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The pinning of a domain wall by weakened bonds in two dimensions

J T Chalker

Department of Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 3NP, England

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Abstract. The pinning of a domain wall by a row of weakened bonds is studied in the solid-on-solid limit of the two-dimensional Ising model. If the weakened bonds lie near the edge of the system the domain wall has a roughening transition, but if they lie in the bulk, then they localise the domain wall at all temperatures. A continuum version of the model shows similar behaviour, in contrast to continuum models of roughening in three dimensions.

1. Introduction

There is a striking contrast between the behaviour of a domain wall in the two-dimensional Ising model and that in the three-dimensional model. In the first case, capillary fluctuations of the wall are sufficiently large that the mean square displacement of the wall from its zero-temperature position diverges with the linear size of the system, at any finite temperature (Abraham and Issigoni 1980). In the second case, the mean square displacement of a wall is more weakly divergent at high temperatures, being proportional to the logarithm of the size of the system, whilst at temperatures below a roughening transition temperature the presence of the lattice is sufficient to localise a wall near its ground-state position (Weeks and Gilmer 1979 and references therein).

Abraham (1980) has shown recently by an exact solution that there is a modification of the planar Ising model, with a row of weakened exchange bonds next to the edge of the system, in which a domain wall also undergoes a transition between localised and rough phases.

In this paper the solid-on-solid limit of the modified system is used to investigate the transition in more detail. It is shown that, in distinction to the usual roughening transition of an interface in a three-dimensional model, there is a continuum version of the system which shows a similar transition at a finite temperature. We conclude that this transition is essentially an unbinding of the wall from the weakened bonds, and that the lattice does not play a vital role. The model is also used to study competition for a domain wall between rows of weakened bonds at opposite edges of the system, and a first-order transition is found in which the wall jumps from one edge to the other as the relative strengths of the bonds next to the two edges is varied.

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2. The model

We begin by describing the model studied by Abraham. Consider spins $\sigma(m, n)$, which occupy the sites (m, n) of a square lattice, with $1 \leqslant n \leqslant N+1$ and $1 \leqslant m \leqslant M$, and take the values $\sigma(m, n) = \pm 1$. The energy of a configuration is

$$E = -\sum_{m=1}^{M} \Big(J_{\parallel} \sum_{n=1}^{N} \sigma(m, n)\sigma(m+1, n) + J_{\perp} \sum_{n=2}^{N-1} \sigma(m, n)\sigma(m, n+1) + (J_{\perp} - \Delta_1)\sigma(m, 2) - (J_{\perp} - \Delta_2)\sigma(m, N) \Big). \tag{1}$$

Thus the periodic boundary condition: $\sigma(M+1, n) = \sigma(1, n)$ has been imposed in the m direction whilst the spins at the edges $n = 1$ and $n = N+1$ have been fixed respectively up and down to guarantee a domain wall.

The limit: $J_{\perp} \to \infty$ gives the solid-on-solid model for which the energy of a configuration relative to that of the ground state, E_0, can also be written

$$E - E_0 = 2 \sum_{m=1}^{M} \Big(J_{\parallel} |h(m) - h(m+1)| - \Delta_1 \delta_{h(m),1} - \Delta_2 \delta_{h(m),N} \Big). \tag{2}$$

Here, m labels sites on a line and the variable $h(m)$ takes the values $1, 2, \ldots, N$; periodic boundary conditions still apply $h(M+1) = h(1)$; and $\delta_{h(m),n}$ is the Kronecker delta. The solid-on-solid limit prevents both excitations of the bulk and also configurations in which the domain wall overhangs itself, so that the dimensionality of the system is effectively reduced from two to one. The special case $\Delta_1 = \Delta_2 = 0$ is known as the Onsager–Temperley string (Temperley 1952): for this, the thermal average $\langle h(m) \rangle$ diverges as $M, N \to \infty$ at any finite temperature. The equivalent two-dimensional model of the interface in three dimensions has been studied extensively (Weeks and Gilmer 1979) and is believed to embody the essentials of the roughening transition.

