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The CLE condition and the correlation length on the square lattice Ising model with first- and second-neighbour interactions

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Abstract. The square Ising lattice with nearest- and next-nearest-neighbour interactions is considered. On the basis of the simplest ansatz on the principal eigenvector of the transfer matrix of the model and of the CLE condition, developed in previous papers, the correlation length along a column is calculated for all $T \geq T_c$, in the ferromagnetic and antiferromagnetic regions. A comparison is made with results obtained through other methods. For competing interactions, it is shown that there is a mechanism which leads to a correlation length made of two analytic pieces.

1. Introduction

In this paper we consider a square lattice Ising model with first- and second-neighbour interactions, described by the Hamiltonian

$$\mathcal{H} = -J_1 \sum_{\langle i,j \rangle} s_i s_j - J_2 \sum_{[i,j]} s_i s_j \tag{1.1}$$

where $\langle i, j \rangle$ refers to the nearest-neighbour pairs, while $[i, j]$ stands for the summation over the next-nearest-neighbour pairs. We will make use of the parameters $K_1 = J_1/kT$, $K_2 = J_2/kT$ and $\rho = K_2/K_1$.

Due to its non-planar character, the above model is not exactly soluble. However, many of its very interesting properties have been conjectured or determined through various approximate methods, ranging from closed-form approximations (Fan and Wu 1969, Gibberd 1969, Burkhardt 1978), renormalization-group (RG) calculations (Nauenberg and Nienhuis 1974, van Leeuwen 1975, Nightingale 1977), Monte Carlo (MC) simulations (Landau 1980), combined MC and RG method (Swendsen and Krinsky 1979), series analysis of high-temperature expansions (Dalton and Wood 1969, Oitmaa 1981), and perturbation theory (Barber 1979).

In this paper we report some calculations on the model (1.1), concerning its correlation length along a column (or a row). The whole region $T \geqslant T_c$ is considered. We follow the approach developed in the previous works (Villani 1990, Angelini *et al* 1992), which is based on the correlation length equality (CLE) for probability distributions on strips of spins.

We start from the probability $P_1(\sigma)$ of a spin configuration $\sigma = (s_1, s_2, \ldots)$ on a column, which is given by $P_1(\sigma) = \Psi_1^2(\sigma)$, where $\Psi_1(\sigma)$ is the eigenvector of the symmetrized

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transfer matrix $L(\sigma|\sigma')$ of our model, associated to its highest eigenvalue. We introduce the simplest parametrization $\widetilde{P}_1(\sigma)$ of $P_1(\sigma)$, in a Boltzmann form, given by

$$\widetilde{P}_1(\sigma) = \widetilde{\Psi}_1^2(\sigma) \qquad \widetilde{\Psi}_1(\sigma) = \exp\left(A\sum_i s_i s_{i+1}\right). \tag{1.2}$$

Essentially, having fixed the attention on a column, we take into account, through $\widetilde{P}_1$, of the summation over the configurations of all the other columns, by replacing the original coupling K_1 between the spins on a column by an effective coupling $2A$, which is a function of K_1 and K_2.

In principle, the above ansatz $\widetilde{\Psi}_1(\sigma)$ makes sense only in some regions of the coupling plane (K_1, K_2). For $K_1 \geqslant 0$, $\rho > -\frac{1}{2}$ (region I) ($K_1 \leqslant 0$, $\rho < \frac{1}{2}$ (region II)) our system has a ferromagnetic (antiferromagnetic) ground state. So $\widetilde{\Psi}_1(\sigma)$ can be a reliable description in region I (II), with $A > 0$ ($A < 0$), as long as ρ ($-\rho$) is not very large; in the limit $|\rho| \to +\infty$, the lattice is decomposed into two independent square sub-lattices. In region III, that is $K_2 < 0$, $|\rho| > \frac{1}{2}$, the ground state, with its extra two-fold degeneracy, is 'superantiferromagnetic'. The simple parametrization (1.2) does not take into account of a such situation. Of course it can be implemented through proper corrections.

However, due to its simplicity, in the following we will make use of (1.2) and we will limit ourselves to region I, also adding the case $\rho = -\frac{1}{2}$. Region II can be analyzed through a similar procedure and we will mention briefly the analogous results. A particular attention will be fixed on the interesting domain $K_1 > 0$, $-\frac{1}{2} \leqslant \rho < 0$ of competing ferromagnetic and antiferromagnetic couplings, where our approach allows to get some further, new insight into the properties of the model. Our results, based on (1.2), are deduced from the CLE condition, whose simplest version is introduced and discussed in the next section.

2. The CLE condition for one and two columns

Besides $P_1(\sigma)$, let us consider the probability $P_2 = P(\sigma_1, \sigma_2)$ of a spin configuration (σ_1, σ_2) on two adjacent columns, regardless of the configurations of the other columns. We have (Villani 1990)

$$P_2 = P(\sigma_1, \sigma_2) = \Psi_1(\sigma_1) L(\sigma_1|\sigma_2) \Psi_1(\sigma_2). \tag{2.1}$$

Obviously, $P_1(\sigma_1)$ is the marginal distribution for the set σ_1, deduced from the joint distribution $P(\sigma_1, \sigma_2)$. Then all the statistical quantities along a column are the same for both of them.

