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Swendsen–Wang Monte Carlo study of the Ising model with external field

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We present a Monte Carlo study of the scaling limit of the two-dimensional Ising model with external field. While no evidence is found for the E_8 mass spectrum, we observe a very good agreement of our numerical data with the theoretical predictions for the magnetization and the correlation length.

It is well known that the scaling limit of the two-dimensional Ising model without external field is described by a free field theory: a single massive Majorana fermion. In the language of perturbed conformal field theory (PCFT), this model corresponds to the perturbation of the critical Ising model, that is the $c=\frac{1}{2}$ minimal CFT, by the energy density operator. The only other relevant primary operator of the model is the local magnetization, usually denoted by σ. When the critical Ising field theory is perturbed by σ, one is dealing with the scaling limit of the Ising model at the critical inverse temperature ($\beta=\beta_c$) but in an external magnetic field h.

A few years ago, in a beautiful and seminal paper, Zamolodchikov put forward an exact on-shell solution for this field theory [1]. By on-shell one means the following. On general grounds, the scaling limit of the IM in an external field should be described by a continuum euclidean-invariant field-theoretic model. Upon Wick rotation "back to real time", a relativistic (1+1)-dimensional quantum field theory is obtained. Then the on-shell solution consists in the explicit knowledge of the exact mass spectrum and of the complete S-matrix of this relativistic QFT model. As it turns out, Zamolodchikov's solution is highly non-trivial (unlike the case of the $\beta\to\beta_c$ limit at $h=0$): there are eight stable scalar particles, all with different masses, satisfying a perfect S-matrix bootstrap based on the numerology of the E_8 exceptional Lie algebra. In particular, the first mass ratio m_2/m_1 is predicted to be the golden number $2\cos(\frac{1}{5}\pi)$. Of course, such a model must possess some remarkable property, for even the limited on-shell exact data are usually beyond reach in interacting QFT. Indeed Zamolodchikov's approach is based on the idea that perturbing by σ the critical IM leads to a completely integrable QFT with no production and purely elastic factorized scattering (the so-called E_8 minimal purely elastic scattering theory or PEST).

In this letter we give a preliminary report on a numerical Monte Carlo study of the scaling limit of the IM with external field. The ingredients are at the fundamental level: a periodic square lattice as large as possible; the Ising action functional

$$\mathscr{A}=-\beta\left(\sum_{\langle xy\rangle}\sigma(x)\sigma(y)+h\sum_{x}\sigma(x)\right), \qquad (1)$$

and an effective non-local Swendsen–Wang MC simulation algorithm to overcome the critical slowing down in the limit $\beta\to\beta_c$ and $h\to 0$ (recall that $\beta_c=\frac{1}{2}\log(1+\sqrt{2})\simeq 0.44068...$). The purpose of this study

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is to see whether the E_8 minimal PEST predictions can really be tested with euclidean computer simulations. This is relevant both on the theoretical side, where many steps and some leap are necessary, and on the "experimental" side, as a check on the effective capability of MC simulations to quantitatively solve field theory models.

Let us mention that numerical checks on the IM with external field have been performed already by several authors [2–6], using a variety of methods. On one hand, within the CFT and exact integrability framework, say by means of the truncated conformal approach [7], perturbed CFT or thermodynamic Bethe ansatz [8], there exists little doubt on the validity of the E_8 minimal PEST. On the other hand, to our knowledge, the status of the numerical studies based "on first principles", with no inputs from CFT or exact integrability, is less satisfactory. There are the positive results of refs. [2,3], where the first two mass ratios are estimated using the hamiltonian limit approach and found to be consistent with Zamolodchikov's prediction; and there are the negative results of ref. [4], where Swendsen–Wang MC simulations are used to measure the $\langle\sigma\sigma\rangle$ correlation function, finding no evidence, in its exponentially small tail, even for the first golden mass ratio. As a matter of fact, the exponential tail of a local correlation function contains also some off-shell information, stored in the one-particle form factors, unlike the low-lying part of the spectrum accessible in the hamiltonian approach. This certainly makes the statistical data for the long distance correlation extremely sensible to form factor ratios, and probably makes them also very dependent on the slight scaling violations unavoidably present in any finite-size simulation. As we shall see, however, it is possible to measure in SW MC experiments a universal field-theoretic quantity other than mass ratios, thus avoiding the troublesome problem of double exponential fitting or dominant exponential filtering.

Let us consider the average magnetization, which is measured on the lattice as expectation value of the local Ising variable σ. According to standard scaling arguments, in the limit $h\to 0$, when $\beta=\beta_c$, the behavior of $\langle\sigma\rangle$ must be

$$\langle\sigma\rangle \simeq Ah^{1/15}, \tag{2}$$

where the critical exponent $\frac{1}{15}$ is uniquely determined by the fixed point hamiltonian, i.e. the $c=\frac{1}{2}$ minimal conformal model, while the numerical constant A is a non-universal quantity proper of the scaling limit of the square lattice Ising model with external field. Our SW MC data for $\langle\sigma\rangle$ are summarized in fig. 1. The critical behavior with exponent $\frac{1}{15}$ is manifest and we can extract the value

$$A=1.003\pm0.002\,. \tag{3}$$

While our results agree with that found in ref. [4] (within two standard deviations), we believe that the increase from $A=0.999\pm0.001$ to our result is indeed significant and it is to be ascribed to finite-size effects. This has been checked on a large lattice (1024×1024 on a CM-2 with two different field values) as reported in fig. 1.

