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To cite this version:
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G. G. Cabrera (*), R. Jullien
Physique des Solides, Bât. 510, Université de Paris-Sud, Centre d'Orsay, 91405 Orsay Cedex, France

E. Brézin and J. Zinn-Justin
Service de Physique Théorique CEN-Saclay, 91191 Gif-sur-Yvette Cedex, France

(Reçu le 24 janvier 1986, révisé le 19 mars 1986, accepté le 10 avril 1986)

Résumé. — Les transitions du premier ordre sont arrondies dans des géométries finies ou dans des bandes de largeur finie (cylindres). Nous avons examiné dans ce travail l'arrondissement du saut d'aimantation d'un modèle d'Ising à température fixée, en dessous de Tc lorsque le champ extérieur passe d'une valeur positive à une valeur négative. Cet arrondi est bien connu dans une géométrie finie mais la situation est plus complexe, et plus intéressante, pour un cylindre. En effet Privman et Fisher ont montré quel était le rôle joué par la longueur de corrélation le long de l'axe du cylindre, qui croît exponentiellement lorsque l'aire A de la section augmente. Il s'ensuit que le champ extérieur correspondant à une aimantation M donnée tend exponentiellement vers sa limite de volume infini, mais le coefficient dans l'exponentielle n'est pas le même si M est supérieur, inférieur ou égal à l'aimantation spontanée du système infini M0. La théorie est testée numériquement de manière satisfaisante à partir de résultats numériques sur le modèle d'Ising en champ à deux dimensions, ou plutôt sur son équivalent, le modèle quantique unidimensionnel en champ transverse.

Abstract. — First order transitions are rounded in finite cells or in infinite strips of finite width (cylinders). In this work we have considered the rounding of the jump of the magnetization of an Ising system at a fixed temperature T below Tc when the external field h goes from a small positive, to a small negative value. This rounding is well-known in a finite cell (block geometry) but the situation is more complicated, and more interesting, in a cylinder. Indeed it is known from the work of Privman and Fisher that these rounding effects are related to the behaviour of the correlation length along the axis of the cylinder which increases exponentially with the cross-sectional area A of the strip. It then follows that if one studies, for a given magnetization M, the external field h, this field approaches exponentially with A its bulk limit, but the coefficient inside the exponential is different if M is smaller, larger than or equal to the bulk spontaneous magnetization M0. We present numerical data for the two-dimensional case (or equivalently for the one-dimensional quantum model in a transverse field) which are in satisfactory agreement with the theory.

1. Introduction.

Finite-size scaling has been proved to be a very useful tool to investigate second order phase transitions in classical as well as quantum systems [1]. In this method, a given quantity such as the magnetization, or the correlation length (or the mass gap in a quantum system) is numerically calculated for an increasing sequence of finite systems. The bulk limit is usually approached exponentially (with periodic boundary conditions) away from Tc and as a power law at Tc.

This exponent is related (through the exponent ν characterizing the divergence of the correlation length at the transition) to the exponent governing the singularity of the quantity in the bulk. Thus a single log-log plot of the numerical results allows to locate the transition and to extract the critical exponents.

Concerning first-order transitions a non-universal behaviour is a priori expected since there is no diverging characteristic length : indeed the correlation length remains finite at the transition temperature and the details of the microscopic structure cannot be forgotten. However it is interesting that the finite size rounding in a block or in a cylinder geometry (in which all the dimensions of the system, except possibly one, remain finite) is nevertheless universal. This is
related to the fact that the correlation length of the finite system $\xi$, below the bulk transition temperature, is considerably larger than the bulk correlation length $\xi_{\infty}$. In a block geometry one cannot define a true correlation length through the exponential decay of the order parameter correlation function. One can define instead a length through moments of the correlation function, but then this length is at most of the order of the size of the block. The corresponding rounding has been recently described by a number of authors [2, 3]. It is found that the jump of the magnetization for the $d$-dimensional Ising model, when the magnetic field is varied through zero, is described by the relation

$$M = M_0 \tanh (\beta L^d HM_0) + \chi_{\infty} H,$$

(1)

where $L$ is the edge length of the hypercubic block, $M_0$ is the spontaneous magnetization of the infinite system, $H$ the magnetic field, and $\chi_{\infty}$ is the bulk zero-field magnetic susceptibility. It is instructive to analyse the finite size effects by solving for the magnetic field, given the magnetization $M$ near $M_0$. The bulk limit of $H$ for given $M$, is zero for $|M| < M_0$, and $(M - M_0)/\chi_{\infty}$ for $M > M_0$. From (1) one sees that this bulk limit is approached exponentially for $M > M_0$, and as a power $L^{-d}$ for $M < M_0$, with an extra $\ln L$ right at $M_0$.