It is also interesting to study two modifications of the system described by (2). In the first, the weakened bonds lie in the bulk rather than next to an edge; that is, $\Delta_2 = 0$ and $h(m)$ takes on the values $0, \pm 1, \pm 2, \ldots, \pm N$. In the second, the lattice in the direction perpendicular to the wall is removed so that $h(m)$ is a continuous variable.

3. Solution of the model

The thermodynamic properties of the model described by (2) can be calculated using the transfer matrix. Define an $N \times N$ matrix

$$(\boldsymbol{T}^{(N)})_{ij} = \exp\{-\beta[2J_{\parallel}|i-j| - \Delta_1(\delta_{i,1} + \delta_{j,1}) - \Delta_2(\delta_{i,N} + \delta_{j,N})]\} \tag{3}$$

where $\beta = 1/kT$, k being the Boltzmann constant and T absolute temperature. Then the partition function is

$$Z_{N,M} = \mathrm{Tr}\{[\boldsymbol{T}^{(N)}]^M\} \tag{4}$$

and if $\lambda_1^{(N)}$ is the largest eigenvalue of $\boldsymbol{T}^{(N)}$, the free energy of the domain wall per unit length in the thermodynamic limit (which is discussed in the appendix) is

$$F = \lim_{N,M \to \infty} -(kT/M) \ln Z_{N,M} = -kT \ln \lambda_1^{(\infty)}. \tag{5}$$

The magnetisation as a function of position in the corresponding Ising model can also be calculated. Let $p(h)$ be the thermal probability that $h(m) < h$. Then

$$\lim_{N,M\to\infty} p(h) = \sum_{j=1}^{h-1} |\phi_j^{(1)}|^2 \tag{6}$$

where $\phi_j^{(1)}$ is the normalised eigenvector of $\boldsymbol{T}^{(N)}$ corresponding to the largest eigenvalue, λ_1. This is related to the magnetisation by

$$\langle\sigma(m, n)\rangle = 1 - 2p(n). \tag{7}$$

The basis of the calculation is therefore the diagonalisation of the transfer matrix, which is outlined in the appendix; the results are described in this section. The eigenvectors of $\boldsymbol{T}^{(N)}$ are of the form

$$\phi_r = a_+ e^{ir\theta} + a_- e^{-ir\theta} \qquad 2 \leqslant r \leqslant N-1 \tag{8}$$

with an associated eigenvalue

$$\lambda = \frac{1-x^2}{x^2 - 2x\cos\theta + 1} \qquad x = \exp(-2\beta J_\parallel).$$

There are N values of θ, $\{\theta_i\}$, in the range $0 \leqslant \mathrm{Re}\,\theta \leqslant \pi$, $\mathrm{Im}\,\theta \geqslant 0$ given by the roots of equation (A2). At high temperatures all θ_i are real and the smallest is $\pi/N + O(N^{-2})$ for large N, so that

$$\lambda^{(1)} = \frac{1+x}{1-x} + O(N^{-1})$$

$$\phi_j^{(1)} = \left(\frac{2}{N}\right)^{1/2} \sin\left(\frac{j\pi}{N}\right) + O(N^{-2}) \tag{9}$$

and the only length scale for $\langle\sigma(m, n)\rangle$ is the size of the system. At sufficiently low temperatures either one or two of the $\{\theta_i\}$ are imaginary so that

$$\lim_{N\to\infty} \lambda^{(1)} = \frac{1-x^2}{1-2x\cosh\kappa + x^2} \tag{10}$$

where $\theta_1 = i\kappa$, $\phi_j^{(1)} \propto e^{-j\kappa}$ or $e^{-(N-j)\kappa}$.

Now κ gives a length scale to $\langle\sigma(m)\rangle$ which remains finite for an infinite system. The critical temperature, T_R, below which the eigenvector with the largest eigenvalue is localised, is given by

$$\exp(-2J_\parallel/kT_R) + \exp(-2\Delta/kT_R) = 1 \qquad \Delta = \max(\Delta_1, \Delta_2) \tag{11}$$

which is also the corresponding limit of equation (8) in Abraham (1980).

