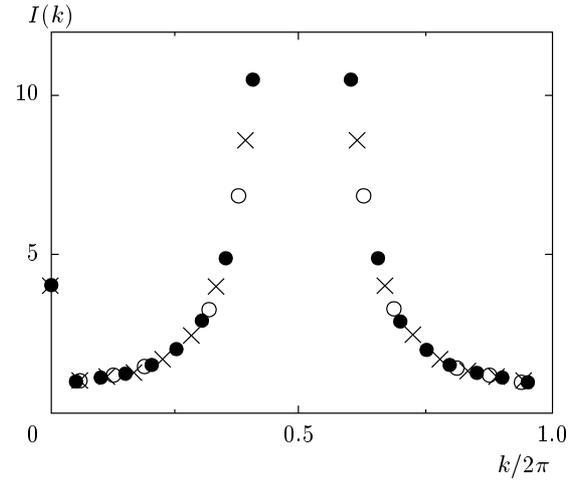


Fig. 6. $I(k)$ for $N = 16$ (\circ), $N = 18$ (\times), and $N = 20$ (\bullet)

In the limit $n \sim n' \rightarrow \infty$, $N \rightarrow \infty$ we have $\mu_{n,N} \rightarrow 0$. This means that every spin within an arbitrarily large but finite distance from the center of the chain has the average magnetization that tends to zero. This does not mean that there is no phase transition in the thermodynamic limit at $H = J_1$ but means only that $m_{n,N}$ is not a correct order parameter for it. As Eq. (40) shows, $m_{k,N}$ is the true (multicomponent) order parameter and there is a first-order transition between the AF and “bow-tie” phases.

The transition at $H = H_c = 2J_1$ in the thermodynamic limit ($n, n', N \rightarrow \infty$) has the features similar to those of odd chains in this field: in the F phase, it is continuous of the second or higher order, while in the “bow-tie” phase, $m_{k,N}$ sharply drops to zero at the transition point.

In finite samples, both transitions become smeared; the factor $1 - Q(-H)^{N/2}$ in (37) rapidly increases from zero to almost unity when H becomes greater than J_1 , while at $H_c < H$, the F order appears gradually in the middle of the chain. Again when $P(J) \rightarrow 0$ as $J \rightarrow -J_1$, we have

$$m_{n,N} = m_\infty(1 + e^{-\kappa N}) + (-1)^n(1 - m_\infty) \times (e^{-\kappa n} - e^{-\kappa n'}) + \mu_{n,N} (e^{-\kappa N} - Q(-H)^{N/2})$$

near H_c , with κ from Eq. (36). At finite κ , we therefore have a distribution of average magnetizations similar to that shown in Fig. 3b,c, while close to H_c when $\kappa \rightarrow 0$, it tends to that in Fig. 4 instead of the straight AF order as in odd chains. When $P(J) \rightarrow \infty$ as $J \rightarrow -J_1$, the magnetization profile shows similar behavior.

We can estimate the temperatures at which the above results for the ground state still hold approximately. The low- T contribution to the partition function is of the order of $\exp(-\Delta E_{min}/T)$, where ΔE_{min} is the lowest excitation energy above the ground state. We can therefore ascertain the validity of the above theory at $T \ll \Delta E_{min}$.

For odd N in the AF phase ($H < H_c$), the low-energy excitations are the flips of spins directed opposite to the field. Each such flip results in the energy change $2H - 2J_k - 2J_{k-1}$, whence

$$\Delta E_{min} = \min_k (-2H - 2J_k - 2J_{k-1}) > 2(H_c - H).$$

In the F phase ($H > H_c$), spin flips to the direction opposite to the field result in

$$\Delta E_{min} = \min_k (2H + 2J_k + 2J_{k-1}) > 2(H - H_c).$$

Hence, in the chains with odd N , the above results certainly hold at

$$T \ll |H - H_c|.$$

In the AF phase ($H < H'_c \equiv J_1$) of even chains, the low-energy excitations are the flips of spins considered for the construction of “kink” states (cf. Fig. 5). For them, we have

$$\Delta E_{min} = \min_k (-2H - 2J_k) > 2(H'_c - H).$$

In the bow-tie phase ($H'_c < H < H_c$), the ordinary spin flips to the field direction can have the lowest energy along with these kink excitations, and hence

$$\begin{aligned} \Delta E_{min} = \min_k (-2H - 2J_k - 2J_{k-1}, 2H + 2J_k) > \\ > 2 \min(H_c - H, H - H'_c). \end{aligned}$$

In the F phase, we also have single spin flips at low T , and therefore in the chains with even N , the range of validity of the ground-state results is

$$T \ll \min(|H - H_c|, |H - H'_c|).$$

We conclude that for all chains, the above results can also hold at sufficiently low T except in the vicinity of the transition points.