The situation is more interesting for a cylinder of cross sectional area $A$ (in $d$ dimensions, $A$ is the generalized area $A = L^{d-1}$ of the section perpendicular to the axis of the cylinder). The bulk correlation length is defined, below the transition temperature, from the order parameter connected correlation function (by convention the bulk order parameter is zero in the bulk limit). The bulk correlation length (4) has a striking effect on the behaviour of the order parameter with the size in a cylinder geometry [5]. In part 2 we investigate analytically the relation between the applied field $H$ and the magnetization $M$. For a given $M$ the field approaches its bulk limit exponentially, but the behaviour is different if $M$ is larger, smaller than or equal to $M_0$. Let us stress that this exponential approach persists even for $M = M_0$, whereas in a block geometry, $H$ goes to zero as the inverse of the volume. In part 3, a numerical diagonalization of the quantum one dimensional Ising chain, in a transverse and longitudinal field, the Hamiltonian version of the 2-D Ising model in a field, is compared with the analytic predictions. A first analysis of naive finite size scaling type (power law approach at $M_0$) leads close to $T_c$ to strange temperature dependent exponents; the fit becomes worse at lower temperatures, whereas on the whole range it fits very well the exponential plus power behaviour of the analytic theory: a blind application of finite size scaling would lead to meaningless results. Furthermore the three different exponential behaviours in the three regions $M > M_0$, $M = M_0$, $M < M_0$, are well reproduced and provide an accurate extrapolation procedure to determine the jump $M_0$ from a finite size calculation.


The result was first derived by Privman and Fisher [3], who considered also the cross-over from a block to a cylinder geometry. We give here for completeness a short derivation of their result.

We consider an Ising, or Ising-like, system on a $d$-dimensional hypercubic lattice, on a cylinder with cross-sectional area $A = L^{d-1}$. Periodic boundary conditions in the $(d-1)$-dimensional section, are assumed.

The free energy is dominated below $T_c$ by the two highest eigenvalues of the transfer matrix, which are exponentially close. Their distance is the inverse of the correlation length (4). All the other eigenstates, at fixed $T$ below $T_c$, lie below these two highest states with a finite gap. Therefore the long distance properties are governed entirely by these two states. In the absence of an external symmetry-breaking field these two states correspond to the quasi-degenerate lowest states (the Hamiltonian is minus the logarithm of the transfer matrix) of the quantum
one-dimensional Hamiltonian

\[ H = \frac{p^2}{L^{d-1}} + L^{d-1} V(q) \]  

(5)

in which \( V(q) \) is an even double-well potential [2] with two degenerate minima away from \( q = 0 \). Indeed the splitting of the even lowest state and the odd one is exponentially small.

If an external field is applied two main effects have to be considered:

i) the field induces matrix elements between the even and odd lowest states. This coupling is proportional to the applied field \( h \) (the external field \( H \) in reduced units), to the magnetization \( M_0 \) and to the area \( A \) of the cross-section;

ii) diagonal matrix elements are shifted quadratically in \( h \), with a coefficient, which is the bulk susceptibility per unit volume \( \chi_\infty \), multiplied by \( A \), (finite size corrections to \( \chi_\infty \) would lead to negligible corrections).

Therefore within the relevant space of the lowest two states, the transfer matrix reduces to

\[
- \ln \tau = \begin{bmatrix}
-1/2 m_L & 0 \\
0 & 1/2 m_L
\end{bmatrix} 
\]

for \( h = 0 \) \( (m_L \equiv \xi_L^{-1}) \)  

(6)

whereas

\[
- \ln \tau = \begin{bmatrix}
-1/2 m_L + 1/2 A \chi_\infty h^2 & \delta A M_0 h \\
\delta A M_0 h & 1/2 m_L + 1/2 A \chi_\infty h^2
\end{bmatrix}
\]

(7)

for non-zero \( h \), in which \( \delta \) is a pure number which will be determined below.