For the modification of the model in which the weakened bonds lie in the bulk the transfer matrix is of rank $2N+1$

$$(\boldsymbol{T}^{(2N+1)})_{ij} = \exp\{-\beta[2J_\parallel|i-j| - \Delta(\delta_{i,0} + \delta_{j,0})]\} \qquad -N \leqslant i, j \leqslant N. \tag{12}$$

The associated eigenvectors have the form

$$\phi_r = a_+ e^{ir\theta} + a_- e^{-ir\theta} \qquad 1 \leqslant r \leqslant N$$

$$\phi_{-r} = \pm\phi_r \tag{13}$$

and the eigenvalues, $\lambda(\theta)$, are as before. However, in this case there are $2N$ real values

of θ and one imaginary one at all temperatures, so that the domain wall is always localised near the weakened bonds.

Lastly, we return to the case of weakened bonds lying at the edge of the system, but now allow $h(m)$ to vary continuously. For the configurational energy

$$E - E_0 = 2 \sum_{m=1}^{M} \{J_{\|}|h(m) - h(m+1)| - \Delta\theta[h(m)]\}$$

where

$$-1 \leqslant h(m) \leqslant L \qquad \text{and} \qquad \theta[x] = \begin{cases} 1 & x \leqslant 0 \\ 0 & x > 0 \end{cases} \tag{14}$$

the transfer matrix is replaced by an integral operator, with eigenfunctions ϕ_i and eigenvalues $\lambda_i^{(L)}$ according to

$$\int_{-1}^{L} T(x, y)\phi_i(y)\,\mathrm{d}y = \lambda_i^{(L)}\phi_i(x)$$

where

$$T(x, y) = \exp\{-\beta[2J_{\|}|x - y| - \Delta(\theta(x) + \theta(y))]\}. \tag{15}$$

At high temperatures the eigenfunctions are all of the form

$$\phi(x) = \begin{cases} A_1 \sin(k_1 x + \phi_1) & x > 0 \\ A_2 \sin(k_2 x + \phi_2) & x < 0 \end{cases} \tag{16}$$

with associated eigenvalues

$$\lambda = \frac{4\beta J_{\|}}{4\beta^2 J_{\|}^2 + k_1^2}$$

but below a critical temperature given by (in the limit $L \to \infty$)

$$\tan[2\beta_{\mathrm{R}} J_{\|}(\mathrm{e}^{2\beta_{\mathrm{R}}\Delta} - 1)^{1/2}] = (\mathrm{e}^{2\beta_{\mathrm{R}}\Delta} - 1)^{-1/2}. \tag{17}$$

There is one eigenfunction of the form

$$\phi(x) = \begin{cases} A_1 \mathrm{e}^{-\kappa x} & x > 0 \\ A_2 \sin(k_0 x + \phi) & x < 0 \end{cases} \tag{18}$$

and an eigenvalue

$$\lambda = \frac{4\beta J_{\|}}{4\beta^2 J_{\|}^2 - \kappa^2}.$$

From this we conclude that the transitions in the discrete and continuous versions of this solid-on-solid model are qualitatively the same.

4. Discussion

The similarity should be set against the differing behaviour of the discrete and continuous two-dimensional solid-on-solid models, which are described by equation (2) with $\Delta_1 = \Delta_2 = 0$, m labelling sites on a two-dimensional lattice, and $h(m) = 0, \pm 1, \pm 2 \ldots$ and $-\infty \leqslant h(m) \leqslant \infty$, respectively. In the discrete case it has been proven

(Abraham and Heilmann 1976) that, at sufficiently low, finite temperatures, $\langle h^2(m)\rangle$ is finite, whilst for the continuum version $\langle h^2(m)\rangle$ is divergent at all finite temperatures (Chui and Weeks 1976). In this sense, the lattice is relevant to the usual roughening transition but not to the transition discussed here.