Now, if we consider the ansatz $\widetilde{\Psi}_1(\sigma_1)$, instead of (2.1) we get the distribution for two adjacent columns

$$\widetilde{P}_2 = \widetilde{P}(\sigma_1, \sigma_2) = \widetilde{\Psi}_1(\sigma_1) L(\sigma_1|\sigma_2) \widetilde{\Psi}_1(\sigma_2). \tag{2.2}$$

$\widetilde{P}_2$ describes a system of spins on two adjacent columns, interacting through the same couplings of the original Hamiltonian (1.1), except along the columns, where K_1 is replaced by the effective coupling $A + K_1/2$.

As a rule, $\widetilde{P}_2$ does not reproduce $\widetilde{P}_1(\sigma_1)$ exactly if we sum over the set σ_2. However, having a parameter in (1.2), the marginality properties of the exact distribution $P_1(\sigma_1)$ can be partially satisfied by $\widetilde{P}_1(\sigma_1)$, if we fix our attention only on one statistical quantity.

Now, a statistical quantity that has a relevant and unique role is provided by the correlation length, so that we impose as a marginality requirement the consistency condition (Villani 1990, Angelini *et al* 1992)

$$\xi_D = \xi_N \tag{2.3}$$

where ξ_D is the correlation length of $\widetilde{P}_1$ and ξ_N is the correlation length along a column, associated with $\widetilde{P}_2$. Equation (2.3), which we call the CLE condition, allows to fix the parameter A and to calculate the correlation length along a column $\xi = \xi_D = \xi_N$.

This approach differs from the standard variational method, where the parameter A is fixed by considering the sup of the Rayleigh–Ritz quotient

$$\sup_A \frac{\sum_{\sigma_1,\sigma_2} \widetilde{P}(\sigma_1,\sigma_2)}{\sum_\sigma \widetilde{P}_1(\sigma_1)} \tag{2.4}$$

in order to get the best approximation to the free energy. It can be seen that (2.4) leads also to a marginality condition. This condition is expressed by the equality for $\widetilde{P}_1$ and $\widetilde{P}_2$ of the short distances correlation function $\langle s_i s_{i+1}\rangle$ along a column (Ruján 1979).

Coming back to (2.3), we have first of all

$$\frac{1}{\xi_D} = \ln\coth 2A\ . \tag{2.5}$$

In order to obtain ξ_N, we note that with the distribution $\widetilde{P}(\sigma_1,\sigma_2)$ is associated with the 4×4 transfer matrix

$$\begin{aligned}\ell = \ell(s_1,s_2|s_1',s_2') \\ &= \exp(K_1 s_1 s_2/2)\ \exp[(A+K_1/2)(s_1s_1'+s_2s_2')] \\ &\quad\times \exp[K_2(s_1s_2'+s_2s_1')]\ \exp(K_1 s_1' s_2'/2)\ .\end{aligned} \tag{2.6}$$

If

$$f_\pm = \mathrm{e}^{\pm K_1}\cosh(2A+K_1\pm 2K_2) \qquad g_\pm = 2\mathrm{e}^{\pm K_1}\sinh(2A+K_1\pm 2K_2) \tag{2.7}$$

we have that δ_1, the highest eigenvalue of ℓ (which is associated with an eigenstate of positive parity), is given by

$$\delta_1 = f_+ + f_- + \sqrt{4+(f_+-f_-)^2} \tag{2.8}$$

while $g_\pm$ are the eigenvalues of ℓ with eigenstates of negative parity. So if

$$\delta_2 = \max\{g_+, g_-\} \tag{2.9}$$

we have

$$\frac{1}{\xi_N} = \ln\frac{\delta_1}{\delta_2} \tag{2.10}$$

and (2.3) becomes

$$\tanh 2A = \frac{\delta_2}{\delta_1} \tag{2.11}$$

This equation can be solved analytically and gives the parameter A, and then the correlation length ξ, in terms of elementary functions of K_1 and K_2. At fixed K_2, we obtain a unique finite value $A(K_1, K_2)$ for every $K_1 < K_{1c}(K_2)$ while for $K_1 \geqslant K_{1c}(K_2)$ (2.11) is satisfied only by $A = +\infty$, giving the usual mechanism of second order phase transition, that is the highest eigenvalues degeneracy.

We also have

$$\lim_{K_1 \to K_{1c}^-(K_2)} A(K_1, K_2) = \lim_{K_1 \to K_{1c}^-(K_2)} \xi(K_1, K_2) = +\infty \, . \tag{2.12}$$

The critical curve so obtained is given explicitly by

$$K_{1c}(K_2) = \tfrac{1}{2}\ln(1 + \sqrt{2}e^{2K_2}) - 2K_2 \tag{2.13}$$

For $K_2 = 0$, we obtain the well known exact value $\frac{1}{2}\ln(1 + \sqrt{2})$.

It turns out that, in order to describe the behaviour of ξ, we have to distinguish between the domains $\rho \geqslant 0$, $-\frac{1}{2} < \rho < 0$ and $\rho = -\frac{1}{2}$.