5. DISCUSSION AND CONCLUSIONS

There are a variety of features specific to the model considered here ($T = 0$, $d = 1$, and the variation of the external parameter H conjugate to the order parameter

m of one of the phases) that distinguish it from a number of conventional smeared first-order transitions. It still must be decided to what extent the present results are universal. Nevertheless, they are a useful example of a strong influence of disorder on a first-order transition in which it becomes a second- or higher-order one (from the F-phase side) with anomalies depending on the bond distribution function.

Thus, we have the first definite evidence that critical indices in an emergent second-order transition can be nonuniversal and that higher-order transitions can appear in the phase coexistence region. Along with this, the model exhibits the unexplored possibility that the first-order jumps can simultaneously be preserved on the other side of the smeared transition.

The model also gives a unique opportunity to elucidate the ordering in finite samples, which is quite necessary for the description of systems with infinite correlation lengths. Here, such systems are exemplified by the even-site AF chains. The existence of the “bow-tie” phase in these chains (either with or without disorder) shows that inhomogeneous size-dependent order can emerge in a system with an infinite correlation length due to the influence of boundary effects on the whole bulk ordering. This conclusion is important for systems with a broken continuous symmetry and other degenerate systems such as frustrated magnets, where similar phenomena can occur. The evidence of the boundary effects spreading throughout large mesoscopic samples are found in numerical studies of the $3d$ uniaxial AF [21] and the $2d$ Heisenberg AF [22].

Physical realization of the continuous distributions considered here, with predefined behavior at the upper end, can possibly be achieved by subjecting AF chains to (artificial) random mechanical stresses that would result in random AF exchanges due to magnetoelastic couplings. But to fully conform to the present model, these random exchanges between nearest neighbors should be independent. This may be difficult to fulfill owing to the long-range nature of deformations caused by random stresses and it is currently not clear whether bond correlations can be neglected for some random-bond patterns produced via such a mechanism. In any case, the present model can be considered a proper starting point to study more realistic models with bond correlations.

We finally note that the method presented here can have generalizations to the random-bond Heisenberg, transverse Ising, or quasi- $1d$ AF models.

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REFERENCES

1. Y. Imry and M. Wortis, *Phys. Rev. B* **19**, 3581 (1979).
2. J. Cardy and J. L. Jacobsen, *Phys. Rev. Lett.* **79**, 4063 (1997).
3. J. L. Jacobsen and J. L. Cardy, *Nucl. Phys. B* **515**, 701 (1998).
4. C. Chatelain, B. Berche, W. Janke, and P.-E. Berche, *Nucl. Phys. B* **719**, 275 (2005).
5. C. Chatelain, B. Berche, and L. N. Shur, *J. Phys. A* **34**, 9593 (2001).
6. P. N. Timonin, *Phys. Rev. B* **69**, 092102 (2004).
7. P. N. Timonin, *Zh. Eksp. Teor. Fiz.* **126**, 1198 (2004).
8. V. G. Baryakhtar, A. N. Bogdanov, and D. A. Yablonskii, *Usp. Fiz. Nauk* **156**, 47 (1988).
9. A. Vilenkin, *Phys. Rev. B* **18**, 1474 (1978).
10. V. Brandt and W. Gross, *Z. Phys. B* **31**, 237 (1978).
11. B. Derrida, J. Vannimenus, and Y. Pomeau, *J. Phys. C* **11**, 4749 (1978).
12. J. Chalupa, *J. Phys. A* **12**, 1257 (1979).
13. S. Katsura and N. Miyamoto, *Physica A* **112**, 393 (1982).
14. B. G. S. Doman, *J. Phys. C* **15**, 5611 (1982).
15. B. G. S. Doman and M. A. Z. Habeeb, *J. Phys. C* **16**, 2591 (1983).
16. E. Gardner and B. Derrida, *J. Stat. Phys.* **39**, 367 (1985).
17. L. Samaj and P. Markos, *J. Phys. A* **24**, 1319 (1991).
18. C. Micheletti, R. B. Griffiths, and J. M. Yeomans, *Phys. Rev. B* **59**, 6239 (1999).
19. U. K. Rößler and A. N. Bogdanov, *Phys. Rev. B* **69**, 094405 (2004).
20. S. V. Goupalov and D. C. Mattis, *Phys. Rev. B* **76**, 224412 (2007).
21. M. Holtschneider, S. Wessel, and W. Selke, *Phys. Rev. B* **75**, 224417 (2007); W. Selke, G. Bannasch, M. Holtschneider et al., *Condens. Matter Phys.* **12**, 547 (2009).
22. Wanzhou Zhang, Wenan Guo, Ling Wang et al., *Phys. Rev. B* **82**, 012401 (2010).