The two transitions also differ in the form of the singularity in the free energy at the critical temperature. The transition in the interface of a simple cubic Ising model is believed to belong to the same universality class as the Kosterlitz–Thouless transition (Chui and Weeks 1976) and so the free energy is thought to have an essential singularity at the roughening temperature. The free energy of the transition in the two-dimensional model is (from equation (5)) of the mean-field type, with a simple discontinuity in the specific heat. It should be noted, however, that roughening transitions of finite order are known for interfaces in three-dimensional systems (Knops 1979).

The transition in the model described by equation (2) is a combined result of an attraction for the domain wall by the weakened bonds and the restriction set by the edge of the system on the configurations which the wall can take up. It may seem surprising initially that the transition should disappear if the weakened bonds lie in the bulk rather than near an edge of the system, and it is interesting to relate this one-dimensional problem in statistical mechanics to the corresponding zero-dimensional quantum field theory (Kogut 1979). First we take the continuum limit of (2) in both directions, so that $h(m)$ becomes a continuous valued function of a continuous argument, m. A configuration $h(m)$ has an energy

$$E\{h(m)\} = \int \mathrm{d}m \left[J\left(\frac{\mathrm{d}h}{\mathrm{d}m}\right)^2 - \Delta\theta[h(m)] \right]. \tag{19}$$

The probability that $h(m_0) = h_0$, given $h(0) = 0$, is proportional to $\int \mathscr{D}(h)\, \mathrm{e}^{-\beta E\{h\}}$, where the functional integral is over all $h(m)$ which satisfy the boundary conditions at 0 and m_0. This is also, within the Feynman formulation of quantum mechanics, the probability that a particle of mass $2J$ moving in the one-dimensional potential, $-\Delta\theta(h)$, will start from the origin and have position h_0 at time m_0. Planck's constant in the quantum mechanical theory takes the place of temperature in the statistical mechanical theory. The two cases of the domain wall in the planar Ising model with bond weakening either at the edge or in the bulk then correspond to a quantum mechanical particle moving in the one-dimensional potentials sketched in figures 1(a) and (b) respectively. As is well known (Landau and Lifshitz 1958) figure 1(b) always has at least one bound state whilst 1(a) has one only for sufficiently large values of $J\Delta/\hbar^2$. The transition might therefore

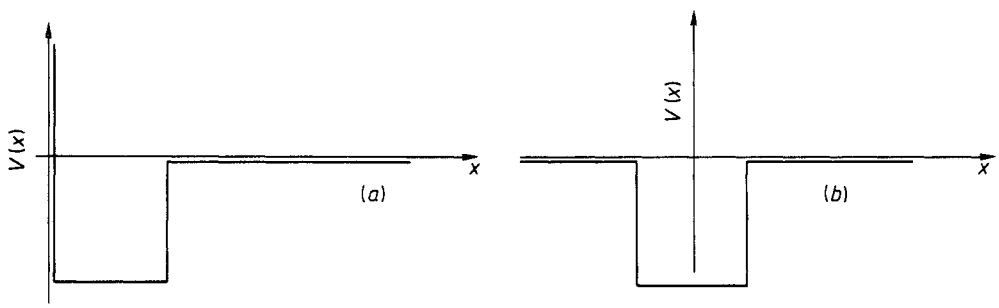

Figure 1. The potential energy for a quantum mechanical particle which corresponds to the domain wall in a model with weakened bonds lying: (a) at the edge and (b) in the bulk.

be described as an unbinding of the domain wall from the attraction of the weakened bonds.

The results of this calculation may be used to test the solid-on-solid approximation by comparing them with those from the solution of the equivalent isotropic Ising model. The roughening temperatures of the discrete and continuous solid-on-solid models and the isotropic Ising model are compared in figure 2. As expected, the discrete solid-on-solid approximation is asymptotically exact as $T \to 0$, when the bulk magnetisation of the Ising model saturates. The continuous and discrete solid-on-solid models have the same asymptotic dependence of T_R on Δ/J, as $\Delta/J \to \infty$, when the energy cost of an excitation is just that of unbinding the wall, and not of bending it.