When $\rho \geqslant 0$, we have that $\delta_2 = g_+$. As a consequence, for $0 \leqslant K_1 \leqslant K_{1c}(K_2)$, from (2.11) we obtain $\xi(K_1, K_2)$ as a unique analytic function of K_1 and K_2, given by

$$\frac{1}{\xi(K_1, K_2)} = -\ln\left\{ \frac{e^{K_1+2K_2}\sinh 2K_1 \sinh(K_1 + 2K_2)}{2(\cosh^2 K_1 - \sinh^2 2K_2)} \times \left[\sqrt{1 + 4e^{-4K_2}\frac{\cosh^2 K_1 - \sinh^2 2K_2}{\sinh^2 2K_1}} + 1\right]\right\} . \tag{2.14}$$

Again, for $K_2 = 0$, we obtain the exact Onsager result (Villani 1990)

$$\frac{1}{\xi(K_1, 0)} = -(\ln\tanh K_1 + 2K_1) \tag{2.15}$$

Furthermore, as a consequence of the analytic behaviour of $1/\xi$, the critical exponent ν deduced from (2.14) is equal to 1, for every fixed ρ, in agreement with previous predictions. Our calculation allows us to see the analytic origin of this value and of the universality concept.

When $-\frac{1}{2} < \rho < 0$, the competition between the ferromagnetic and the anti-ferromagnetic interactions gives rise to a relevant phenomenon. While for $\rho \geqslant 0$ we always have $g_+ > g_-$, for $\rho < 0$ these two eigenvalues of negative parity may cross each other at some values of A, K_1 and K_2. This crossing does not take place in the proximity of the critical point. There is a finite value $K_{1s}(K_2)$ of K_1, such that $K_{1s}(K_2) < K_{1c}(K_2)$ and, for $K_{1s}(K_2) \leqslant K_1 \leqslant K_{1c}(K_2)$, the equation (2.11) is solved with $\delta_2 = g_+$, as happens in the case $\rho \geqslant 0$. In this interval of K_1, the correlation length is given again by (2.14). So the above comment about the exponent ν is also valid for $-\frac{1}{2} < \rho < 0$. However, for $0 \leqslant K_1 \leqslant K_{1s}(K_2)$, (2.11) is solved with $\delta_2 = g_-$. In this last interval we have

$$\frac{1}{\xi(K_1, K_2)} = -\ln\left\{ \frac{e^{2K_2-K_1}\sinh 2K_1 \sinh(K_1 - 2K_2)}{2(\cosh^2 K_1 - \sinh^2 2K_2)} \times \left[\sqrt{1 + 4e^{-4K_2}\frac{\cosh^2 K_1 - \sinh^2 2K_2}{\sinh^2 2K_1}} - 1\right]\right\} . \tag{2.16}$$

Thus we obtain a correlation length which is continuous, but made of two analytic pieces, which match at the singular point K_{1s}. This point is a monotonic decreasing function of K_2, given by

$$K_{1s}(K_2) = \tfrac{1}{2}\ln\left[\cosh 2K_2 - e^{-2K_2}\sinh 2K_2 + \sqrt{(\cosh 2K_2 - e^{-2K_2}\sinh 2K_2)^2 - 1}\right] \tag{2.17}$$

In terms of ρ, we have

$$\lim_{\rho\to -1/2^+} K_{1s}(\rho) = +\infty \qquad \lim_{\rho\to 0^-} K_{1s}(\rho) = 0\,. \tag{2.18}$$

From (2.13) it also follows that

$$\lim_{\rho\to -1/2^+} K_{1c}(\rho) = +\infty\,. \tag{2.19}$$

Then we deduce that, for $\rho = -\frac{1}{2}$, $K_1 \geqslant 0$, the correlation length is given by a unique analytic function of K_1, which can be obtained from (2.16) by putting $K_2 = -\frac{1}{2}K_1$. We have

$$\frac{1}{\xi(K_1)} = \ln\frac{1}{2}\left(\sqrt{1+\frac{4e^{2K_1}}{\sinh^2 2K_1}} + 1\right). \tag{2.20}$$

We obtain $T_c(-\frac{1}{2}) = 0$, in agreement with previous arguments given in the literature. Near the critical point, that is for large values of K_1, we deduce from (2.20) the exponential behaviour

$$1/\xi(K_1) \simeq 4e^{-2K_1}\,. \tag{2.21}$$

We could say that the critical exponent ν, at $\rho = -\frac{1}{2}$, is $+\infty$.

The above results have been obtained in a simple and analytic way by making use of the distributions $\widetilde{P}_1$ and $\widetilde{P}_2$ in the CLE condition. Now we discuss a test of their reliability, which, at the same time, allows us to improve, as far as possible, the calculations done before.