Neglecting higher orders in \( h \), the two eigenvalues of (7) are simply

\[
e_\pm = 1/2 A \chi_\infty h^2 \pm \left( \frac{m_L^2}{4} + \delta^2 A^2 M_0^2 h^2 \right)^{1/2}.
\]

(8)

The magnetization (per site) in the plus state is given by

\[
M = \frac{1}{A} \frac{\partial e_+}{\partial h} = \chi_\infty h + \frac{\delta^2 M_0^2 A h}{\left( \frac{m_L^2}{4} + \delta^2 M_0^2 A^2 h^2 \right)^{1/2}}.
\]

(9)

If \( A \) goes to infinity first, \( M \) should approach the (small \( h \)) bulk law

\[
M = M_0 + \chi_\infty h.
\]

(10)

Comparing (9) and (10) we see that the undetermined number \( \delta \) has to be equal to

\[
\delta = 1.
\]

(11)

We thus obtain the rounded field-magnetization relation (for small \( h \))

\[
M = \chi_\infty h + \frac{L^{d-1} h M_0^2}{\left[ 4 m_L^2 + (h M_0 L^{d-1})^2 \right]^{1/2}}
\]

(12)

with \( m_L^{-1} = \xi_L \), given by (4).

It is interesting to analyse this rounding for various parts of the curve, and determine the value of the field corresponding to a given magnetization:

i) \( M = r M_0 \) with \( 0 < r < 1 \) finite. Solving (12) one finds, for large \( L \)

\[
h M_0 L^{d-1} = 1/2 - \frac{r}{\sqrt{1 - r^2}} m_L
\]

and thus, with (4)

\[
h \propto L^{-1/2(d+1)} \exp - (\sigma L^{d-1})
\]

(13)

Clearly the point \( r = 1 \) \( (M = M_0) \) is singular and must be treated separately.

ii) \( M = M_0 \)

The equation (12) is quartic in \( h \), but keeping the leading terms for small \( h \), large \( L \), one obtains

\[
h^2 = \frac{1}{8 M_0 \chi_\infty L^{2(d-1)}},
\]

i.e.

\[
h \propto L^{-1/3(d+1)} \exp - (2/3 \sigma L^{d-1})
\]

(15)
For $M = (1 + r) M_0$, $r > 0$ we have to compare $h$ to the bulk solution $h_\infty$

$$h_\infty = \frac{r M_0}{\chi_\infty}.$$  \hspace{1cm} (16)

The same algebra leads from (12) to

$$h - h_\infty \propto L^{- (d + 1)} \exp - (2 \sigma L^{d-1}).$$  \hspace{1cm} (17)

We see thus from (13), (15), (17) that the three parts of the curve, $M < M_0$, $M = M_0$, $M > M_0$ scale differently. They all approach exponentially their bulk limit, but the coefficient of the interfacial energy is equal to 1, 2/3 or 2. The prefactor has also three different behaviours. In two dimensions the respective powers are $L^{-3/2}$, $L^{-1}$, $L^{-3}$, and since $m_\ell$ is known exactly these three powers are known without ambiguity. For $d > 2$, since the derivation of equation (9) is more delicate (in particular in three dimensions, an extra logarithm could be present) it would be interesting to compare the predictions of this analysis to a finite size calculation. To summarize let us collect the above formulae for the case $d = 2$.

The surface tension below $T_c$ has been calculated by Onsager [6] for the plane square lattice

$$\sigma_\perp(T) = \frac{2 J_\perp}{k_B T} - \ln \coth \left(\frac{J_\perp}{k_B T}\right),$$  \hspace{1cm} (18)

for an interface parallel to the $x$ axis.

The finite-size behaviour of finite two-dimensional strips of width $L$ is given by

$$h = \begin{cases} 
Cte \times L^{-3/2} \exp[- L \sigma(T)], & \text{if } M < M_0; \\
Cte \times L^{-1} \exp[- 2/3 L \sigma(T)], & \text{if } M = M_0; \\
h_\infty + Cte \times L^{-3} \exp[- 2 L \sigma(T)], & \text{if } M > M_0.
\end{cases}$$  \hspace{1cm} (19)

We will test these results numerically in the next section.

### 3. Numerical analysis in two dimensions.

For convenience the numerical analysis will be performed with the Hamiltonian version of the two-dimensional Ising model, which is the quantum Ising chain in a transverse field.