Finally, we discuss competition for a domain wall between weakened bonds at opposite edges of the system. Since the free energy, F, of the model described by equation (2) depends on $J_\parallel$, kT and only the larger of Δ_1 and Δ_2, if Δ_2 is varied whilst the

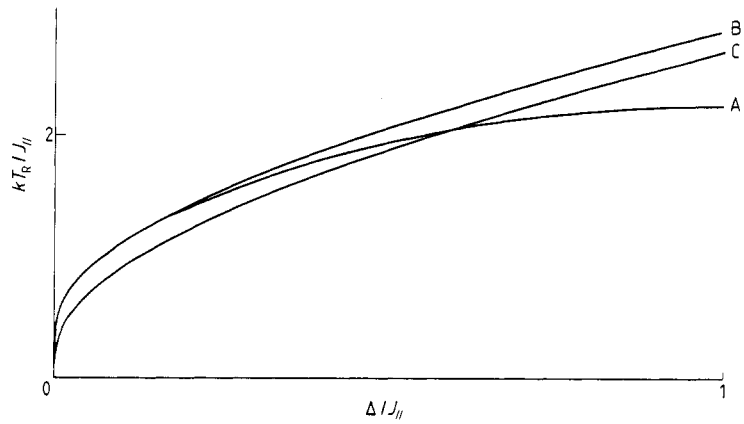

Figure 2. The dependence of the roughening temperature on the strength of the weakened bonds in: A, the isotropic Ising model; B, the discrete solid-on-solid model and C, the continuous solid-on-solid model.

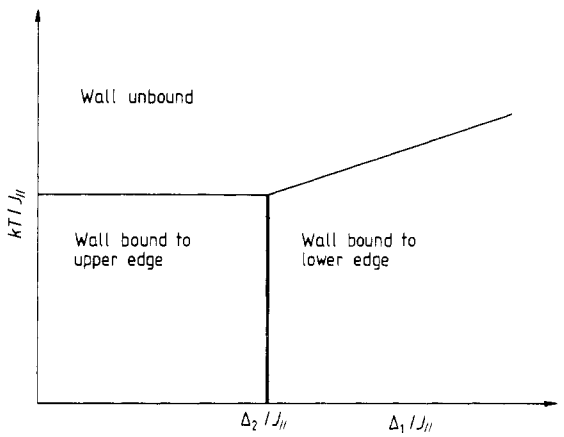

Figure 3. A representative plane of the phase diagram for the domain wall in a model with lines of weakened bonds next to both edges.

other parameters are held constant there is a discontinuity in $\partial F/\partial \Delta_2$ at the point $\Delta_1 = \Delta_2$. The full phase diagram for the system is three-dimensional; a representative plane is shown in figure 3.

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Appendix. The eigenvectors and eigenvalues of the transfer matrices and integral

If one assumes the form given in equation (8) for the eigenvectors, $\boldsymbol{\phi}$, of $\boldsymbol{T}^{(N)}$, then ϕ_1, ϕ_N, a_+, a_- and θ remain to be determined. By direct substitution, $\boldsymbol{T}^{(N)}\boldsymbol{\phi} = \lambda\boldsymbol{\phi}$, where the eigenvalue λ is as in (8), provided that

