One-Dimensional Ising Model and the Complete Devil's Staircase

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It is shown rigorously that the one-dimensional Ising model with long-range antiferromagnetic interactions exhibits a complete devil's staircase.

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Periodic modulated systems are quite common in solid-state physics. In general there is a tendency for the periodicity to lock into values which are commensurable with the lattice constant.[1] As a parameter is changed, the system may pass through several commensurate phases which may or may not have incommensurate phases between them. In particular, Bak and von Boehm argued that the three-dimensional anisotropic Ising model with next-nearest-neighbor interactions has an *infinity* of commensurate phases.[2] At high temperatures there are probably also incommensurate phases,[3] but at low temperatures the commensurate phases are generally separated by first-order transitions in this model.[4]

In principle the periodicity may assume *every single* commensurable value in an interval. Since the rational numbers are everywhere dense, two steps in the function showing the periodicity versus the parameter are then always separated by an infinity of more steps. This structure is called the *devil's staircase*.[5] If the commensurate phases "fill up" the whole phase diagram the staircase is called *complete*. It has been speculated that the Frenkel-Kontorowa model (an array of classical particles, connected by springs, in a periodic potential) exhibits the complete devil's staircase, but until now only numerical arguments have been available.[6] In this paper it is shown rigorously that the ground state of the one-dimensional Ising model with convex long-range antiferromagnetic interactions has a complete devil's-staircase structure. To our knowledge, this constitutes the first proof of the existence of the complete devil's staircase in any model.

For simplicity we write the Hamiltonian in the following asymmetric form (which, of course, is completely general):

$$H=\sum_i HS_i+\tfrac{1}{2}\sum_{ij}J(i-j)(S_i+1)(S_j+1), \qquad (1)$$

where the summation is over the N spins in the chain, and $S_i=\pm 1$. Only "up" spins ($S=+1$) interact.

The model has some rather direct physical applications. Safran[7] has applied the model to the phenomenon of "staging" in graphite intercalation compounds. $S_i=1$ indicates the existence of a layer of intercalated atoms at the ith graphite layer and $S_i=-1$ indicates the absence of intercalated ions. $J(i-j)$ is thus essentially the interaction between intercalated layers, and H is a chemical potential for the layers. Hubbard and Torrance[8] suggested that the model may explain certain features of the "neutral-ionic" transitions observed in some mixed-stack organic charge transfer salts by Torrance *et al.*[9] $J(i-j)$ is then the Coulomb repulsion between ionic planes and H is the difference $I-A$ between the donor ionization potential I and the acceptor electron-affinity A. Both argue that an infinity of phases may occur, but the precise nature of the phases has not been specified.

For a given magnetization (number of "up" spins minus number of "down" spins) the problem of minimizing (1) is equivalent to the problem of arranging a number of charged particles on N sites so as to minimize the Coulomb energy. This problem has been solved by Hubbard[10] and by Pokrovsky and Uimin.[11] Some simple properties of the stable configurations are important for our purpose. Let X_i^0 denote the position of the ith up spin, and let X_i^1 be the distance to the next up spin. Similarly, X_i^p is the distance to the pth-nearest up spin, $X_i^p=X_{i+p}^0-X_i^0$. If the fraction of up spin is $q=m/n$ it can be shown that the energy is minimized if for all sites, then

$$X_i^p=r_p \ \text{ or } \ r_p+1, \qquad (2)$$

where $r_p<np/m<r_p+1$. For $p/q=pn/m$ integer,

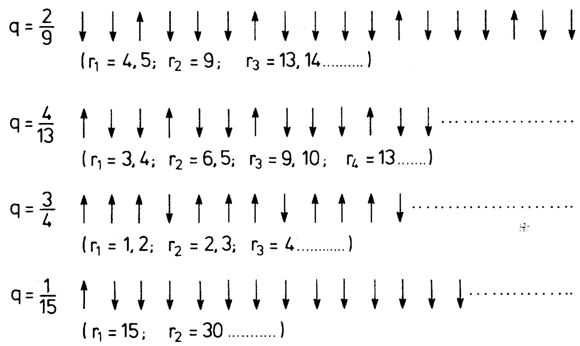

FIG. 1. Typical stable spin configurations with q the ratio of up spins over down spins.

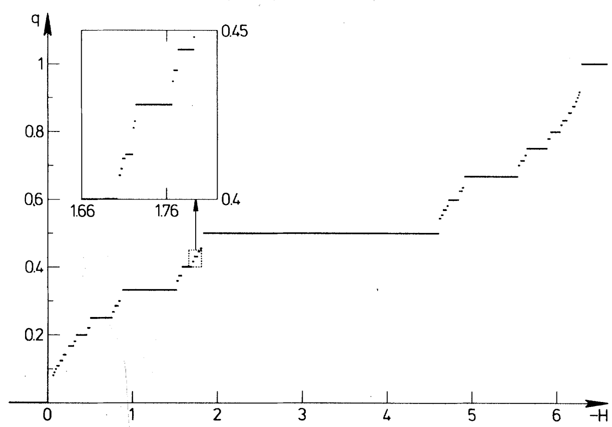

FIG. 2. The devil's staircase. The ratio of up spins over down spins q is plotted vs the applied field H for an interaction $J(i) = i^{-2}$. Inset: The area in the square magnified 10 times.

$X_i^p = r_p = np/m$. The sum of all pth-nearest-neighbor distances must fulfill the obvious relation

$$\sum_i X_i^p = pN. \tag{3}$$

Figure 1 shows some typical configurations. The relations (2) and (3) are all we need to calculate exactly the stability intervals for all possible rational fractions of up spins.