As it is well-known [7] this model corresponds to an extreme anisotropic limit of the usual 2-D Ising model, when the two (reduced) coupling constants $K_1$, along the axis of the cylinder (« time » direction) and $K_2$ in the transverse direction are sent respectively to infinity and zero,

$$K_1 \to \infty \quad K_2 \to 0$$  \hspace{1cm} (20a)

in such a way that

$$K_2 \exp 2 K_1 = 1/\gamma$$  \hspace{1cm} (20b)

remains finite; the parameter $\gamma$ is the transverse field in reduced units.

The correlation length is the inverse of the mass gap between the two lowest states of the Hamiltonian

$$H = - \sum_{n=1}^{N} \sigma_n(n) \sigma_n(n + 1) - \gamma \sum_{n=1}^{N} \sigma_n(n) - h \sum_{n=1}^{N} \sigma_n(n).$$  \hspace{1cm} (21)

The finite size behaviour of the (zero field) mass gap can be obtained analytically for $d = 2$, either from an explicit finite size solution [8], by performing the anisotropic limit (20), or directly from the Hamiltonian (21) [9]. Finite-size scaling methods in this Hamiltonian language have been also developed by Hamer and Barber [10]. The result for the zero field mass gap

$$m(\gamma, N) \sim N^{-1/2} \exp - N \sigma(\gamma)$$  \hspace{1cm} (22)

in which $N$ is the transverse size in units of the lattice spacing, with

$$\sigma(\gamma) = - \ln \gamma.$$  \hspace{1cm} (23)

When a longitudinal field is applied, the calculation has to be performed numerically. A first order transition takes place when the longitudinal field $h$ goes through zero in the region $\gamma < 1$. We have studied numerically the size dependence of this first order transition and compared it with the description of the previous section. We have studied values of $N$ up to 14, but in some cases (at lower temperatures) it was not necessary to go beyond $N = 8$. The computational work can be summarized as follows:

i) the magnetization is calculated exactly as a function of the size, for fixed values of both the transverse and the longitudinal fields;

ii) for a given value of the magnetization $0 < M < 1$, we obtain the corresponding longitudinal field using an inversion sub-program;

iii) we plot this longitudinal field as a function of the size and compare it with (19) or with a power law.

This procedure has been chosen because it provides a general and simple tool which allows to check the experimental data and to localize the spontaneous magnetization when it is unknown.

Near the critical value of $\gamma$ ($\gamma_c = 1$), we face a difficulty: indeed the surface tension is going to zero and it becomes more difficult to distinguish a power-law from an exponential behaviour. Therefore we deal with higher value of $N$ by the Lanczos method [10] which approximates accurately the ground state and the first excited level. The cross-over to an exponential behaviour at larger $N$ is then observed. On the other
hand, far from the critical point, the exponential behaviour is much more pronounced. Therefore the magnetization is rapidly saturated and this makes an accurate calculation of $h(M)$ more difficult.

The analysis shows that the present study is useful to answer the following question: as long as the size is finite, the magnetization as a function of the field is analytic; $M$ vanishes with $h$, whereas the bulk magnetization would jump from $+M_0$ to $-M_0$. Can one thus find an efficient extrapolation procedure which allows one to determine $M_0$ from a finite size calculation? It is shown below that the three different exponential behaviours of $h(M)$, as a function of the size, for $M > M_0$, $M < M_0$, and $M = M_0$ provide an accurate determination of $M_0$.

Assuming that the expression (19) is asymptotically valid, we write the longitudinal field, for $M > M_0$, in the following form for arbitrary $N$:

$$\ln h(N) = -\alpha(N) \ln N - N\sigma(N) + C + 0(1/N)$$

(24)

where $\alpha(N)$ and $\sigma(N)$ are « weakly » $N$-dependent quantities (they differ from their infinite size values by quantities which are at worst of order $1/N$). To improve the convergence with the size we define a new quantity

$$Y \equiv \ln \left[ \frac{h(N)}{h(N-1)} \right]$$

(25)

which by using relation (24) and the fact that $\sigma(N-1) \approx \sigma(N)$, $\alpha(N-1) \approx \alpha(N)$, can be cast into the form

$$Y = \ln \left[ \frac{h(N)}{h(N-1)} \right] = -\alpha(N) \ln (N/N - 1) -

- \sigma(N) + B(N),$$

(26)

where $B(N)$ is hopefully of order $1/N^2$.