$$\begin{pmatrix} \dfrac{y_1}{x}, & \dfrac{e^{i2\theta}}{x(x-e^{i\theta})}, & \dfrac{e^{-i2\theta}}{x(x-e^{-i\theta})}, & 0 \\ y_1 x^{N-1}, & \dfrac{e^{i2\theta}}{x(x-e^{i\theta})}(x^N - x^2 e^{i(N-2)\theta}), & \dfrac{e^{-i2\theta}}{x(x-e^{-i\theta})}(x^N - x^2 e^{-i(N-2)\theta}), & y_2 - \dfrac{\lambda}{y_2} \\ y_1 - \dfrac{\lambda}{y_1}, & \dfrac{e^{i\theta}}{x(x-e^{-i\theta})}(x^N e^{i(N-2)\theta} - x^2), & \dfrac{e^{-i\theta}}{x(x-e^{i\theta})}(x^N e^{-i(N-2)\theta} - x^2), & y_2 x^{N-1} \\ 0, & \dfrac{e^{i(N-1)\theta}}{x(x-e^{-i\theta})}, & \dfrac{e^{-i(N-1)\theta}}{x(x-e^{i\theta})}, & \dfrac{y_2}{x} \end{pmatrix} \begin{pmatrix} \phi_1 \\ a_+ \\ a_- \\ \phi_N \end{pmatrix} = \mathbf{0} \tag{A1}$$

where $x = e^{-2\beta J_\parallel}$ and $y_i = e^{\beta \Delta_i}$.

The allowed values of θ, and hence of λ, are found from the zeros of the determinant of this 4×4 matrix. The condition for this determinant to be zero can be written as:

$$\tan(N-1)\theta = F(\theta) \tag{A2}$$

where

$$F(\theta) = \frac{R_1 I_2 + I_1 R_2}{R_1 R_2 - I_1 I_2}$$

$$R_i = \mathrm{Re}\{f_i(\theta)\} \qquad I_i = \mathrm{Im}\{f_i(\theta)\}$$

$$f_i(\theta) = (x - e^{i\theta})y_i + (e^{i\theta} - x^{-1})(y_i - \lambda/y_i).$$

It is helpful to note that since $\boldsymbol{T}^{(N)}$ is Hermitian, λ is real and so θ is either purely real or purely imaginary. Also, all values of λ are encompassed by the range for θ: $0 \leqslant \mathrm{Re}\ \theta \leqslant \pi$, $\mathrm{Im}\ \theta \geqslant 0$. Hence the roots of (A2) can be found graphically as the points of intersection of the curves $y = \tan(N-1)\theta$ and $y = F(\theta)$, plotted for real θ over the range $0 \leqslant \theta \leqslant \pi$ and for imaginary θ over the range $0 \leqslant \theta < i\infty$. The forms of these

curves are sketched for the three possible cases of 0, 1 or 2 imaginary roots for θ in figure 4. It is clear that the smallest real root for θ lies between $\theta = 0$ and $\theta = \pi/(N-1)$ ($\theta = 0$ is not, in general, a solution). In the limit $N \to \infty$ the roots for imaginary θ are the solutions to $F(\theta) = \mathrm{i}$. This can be written as

$$e^{\kappa} = \frac{y_i^2 - 1}{xy_i^2} \qquad \theta = \mathrm{i}\kappa. \tag{A3}$$

As $T \to T_R^-$, $\kappa \to 0$ which gives equation (10) for T_R.