On the basis of the spectral representation of the transfer matrix $L(\sigma|\sigma')$ and of the Perron–Frobenius theorem, we have that, if L is applied repeatedly to $\widetilde{\Psi}_1(\sigma)$, we reach an 'equilibrium' state which, actually, is described by $\Psi_1(\sigma)$ (Mattis 1985). So, if $\widetilde{\Psi}_1(\sigma)$ is an approximation to $\Psi_1(\sigma)$, we expect that the action of L on $\widetilde{\Psi}_1(\sigma)$ allows us to get closer to the properties of $\Psi_1(\sigma)$. If, hypothetically, $\widetilde{\Psi}_1(\sigma) = \Psi_1(\sigma)$, the repeated action of L would not change the state. Then we are led to consider the further distributions

$$\begin{aligned}
\widetilde{P}_3 &= \widetilde{P}(\sigma_1,\sigma_2,\sigma_3) = \widetilde{\Psi}_1(\sigma_1)L(\sigma_1|\sigma_2)L(\sigma_2|\sigma_3)\widetilde{\Psi}_1(\sigma_3) \\
\widetilde{P}_4 &= \widetilde{P}(\sigma_1,\sigma_2,\sigma_3,\sigma_4) = \widetilde{\Psi}_1(\sigma_1)L(\sigma_1|\sigma_2)L(\sigma_2|\sigma_3)L(\sigma_3|\sigma_4)\widetilde{\Psi}_1(\sigma_4) \\
&\ \vdots
\end{aligned} \tag{2.22}$$

for strips made of three adjacent columns, four adjacent columns, and so on. A similar procedure appears in a recent approach to the calculation of the critical temperature (Lipowski and Suzuki 1992).

Now, if we consider two distributions $\widetilde{P}_i$ and $\widetilde{P}_j (i \neq j)$ and demand that they have the same correlation length along the columns, we obtain generally a new equation and a new evaluation of ξ. These evaluations can be considered reliable if they show a significant consistency between them or if they are not changed significantly by going to distributions of higher order.

The calculation of the correlation length as a function of A, for each $\widetilde{P}_i$, can be done by making use of the transfer matrix formalism. With $\widetilde{P}_i$ is associated a $2^i \times 2^i$ transfer matrix, which can be reduced and simplified considerably due to its symmetry properties.

3. The CLE condition for strips of size two and three and its consequences

In this paper we report the results based on the CLE condition applied to the pair $\widetilde{P}_2, \widetilde{P}_3$, and to the pair $\widetilde{P}_3, \widetilde{P}_4$, which leads to the evaluations $\xi^{(2)}$ and $\xi^{(3)}$ of ξ, respectively. We also call $\xi^{(1)}$ our simple calculation of section 2, based on the $\widetilde{P}_1, \widetilde{P}_2$, and $T_c^{(i)}(\rho)$ the critical curve where $\xi^{(i)}$ diverges. For the calculation of $\xi^{(2)}$ and $\xi^{(3)}$ we need the higher eigenvalues of Hermitian matrices of order three, four and six.

We obtain that both the sequences $\xi^{(1)}, \xi^{(2)}, \xi^{(3)}$ and $T_c^{(1)}, T_c^{(2)}, T_c^{(3)}$ are monotonic decreasing. Depending on the values of ρ, it is useful to give the critical curves $T_c^{(i)}(\rho)$ either in terms of the parameter K_1 or in terms of the parameter K_2.

(In (*b*) the dashed line lies between the full and dotted lines.)

For a large interval of positive values of ρ, the functions $K_{2c}^{(i)}(\rho)$ $(i = 1, 2, 3)$ are shown in figure 1(*a*). For $0 \leqslant \rho \leqslant \frac{1}{2}$, the $K_{2c}^{(i)}$ are practically coincident; in this interval, our first simple evaluation (2.13) gives an excellent description of the critical curve. The numerical results obtained through a series-expansion method by Dalton and Wood (1969), are well reproduced . However, while the numerical data for $T_c(\rho)/T_c(0)$ are fitted through a linear law (for $0 \leqslant \rho \leqslant 1$)

$$T_c(\rho)/T_c(0) = 1 + m\rho \tag{3.1}$$

giving $m \simeq 1.45$, we obtain the slope at $\rho = 0$ of the same quantity equal to $\sqrt{2}$, which presumably is the exact value.

As a matter of fact our $K_{1c}^{(1)}(\rho)$ (2.13) has been already obtained by Fan and Wu (1969), through a quite different elaborate procedure, the so-called free fermion approximation. However, if one attempts to go beyond this approximation by making use of the perturbation theory, the result on the critical curve is not modified.

On the other hand our approach, through strips of higher size, allows to get some improvement. Figure 1(*a*) shows that, in the interval $\frac{1}{2} < \rho < 2$, the critical curve is well described by $K_{2c}^{(2)}(\rho)$, while, for $2 < \rho < 10$, the same property is shared by $K_{2c}^{(3)}(\rho)$. Our predictions are in excellent agreement with the more extensive numerical results obtained by Oitmaa (1981) through the series expansion method.

As we see from figure 1(*a*), in the limit $\rho \to +\infty$, $K_{2c}^{(i)}(\rho)$ do not reproduce the exact value $K_{2c}(+\infty) = \frac{1}{2}\ln(1+\sqrt{2})$. Furthermore, for large ρ, the convergence of the sequence $K_{2c}^{(1)}(\rho), K_{2c}^{(2)}, K_{2c}^{(3)}(\rho), ..$ seems very weak. Of course, it could be accelerated by making use of some standard algorithm. As a matter of fact, when $\rho \to +\infty$, the sets of spins on a column splits into two independent subsets. As a consequence, our parametrization (1.2) is not appropriate for large ρ and near the critical point, since the above subsets are strongly coupled through the effective parameter A. However if we take into account of the geometry of our lattice, we have that the simplest parametrization of $P(\sigma)$, in the limit $\rho \to +\infty$, is given by

$$\widetilde{P}_1'(\sigma) = \widetilde{\Psi}_1'^2(\sigma), \widetilde{\Psi}_1'(\sigma) = \exp\left(B\sum_i s_i s_{i+2}\right) \tag{3.2}$$