A finite-size calculation of $Y$ as a function of the variable $X \equiv -\ln (1 - 1/N)$ should allow us to extrapolate the surface tension $\sigma$ and the exponent $\alpha$ of the prefactor in the relation (19). In fact, for large sizes and for $M < M_0$, the graph $Y$ vs. $X$ should yield a straight line with slope $\alpha$, $\sigma$ being the intercept with the $Y$ axis. The same procedure for $M = M_0$ should lead instead to a slope $2/3$ $\alpha$ and an intercept $2/3$ $\sigma$.

For $M > M_0$, we obtain the limits

$$h(N), h(N-1) \rightarrow h_\infty, \quad N \rightarrow \infty,$$

(27)

and

$$Y(N) \rightarrow 0, \quad N \rightarrow \infty.$$ 

(28)

Our numerical results are in complete agreement with the considerations presented above and in the previous section. Before presenting the results of $Y$ versus $X$ let us show what would give the « standard » (i.e. power law) finite-size scaling analysis.

In figure 1 we show the results obtained when the numerical data are analysed with a simple power law of the form

$$h(M, N) = h_\infty(M) + CN^{-A}$$

(29)

as it is usually done in finite-size methods. In formula (29) $C$ is a constant and $h_\infty(M)$ is the longitudinal field in the infinite-size limit

$$h_\infty(M) = \begin{cases} 
0 & \text{for } M \leq M_0, \\
\neq 0 & \text{for } M > M_0.
\end{cases}$$

(30)

The quantity plotted in figure 1 has been calculated using the expression given below

$$A(N) = \lim_{N \rightarrow \infty} \frac{\ln h(N) - \ln h(N-1)}{\ln (N/N - 1)} =

= \frac{\ln [h(N)/h(N-1)]}{\ln (N/N - 1)}.$$ 

(31)

For $M > M_0$, the field $h(M, N)$ will saturate to a finite value, and consequently $A(N) \rightarrow 0$, for $N \rightarrow \infty$. For $M = M_0$, the above quantity should yield the exponent $A$ of relation (29), if this exponent really existed. Indeed, it can be noted from the figures that the quantity calculated does not stabilize with the size for $M \leq M_0$. This fact is more apparent when $\gamma$ is far from the critical value $\gamma_c = 1$. No meaningful exponent can be defined either for values of $\gamma$ close to $\gamma_c$ (as in Fig. 1 for $\gamma = 0.9$), although for small sizes the power-law seems to work well (due to the fact that the surface tension $\sigma$ is itself small), and only much larger sizes reveal a crossover towards an exponential behaviour. This illustrative example shows that some caution is needed in order to obtain significant results from finite size extrapolations. More specific details are given in the corresponding figure captions.

In figure 2 we plot $Y$ vs. $X$ for the same cases as in figure 1. The curve corresponding to the spontaneous magnetization is indicated in each case. The results for $\gamma = 0.9$ are encouraging but not really conclusive. For $\gamma = 0.5$ we see that the graph is quite similar to those usually appearing in finite-cell calculations. The curve corresponding to the spontaneous magnetization clearly separates two regimes converging to different values. Finite-size effects are strong in the close vicinity of $M_0$.

We have then determined the $N$-dependent parameters $\sigma(N)$ and $\alpha(N)$ defined from two points of the upper curve through the formulae:

$$\alpha(N) = -\frac{Y(N) - Y(N-1)}{X(N) - X(N-1)}$$

(32)

and

$$\sigma(N) = -\frac{Y(N) + X(N) \alpha(N)}{2}.$$
The quantity $A(N)$ defined in relation (31) is plotted as a function of the inverse of the size $(1/N)$ for several values of the magnetization parameter around the bulk spontaneous value (which is shown in the figures with blank circles). The upper graph corresponds to $\gamma = 0.9$, which is close to the critical value $\gamma_c = 1$. The size $N = 14$ has been reached in order to test the power law. A naive analysis using the standard finite-cell procedure would predict a spontaneous magnetization a little larger than the actual value (between the curves labelled as 2 and 3), with an exponent $A$, such that $A \approx 1.6$. However, the spontaneous magnetization is known exactly from reference [8] to be $M_s = 0.81250$. For this value no meaningful exponent can be obtained. The fact that the power-law seems to work well in this case, is related to the value of $\gamma$ close to the critical value $\gamma_c = 1$. The exponential behaviour shows up markedly when $\gamma$ decreases, and this is apparent in the lower curve for $\gamma = 0.5$. Again the curve for the spontaneous magnetization is displayed with open circles. If we force a description in terms of a power-law we will obtain an exponent which is strongly $\gamma$-dependent. We also observe that the exponential behaviour is already apparent for smaller sizes ($N = 8$). The numerical calculation shown here, has been performed for the following values of the magnetization parameter:

A) upper curve ($\gamma = 0.9$): $M(1) = 0.90000$, $M(2) = 0.82250$, $M(3) = M_0 = 0.81250$, $M(4) = 0.78250$, and $M(5) = 0.69250$;

B) lower curve ($\gamma = 0.5$): $M(1) = 0.97468$, $M(2) = 0.96568$, $M(3) = M_0 = 0.96468$, $M(4) = 0.96368$, and $M(5) = 0.70000$.

In figure 3, we display the plot obtained in determining the parameter $\sigma(N)$ (surface tension) by finite-size calculations; the spontaneous magnetization for the infinite system has been exactly calculated by Pfeuty [9] as a function of the transverse field $\gamma$. Well below $M_0$, the calculation of $\sigma(N)$ is stabilized, yielding a series of values converging to $\sigma = - \ln \gamma$. The factor $(2/3)$ is also visible at $M = M_0$. Size effects are enhanced in the close neighbourhood of $M_0$, producing the large discontinuity depicted in figure 4. The location of this discontinuity will provide an excellent estimate of the spontaneous magnetization for a system whose equation of state is not known.

When $M > M_0$, the longitudinal field saturates to a finite value exponentially fast with size (see Fig. 3).

In figure 5 we show the plot aimed at finding the exponent of the prefactor in the relation (19). The results are not conclusive but there is a clear tendency of converging to the predicted values : $\alpha = 1.5$ for $M < M_0$ and $\alpha = 1$ for $M = M_0$. At this point, a comment concerning the Lanczos method is in order. As stated before, for large sizes and small longitudinal fields, the magnetization is determined by the two low-lying levels which are linearly coupled by the longitudinal field. Asymptotically these two levels are exponentially close in finite systems, and this makes a clear numerical separation of the two states extremely difficult. We expect therefore a poor convergence of the Lanczos method within the exponential region. This fact has been verified in our numerical calculation using from 35 to 50 steps in the Lanczos procedure [11].

The calculation has been stopped at the size where no convergence is attained ($N = 14$ being the maximum size available).

The finite-size exponential rounding of the first order phase transition described here, is a direct consequence of the exponential dependence of the mass gap given by (22). In order to check this behaviour and compare it with the magnetization results, exact finite-size calculations for the mass gap have been performed. The results are shown in figures 6 and 7. They are consistent with the expression given by (23), which in turn reproduces the formula given in references [8] and [9] for the mass gap. Again, the results are consistent with the expression given by (23), which in turn reproduces the formula given in references [8] and [9] for the mass gap. Again, the results for $\gamma$ close to the critical value $\gamma_c = 1$ are not very conclusive. For $\gamma = 0.9$ (Fig. 7) we can see a crossover between two regimes governed by different exponents $A(N)$. By exact calculation we mean that the diagonalization of the full Hamiltonian matrix has been performed numerically without the truncation usually present in the Lanczos method. The agreement with the considerations presented in the previous sections is excellent, confirming the hypothesis of a two-level phenomenon.

4. Conclusion

We have confirmed numerically that the finite-size scaling behaviour near a first order phase transition
Fig. 2. — Analysis of the numerical data assuming that the exponential behaviour given by relation (19) is asymptotically valid. If the above law is confirmed, the curves $Y$ vs. $X$ should extrapolate, for asymptotically large sizes, to zero for $M > M_0$, to $\sigma$ for $M < M_0$, and to $2/3 \sigma$ for $M = M_0$. The difference between both graphs ($\gamma = 0.9$ and $\gamma = 0.5$) can be immediately visualized. The results for $\gamma = 0.9$ are again not conclusive. The curve for the spontaneous magnetization is shown with blank circles for both cases. The lower figure ($\gamma = 0.5$) strongly suggests that the predicted dependence is correct, displaying a rapid convergence on both sides of the spontaneous value. As in the previous figure, the critical size for the exponential behaviour is smaller for smaller transverse fields. The cases shown in the figure correspond to

A) upper figure ($\gamma = 0.9$)