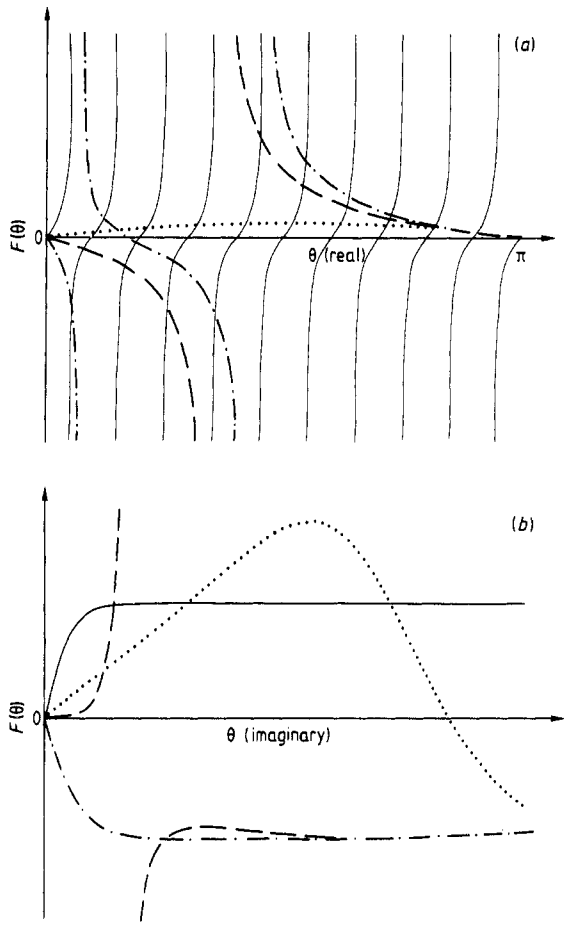

Figure 4. Graphs of $\tan(N-1)\theta$ and $F(\theta)$ for (*a*) θ real and (*b*) θ imaginary. The cases of 0, 1 and 2 imaginary values for θ_i are represented by the curves: -·-·-, --- and ····· respectively.

The transfer matrix for the model in which the weakened bonds lie in the bulk (equation (12)) is diagonalised in a similar way. The largest eigenvalue will be associated with an eigenvector which has even symmetry, $\phi_r = \phi_{-r}$, and substitution of the form given in equation (13) leads to three equations for a_+, a_- and ϕ_0.

$$\begin{pmatrix} \dfrac{x^2-2x\,e^{i\theta}+1}{(1-x\,e^{i\theta})(1-x\,e^{-i\theta})}+\dfrac{(x\,e^{i\theta})^{N+1}}{1-x\,e^{i\theta}}, & -y, & \dfrac{x^2-2x\,e^{-i\theta}+1}{(1-x\,e^{i\theta})(1-x\,e^{-i\theta})}+\dfrac{(x\,e^{-i\theta})^{N+1}}{1-x\,e^{-i\theta}} \\ 2x\,e^{i\theta}\dfrac{1-x^N\,e^{iN\theta}}{1-x\,e^{i\theta}}, & y^2-\lambda, & 2x\,e^{-i\theta}\dfrac{1-x^N\,e^{-iN\theta}}{1-x\,e^{-i\theta}} \\ x\,e^{i\theta}\dfrac{x^N\,e^{iN\theta}}{1-x\,e^{i\theta}}, & 0, & x\,e^{-i\theta}\dfrac{x^N\,e^{-iN\theta}}{1-x\,e^{-i\theta}} \end{pmatrix} \begin{pmatrix} a_+ \\ \phi_0 \\ a_- \end{pmatrix} = \mathbf{0}. \tag{A4}$$

The determinant of this 3×3 matrix is zero if

$$\tan N\theta = \frac{(y^2-\lambda)\sin\theta}{(y^2-\lambda)(x-\cos\theta)-2x} \equiv F'(\theta). \tag{A5}$$

As before, the largest eigenvalue, $\lambda(\theta)$, and an associated localised eigenvector, will result from a purely imaginary solution for θ. In the limit $N\to\infty$ this is the solution to $F'(\theta)=\mathrm{i}$ which can be written as

$$\frac{1+x^2}{2x} = \cosh\kappa + \frac{1}{y^2-1}\sinh\kappa \qquad \theta = \mathrm{i}\kappa. \tag{A6}$$

If $\Delta>0$ (i.e. if there are weakened bonds), then there is a finite real value of κ which satisfies equation (A6) at all temperatures, so that the domain wall is always pinned in this model.