Now, if we apply the CLE condition to $\widetilde{P}_1'$ and to

$$\widetilde{P}_2' = \widetilde{P}'(\sigma_1, \sigma_2) = \widetilde{\Psi}_1'(\sigma_1) L(\sigma_1|\sigma_2) \widetilde{\Psi}_2'(\sigma_2) \tag{3.3}$$

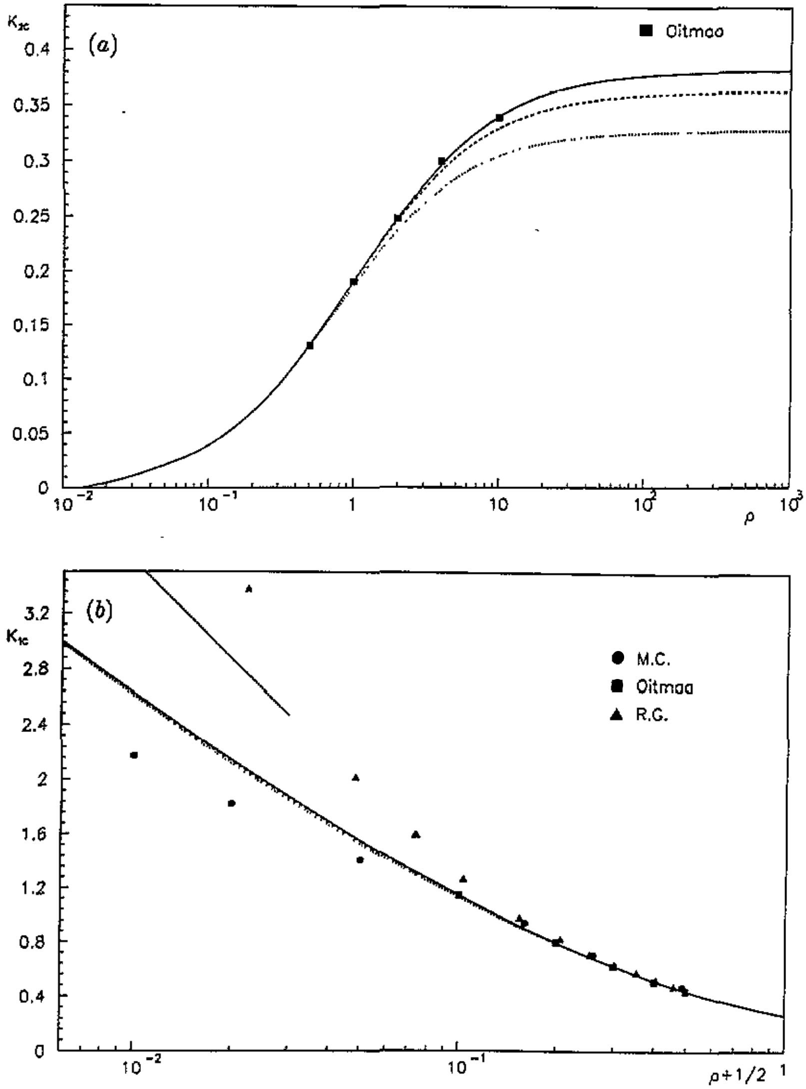

Figure 1. The critical curve calculated from strips of size one (dotted line), two (dashed line) and three (full line). (*a*) K_{2c} versus ρ for a large range of positive ρ's, compared with the results of Oitmaa. (*b*) K_{1c} versus ρ for negative ρ's, compared with the results of Oitmaa, of Nauemberg and Nienhuis (RG), and of Landau (MC). The straight line shows our asymptotic behaviour (3.5) for $\rho \to -\frac{1}{2}^{+}$.

in the limit $K_1 \to 0$, we obtain again the exact value: $K_{2c}^{(1)'}(+\infty) = \frac{1}{2}\ln(1+\sqrt{2})$. So an improved parametrization over the whole range of positive values of ρ, would be

$$\widetilde{P}_1''(\sigma) = \widetilde{\Psi}_1''^2(\sigma),\ \widetilde{\Psi}_1''(\sigma) = \exp\left(A\sum_i s_i s_{i+1} + B\sum_i s_i s_{i+2}\right). \qquad (3.4)$$

Now, coming back to our $\widetilde{\Psi}_1(\sigma)$, let us consider the interesting interval $-\frac{1}{2} \leqslant \rho < 0$. Our results on the critical curve are shown in figure 1(*b*). For $-0.3 < \rho < 0$, the three functions $K_{1c}^{(i)}(\rho)$ are practically coincident, while for $-\frac{1}{2} \leqslant \rho \leqslant -0.3$ there is only a small difference. In agreement with several arguments we obtain $T_c^{(i)}(-\frac{1}{2}) = 0$. Furthermore, asymptotically for $\rho \to -\frac{1}{2}^+$ we have

$$K_{1c}^{(i)}(\rho) \simeq -\ln 2\sqrt{2}(\tfrac{1}{2}+\rho) \qquad (i = 1, 2, 3)\,. \tag{3.5}$$

There are further diverging log–log corrections to this behaviour, so that the asymptotic regime is reached for ρ very near $-\frac{1}{2}$. In figure 1(*b*) the straight line gives the function $-\ln 2\sqrt{2}(\rho+\frac{1}{2})$; we see that, in the range of values of ρ reported, it differs considerably from the functions $K_{1c}^{(i)}(\rho)$.