Consider the situation where the chain is deformed into a loop of length N. The phase characterized by $q = m/n$ is stable as long as it costs energy to flip one up spin down, or flip one down spin up, and rearrange the new configuration to minimize the energy.

We calculate first the cost of flipping one down spin. There is now one more pth-nearest-neighbor interaction. Since (2) and (3) must still hold, r_p pth-nearest-neighbor distances $r_p + 1$ must be replaced by $r_p + 1$ pth-nearest-neighbor distances $X_i^p = r_p$, and the total change in energy is

$$\Delta U(\downarrow \to \uparrow) = 2H + 4(r_1+1)J(r_1) - 4r_1 J(r_1+1) + 4(r_2+1)J(r_2) - 4r_2 J(r_2+1) + \ldots$$
$$+ 4nJ(n-1) - 4(n-1)J(n) + \ldots + 8nJ(2n-1) - 4(2n-1)J(2n) + \ldots, \tag{4a}$$

where $r_m = n$, $r_{2m} = 2n, \ldots$, have been inserted. Similarly the energy cost of flipping one up spin is

$$U(\uparrow \to \downarrow) = -2H - 4(r_1+1)J(r_1) + 4r_1 J(r_1+1) - 4(r_2+1)J(r_2) + 4r_2 J(r_2+1) - \ldots$$
$$- 4(n+1)J(n) + 4nJ(n+1) - \ldots - 4(2n+1)J(2n) + 8nJ(2n+1) - \ldots . \tag{4b}$$

The interval in H, $\Delta H(m/n)$, where the phase is stable is determined simply by setting (4a) and (4b) equal to zero, respectively:

$$\tfrac{1}{2}\Delta H(q = m/n) = nJ(n+1) + nJ(n-1) - 2nJ(n) + 2nJ(2n+1) + 2nJ(2n-1) - 4nJ(2n) + \ldots$$
$$+ pnJ(pn+1) + pnJ(pn-1) - 2pnJ(pn) + \ldots . \tag{5}$$

Note that ΔH is independent of the numerator m. If we make the assumption that the interaction J is of infinite range and convex, $J(i+1) + J(i-1) - 2J(i) > 0$, then $\Delta H(m/n)$ is positive and *finite* for all values of m and n. Also, it is easy to show that if ΔH is summed over all rational values the whole interval of H is "filled up." We have thus proven the existence of the complete devil's staircase for a very general class of interactions, including the power-law interactions expected for the intercalation compounds, and the exponentially decaying Coulomb interactions expected for the neutral-ionic transition.

Figure 2 shows q vs H. An interaction $J(i) = i^{-2}$ was chosen. Only phases which are stable in an interval $\Delta H/J(1) > 10^{-3}$ are shown. The curve has no finite jumps. To illustrate the self-similarity of the function a part of it has been magnified by a factor 10 in the inset.

The states formed by flipping *one* spin starting from a simple commensurate phase with $q = 1/m$ have a simple structure. Figures 3(a) and 3(b) show the $q = \frac{1}{3}$ phase and the configuration which has one more up spin. *Three* defects are formed (infinitely far apart for an infinite system) al-

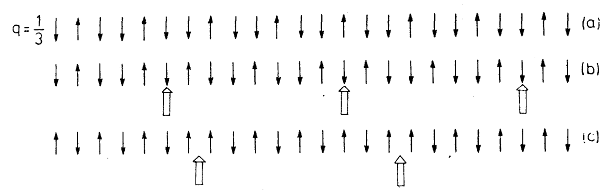

FIG. 3. (a) The commensurate structure with $q = \frac{1}{3}$, and (b) the configuration with one more "up" spin (the lowest excited states for values of H where the $q = \frac{1}{3}$ phase is stable). Note the formation of defects or "solitons" with fractional spin $S^* = \frac{1}{3}$, indicated by an arrow below the array. (c) The lowest excited state of the $q = \frac{1}{2}$ phase, with $S^* = \frac{1}{2}$ solitons.

though only *one* spin has been flipped. Hence, the spin of each defect is $S^* = \frac{1}{3}$. The nature of this fractional spin is very similar to the fractional charges discussed by Su, Schrieffer, and Heeger.[12] The situation for $q = \frac{1}{2}$ is topologically equivalent with the situation for the antiferromagnetic Heisenberg model as worked out by Fadeev.[13] Topological solitons with spin $S^* = \frac{1}{2}$ are expected in this case [Fig. 3(c)].

Until now, we have addressed only the problem of finding the ground state. What happens at nonzero temperature? A d-dimensional model can be constructed by adding ferromagnetic interactions in the d-1 perpendicular directions.

Drawing on the general insight achieved in Refs. 1–4 we expect that in three dimensions *all* commensurate phases extend to finite temperature, probably all the way to the transition temperature T_c where the system becomes paramagnetic. At nonzero temperature, in particular near T_c, there may be incommensurate phases, of finite measure, between the C phases.

Generalizing the results derived by Villain and Bak,[14] we expect that in two dimensions the high-order commensurate phases vanish at some temperature $T_n \sim 16T_c/n^2$. At a given nonzero temperature there are thus only a finite number of phases. The high-order C phases give way to a floating incommensurate phase. The phase with $q = \frac{1}{2}$ plays a special role: We expect a transition directly to a paramagnetic phase all the way down to $T = 0$.

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