We now derive the eigenvalues of the transfer integral (equation (15)) which describes the model in which $h(m)$ is a continuous variable. By differentiation of (15), the eigenfunction, $\phi(n)$, obeys the differential equation

$$\lambda\frac{\mathrm{d}^2\phi}{\mathrm{d}n^2} = \begin{cases} 4\beta J_\parallel(\lambda\beta J_\parallel - 1)\phi(n) & L\geqslant n>0 \\ 4\beta J_\parallel(\lambda\beta J_\parallel - \mathrm{e}^{2\beta\Delta})\phi(n) & -1\leqslant n<0 \end{cases} \tag{A7}$$

hence the forms (16) and (18) for $\phi(n)$. Substitution of these into the integral equation leads to boundary conditions for $\phi(n)$:

$$\phi(n) \text{ and } \mathrm{d}\phi/\mathrm{d}n \text{ continuous} \qquad \text{at } n=0$$
$$\mathrm{d}\phi/\mathrm{d}n = 2\beta J_\parallel\phi \qquad \text{at } n=-1 \qquad \text{and} \qquad \mathrm{d}\phi/\mathrm{d}n = -2\beta J_\parallel\phi \qquad \text{at } n=L. \tag{A8}$$

In the limit, $L\to\infty$, the smallest allowed value of k_1 tends to zero (with $k_1 L\to\pi$), so that the largest eigenvalue above the transition temperature is $\lambda = 1/\beta J_\parallel$. Below the critical point there is a localised eigenfunction with κ and k_0 determined by

$$\kappa^2 = 4\beta^2 J_\parallel^2 - \mathrm{e}^{-2\beta\Delta}(4\beta^2 J_\parallel^2 + k_0^2)$$
$$\tan k_0 = \frac{k_0(\kappa+2\beta J_\parallel)}{k_0^2 - 2\kappa\beta J_\parallel}. \tag{A9}$$

As $T\to T_{\mathrm{R}}^-$, $\kappa\to 0^+$, which yields equation (17) for T_{R}.

The thermodynamic limit given in equation (5) requires some justification. The partition function, $Z_{M,N}$, describes the solid-on-solid limit of an $M\times N$ site Ising model, so that in the thermodynamic limit $M, N\to\infty$ with M/N fixed. Order the eigenvalues of $\boldsymbol{T}^{(N)}$ by magnitude, $|\lambda_1^{(N)}|>|\lambda_2^{(N)}|>\cdots>|\lambda_N^{(N)}|$, and set $M=N$. Then

$$\ln[\lambda_1^{(N)}] < N^{-1}\ln Z_{N,N} < N^{-1}\ln[N(\lambda_1^{(N)})^N]. \tag{A10}$$

The right-hand side can be written

$$\ln[\lambda_1^{(N)}]+N^{-1}\ln N \xrightarrow[N\to\infty]{\lim} \ln[\lambda_1^{(N)}] \tag{A11}$$

which proves equation (5).

The transfer integral (equation (15)) has an infinite number of eigenvalues, even for finite L, so that it is not immediately obvious that the free energy of the continuum model is dominated by the largest of these. However, the distribution of eigenvalues, apart from the one belonging to the localised eigenfunction, is qualitatively independent of Δ. In the special case, $\Delta = 0$, the Hamiltonian (14) is diagonalised by the change of variable, $k(m) = h(m) - h(m+1)$. Then we have

$$\ln[\lambda_1^{(L)}] < M^{-1}\ln Z_{M,L} < M^{-1}\ln \int_{-\infty}^{\infty} \mathrm{d}k(1) \ldots \int_{-\infty}^{\infty} \mathrm{d}k(M-1) \times \int_{-1}^{L} \mathrm{d}h(M)\exp[-\beta(E-E_0)] \tag{A12}$$

where $Z_{M,L}$ is the partition function for (14) and $\lambda_1^{(L)}$ is the largest eigenvalue of the form (16). In the limit $M, L \to \infty$ with $M \propto L$, the right-hand side of (A12) becomes

$$\ln\left[\int_{-\infty}^{\infty} \mathrm{d}k(1)\exp(-2\beta J_{\|}|k(1)|)\right] = \ln\left(\frac{1}{\beta J_{\|}}\right) = \ln(\lambda_1^{(L)}). \tag{A13}$$

This proves that, for $\Delta = 0$, the free energy in the thermodynamic limit depends only on the largest eigenvalue of the transfer integral, and it appears reasonable to suppose the same for general Δ.

Note added in proof. Since this work was completed the author has learned of the following related publications.

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