When we have competing interactions, the series expansion method is faced with oscillating or, eventually, irregular results. As a matter of fact, Dalton and Wood, having a short series, were unable to obtain the critical curve for $\rho < 0$. However Oitmaa, by calculating a further five terms in the high-temperature expansion, obtained the critical points for $-0.4 \leqslant \rho \leqslant 0$. But again, for $-\frac{1}{2} \leqslant \rho \leqslant -0.4$, the series becomes irregular and no conclusion has been reached. The first results on the critical curve for $-\frac{1}{2} \leqslant \rho < 0$ have been obtained by Nauemberg and Nienhuis (1974), through approximate RG transformations. Other estimates have been obtained by Landau (1980) through the MC method. The above results, denoted by RG and MC respectively, and the calculations of Oitmaa are reported in figure 1(*b*). While for $-0.4 \leqslant \rho \leqslant 0$, there is a general agreement with our predictions, for $-\frac{1}{2} < \rho < -0.4$ the MC and RG methods get respectively lower and higher values than our critical curve. The last MC points on the left are consistent with a straight line; as a matter of fact Landau makes such a linear fit, in order to get consistency in the crossover scaling analysis. However, as we have observed, at these points we are not in the asymptotic regime.

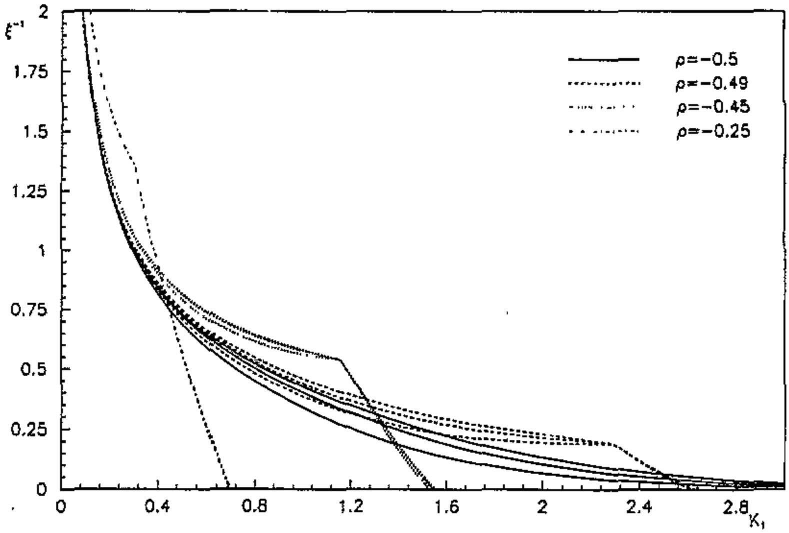

Figure 2. The inverse correlation length ξ^{-1} as a function of K_1 for some negative values of ρ, obtained from our three calculations.

In the above interval $-\frac{1}{2} \leqslant \rho < 0$, the correlation lengths $\xi^{(i)}(K_1, \rho)$ are shown in figure 2, for several values of ρ. The crossing phenomenon involving the highest eigenvalues of negative parity, is confirmed by the further CLE conditions which lead to $\xi^{(2)}(K_1, \rho)$ and $\xi^{(3)}(K_1, \rho)$. It occurs at the same point $K_{1s}(\rho)$ given by (2.17) and, as we see in figure 2, it is responsible for a singularity in the temperature dependence of the correlation length, given by a discontinuity in the first derivative. Furthermore the phenomenon is present for every ρ such that $-\frac{1}{2} < \rho < 0$, anticipating the behaviour which occurs at $\rho \simeq -\frac{1}{2}$. As a matter of fact, as $\rho \to -\frac{1}{2}^+$, the above crossing gives the mechanism of the crossover behaviour between the $T = 0$, $\rho = -\frac{1}{2}$ transition and the asymptotic critical behaviour near $K_{1c}^{(i)}(\rho)(\rho \neq -\frac{1}{2})$, which is characterized by the critical exponent $\nu = 1$.

In the limit $\rho \to -\frac{1}{2}$, the trend at the left of $K_{1s}(\rho)$ dominates over the whole interval $0 < K_1 < +\infty$. It is exponentially decreasing, when $K_1 \to +\infty$, for the three evaluations $1/\xi^{(i)}(K_1)(\rho = -\frac{1}{2})$, as in (2.21), the difference for $1/\xi^{(2)}$ and $1/\xi^{(3)}$ being in the multiplicative coefficient. Some features of the above crossover behaviour have been already observed by Landau in the MC calculations; however, it is difficult to get definite conclusions by the MC approach as $\rho \to -\frac{1}{2}$, and only consistency arguments with some ansatz of the crossover scaling theory, like the exponential behaviour, can be given.