$M(1) = 0.85250 \quad M(2) = 0.82250$

$M(3) = M_0 = 0.81250 \quad M(4) = 0.80250$

$M(5) = 0.69250$

B) lower figure ($\gamma = 0.5$)

$M(1) = 0.97468 \quad M(2) = 0.96968$

$M(3) = 0.96868 \quad M(4) = 0.96768$

$M(5) = 0.96668 \quad M(6) = 0.96568$

$M(7) = M_0 = 0.96468 \quad M(8) = 0.96368$

$M(9) = 0.96268 \quad M(10) = 0.96168$

$M(11) = 0.96068 \quad M(12) = 0.95968$

$M(13) = 0.95468$

Fig. 3. — The coefficient $\sigma(N)$ as a function of the size for $\gamma = 0.5$, for various values of the magnetization parameter around the spontaneous value (curve with blank circles). The marks in the vertical axis show the asymptotic limits given by relations (19) and (22) for the cases $M < M_0$, $M = M_0$ and $M > M_0$. Close to $M_0$ strong size-effects develop in the form of large oscillations. Excellent convergence is obtained for values far from $M_0$. The values of $M$ depicted here are given by:

$M(1) = 0.98468 \quad M(2) = 0.97468$

$M(3) = 0.96568 \quad M(4) = M_0 = 0.96468$

$M(5) = 0.96368 \quad M(6) = 0.96168$

$M(7) = 0.95468 \quad M(8) = 0.92468$

$M(9) = 0.89468 \quad M(10) = 0.70000$

in a cylindrical geometry is of exponential type. Everywhere a leading exponential behaviour is observed with the size, and the singularity only appears in the argument of the exponential. The behaviour is controlled by the finite-size dependence of the mass gap between the exponentially degenerate eigenvalues of the transfer matrix. An extension of the numerical calculations to the three dimensional case is under progress to test the predictions on the size dependence of the mass gap [12].

Acknowledgments.

The computations were made with the help of the Centre de Calcul Vectoriel pour la Recherche (CCVR), Palaiseau. One of US (G.C.) would like to acknowledge financial support from the CNPq (Brasil).
Fig. 4. — The coefficient $a(N)$ for $\gamma = 0.5$ as a function of the magnetization parameter for the largest size available in the previous figure ($N = 8$). The size effects developed in the neighbourhood of the spontaneous magnetization $M_0$ represent an excellent method to locate the latter (generally, the exact equation of state is not known). Far from $M_0$, we can also see the saturation to the predicted values. If the exact value of $M_0$ is not known, the $2/3$ prefactor in the exponential will be masked by size effects.

Fig. 5. — Plot of $a(N)$ as a function of size for $\gamma = 0.5$ and for various values of the magnetization. The quantity $a(N)$ extrapolates to the exponent $\alpha$ in the prefactor of the exponential in relation (19). The asymptotic limits are marked on the vertical axis. The values of $M$ displayed are given below:

- $M(1) = 0.97468$
- $M(2) = M_0 = 0.96468$
- $M(3) = 0.95468$
- $M(4) = 0.92468$
- $M(5) = 0.89468$

Fig. 6. — The coefficient $\sigma(N)$ of the mass gap as a function of the size for various values of the transverse field. The convergence towards the asymptotic limit given by relation (23) is very rapid. The results shown here were obtained through exact numerical diagonalization of the Hamiltonian. The curves labelled from 1 to 4 correspond to the following transverse fields:

- $\gamma_1 = 0.3$
- $\gamma_2 = 0.5$
- $\gamma_3 = 0.7$
- $\gamma_4 = 0.9$

Fig. 7. — The plot of $\lambda(N)$ as a function of the size will extrapolate towards the exponent $\lambda$ in the prefactor of the exponential, in the asymptotic limit (22) of the mass gap. We display here the values corresponding to $\gamma_1 = 0.3$, $\gamma_2 = 0.5$, $\gamma_3 = 0.7$ and $\gamma_4 = 0.9$, which are the values of the transverse field depicted in the previous figure. The case $\gamma = 0.9$ is interesting, since it shows the crossover from an exponent $\lambda \approx 1$, typical of the critical region, to an exponent $\lambda < 1$. The theoretical limit for large sizes is $\lambda = 1/2$. 
References


[12] We have been informed that Hamer C. J. and Johnson H. J., have recently tested the $(2 + 1)$ dimensional triangular lattice, J. Phys. A (in press).