A further insight into the above transition phenomenon is provided by our approach, if we analyse the asymptotic critical behaviour near $K_{1c}(\rho)(\rho > -\frac{1}{2})$. We fix our attention on the amplitude $\sigma(\rho)$ given by

$$\xi(K_1, \rho) \simeq \frac{\sigma(\rho)}{1 - K_1/K_{1c}(\rho)} . \tag{3.6}$$

We obtain the result that, for the three evaluations $\xi^{(i)}(K_1, \rho)$, the leading behaviour of $\sigma(\rho)$, as $\rho \to -\frac{1}{2}^+$, is given by

$$\sigma(\rho) \simeq \frac{1}{16(\rho + \frac{1}{2}) \ln^2(\rho + \frac{1}{2})} . \tag{3.7}$$

So the transition to the regime of strong competition between the ferromagnetic and antiferromagnetic couplings, is characterized by a further divergence in the correlation length, which appears through its amplitude. In this way we have a kind of matching between the exponential behaviour to the left of $K_{1s}(\rho)$ and the linear behaviour to the right of the same point.

Concerning the reliability of the three evaluations $\xi^{(i)}(K_1, \rho)$, we have that up to $\rho \simeq -0.3$, they practically overlap, so that it is sufficient to consider, in this interval, $\xi^{(1)}(K_1, \rho)$; on the other hand, for ρ between -0.3 and -0.45, we can limit ourselves to $\xi^{(2)}(K_1, \rho)$. For ρ smaller and up to $-\frac{1}{2}$, $\xi^{(3)}(K_1, \rho)$ provides a more reliable result. In any case, for ρ near $-\frac{1}{2}$, the values of K_1, for which there is less stability, are not in the proximity of the critical point, but at the left of the singular point $K_{1s}(\rho)$.

For $\rho \geqslant 0$, all the three quantities $\xi^{(i)}(K_1, K_2)$ are each described by a unique analytic function. The maximum of the discrepancy between $\xi^{(1)}, \xi^{(2)}$ and $\xi^{(3)}$ appears at the critical point, as shown in figure 3, in the case $\rho = 10$. As we leave the critical point, they become closer and closer. This feature is common to every positive ρ. As a consequence, for $\rho \epsilon [0, \frac{1}{2}]$, $\xi^{(1)}(K_1, \rho)$ provides a quite good description of the correlation length for every $T \geqslant T_c(\rho)$, while this happens for $\xi^{(2)}(K_1, \rho)$ if $0 \leqslant \rho \leqslant 2$. Up to $\rho \simeq 10$, we have that $\xi^{(3)}$ is a reliable evaluation of the correlation length for every $T \geqslant T_c(\rho)$.

For large ρ , we see, through the calculation of the three functions $\xi^{(i)}(K_2, \rho)$, that our parametrization (1.2) is not appropriate only near the critical point, where large value of

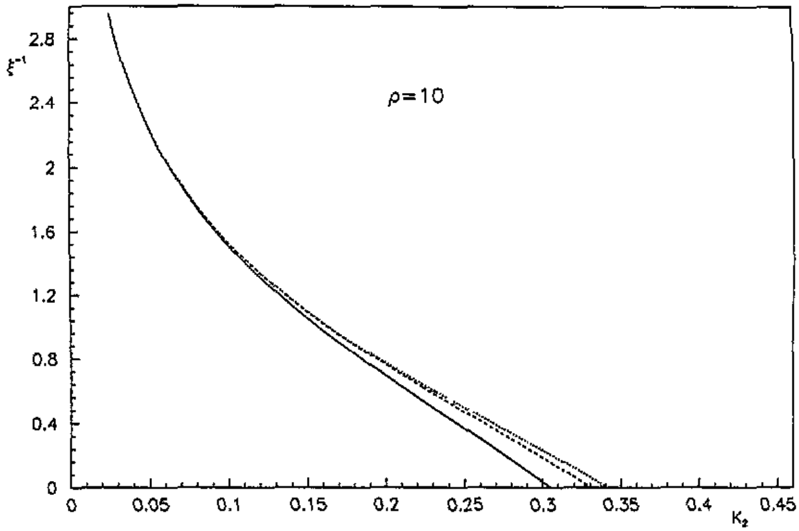

Figure 3. The inverse correlation length ξ^{-1} as a function of K_2 at $\rho = 10$ calculated for strips of size one (dotted line), two (dashed line) and three (full line).

A are required in order to have long-range correlations. However, if we leave the critical point, than $\xi^{(3)}(K_2, \rho)$ gives a reliable result even for large ρ. In figures 4(a) and 4(b) we show $\xi^{(3)}$ as a function of K_1 and K_2 respectively, for several values of ρ. At $\rho = 0$, we have that $\xi^{(3)} = \xi^{(2)} = \xi^{(1)}$ gives the exact Onsager result. In figure 4(b) we show also $1/\xi$ for $\rho = +\infty$, calculated through (3.2) and (3.3); we get then the exact answer over the whole range $T \geqslant T_c$. We note that, when $K_1 = 0$, our correlation length along a column becomes the correlation length along a diagonal of a square lattice.

4. Conclusions

The above results have been obtained by fixing the attention on region I of the coupling plane (K_1, K_2). In region II of the antiferromagnetic behaviour ($K_1 < 0, \rho < \frac{1}{2}$), the correlation lenghth along a column can be deduced quite easily from the previous calculations.

First of all, for $K_1 < 0$ and $\rho < \frac{1}{2}$, we consider in (1.2) a negative effective coupling parameter A. It is the same as introducing

$$\widetilde{\Phi}_1(\sigma) = \exp\left(-A \sum_i s_i s_{i+1}\right) \qquad (A > 0) \tag{4.1}$$

while, for $K_1 > 0$, we always have

$$\widetilde{\Psi}_1(\sigma) = \exp\left(A \sum_i s_i s_{i+1}\right) \qquad (A > 0)\,. \tag{4.2}$$

Now, if we consider the distributions

$$\widetilde{\Phi}_1^2(\sigma),\;\; \widetilde{\Phi}_1(\sigma_1)L(\sigma_1|\sigma_2)\widetilde{\Phi}_1(\sigma_2),\;\; \widetilde{\Phi}_1(\sigma_1)L(\sigma_1|\sigma_2)L(\sigma_2|\sigma_3)\widetilde{\Phi}_1(\sigma_3),\;\ldots$$

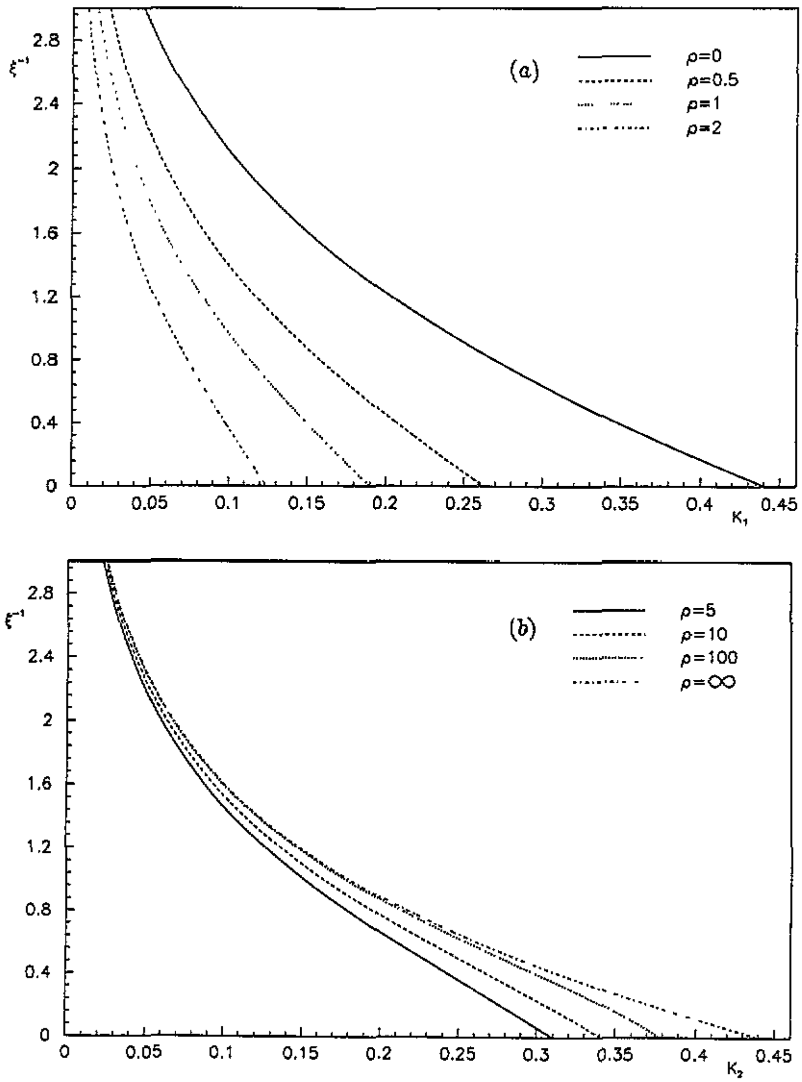

Figure 4. The inverse correlation length ξ^{-1} (*a*) as a function of K_1 for small values of ρ, and (*b*) as a function of K_2 for large values of ρ, deduced from our last calculation.

we see that the pair correlation functions on a column can be obtained, up to a possible change in the sign, from the distributions

$$\widetilde{\Psi}_1^2(\sigma),\ \widetilde{\Psi}_1(\sigma_1)L(\sigma_1|\sigma_2)\widetilde{\Psi}_1(\sigma_2),\ \widetilde{\Psi}_1(\sigma_1)L(\sigma_1|\sigma_2)L(\sigma_2|\sigma_3)\widetilde{\Psi}_1(\sigma_3),\ \ldots$$

by replacing K_1 by $-K_1 = |K_1|$ in $L(\sigma_1|\sigma_2)$. As a consequence our $\xi^{(i)}$ are functions of $(|K_1|, K_2)$.

In region III, neither $\widetilde{\Phi}_1(\sigma)$ nor $\widetilde{\Psi}_1(\sigma)$ are appropriate to describe the extra twofold degeneracy in the 'superantiferromagnetic' behaviour. However, such a situation could be analysed through a linear combination of (4.1) and (4.2). In any case, when ρ is large, it seems more appropriate to add a further parameter, like the coupling B in (3.4). In order to fix both the parameters A and B, we can consider a variational procedure constrained by the CLE condition (Angelini *et al* 1992).

These further analyses, together with generalizations of the model (1.1), will be reported elsewhere.

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