Now consider the correlation length ξ of the model, whose inverse defines the (dimensionless) mass m_1 of the lightest particle of the spectrum. As h vanishes and the theory becomes critical, also m_1 goes to zero in a way dictated by the fixed point hamiltonian, namely

$$m_1 \simeq Ch^{8/15}\,. \tag{4}$$

Just as the constant A, the number C is a non-universal parameter proper of our "regularization" of the

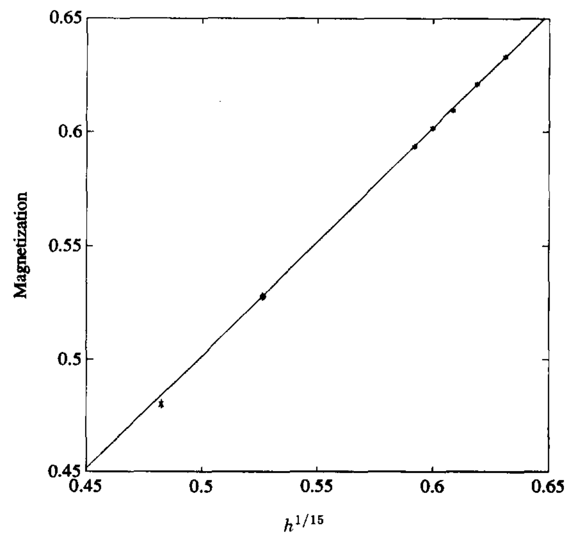


Fig. 1. The magnetization as a function of $h^{1/15}$: (∗) lattice size=240–400, (○) lattice size=1024. Also the point (×) refers to a lattice 1024×1024; since h is smaller, correlation length and finite-size effects are larger.

model. An approximate value for C can be extracted from our MC data for the two-point function $\langle \sigma_x \sigma_0 \rangle$ of the Ising variable. Our findings are summarized in fig. 2, and from them one reads off

$$C = 1.839 \pm 0.007 . \quad (5)$$

The non-universality of the constant C can be verified by comparing our square lattice result to that derived by Klassen and Melzer, in the continuum and on the cylinder, by checking first order conformal perturbation theory against (partly numerical) TBA calculations [6]. The coupling constant denoted by λ in ref. [6] should be identified with our product $\beta_c h$; then their result $\lambda m_1^{-15/8} \simeq 0.062033$ would correspond to $C = 2.845352$.

Finally, consider the ratio A/C^2. Let us show that it is a universal parameter characterizing the field theory which describes the scaling limit of the Ising model in an external field. The argument is quite simple: let f be the specific free energy of the model at $\beta = \beta_c$, that is

$$f(h) = -\lim_{N \to \infty} \frac{1}{N^2} \log Z_N(\beta_c, h) , \quad (6)$$

where $Z_N(\beta, h)$ is the partition function on the periodic $N \times N$ lattice. f is singular at $h = 0$, with a singular part which must scale like the squared inverse of the correlation length, $f \sim \xi^{-2}$. This follows from pure dimensional arguments, since $f(h)$ is the physical density. In field theory language, $f(h)$ corresponds to a physical observable with dimension two. It follows that

$$f(h) = -b m_1^2 + ... , \quad h \to 0 , \quad (7)$$

where the dots stand for terms analytic in h and b is a universal numerical constant, proper of the field theory describing the $h \to 0$ critical limit. Comparing with eq. (4), one gets

$$f(h) = -bC^2 h^{16/15} + ... \quad (8)$$

On the other hand, the explicit form of Ising action, eq. (1), implies

$$\beta_c \langle \sigma \rangle = -\mathrm{d}f/\mathrm{d}h , \quad (9)$$

which correctly reproduces eq. (2) and allows us to make the identification

$$\frac{A}{C^2} = \frac{16b}{15\beta_c} . \quad (10)$$

This completes our argument.

Strictly speaking, of course, eq. (10) is exact only at the thermodynamical limit $N \to \infty$, when the volume of the system is infinite as compared to the physical correlation length. On a finite lattice, the only one available on a computer, eq. (10) is corrected by finite-size effects. However, by general arguments, these should be exponentially small in the ratio N/ξ. In our simulations, as h is lowered toward zero, the linear size of the lattice N is also increased as $h^{-8/15}$, in such a way that the correlation length ξ is kept fixed to roughly $\frac{1}{10} N$. This should maintain the finite-size effects well below our statistical errors.

Eq. (10) is quite important, for it allows us to perform a rather stringent test on the predictions of Zamolodchikov's E_8 PEST model. Indeed the universal number b can be theoretically predicted through a combination of perturbed CFT and TBA. The general ideas as well as most details on this approach can be found in the original works [8,6]. Here we give a sketchy outline, mostly to show how indirect and involved is the argument leading to the determination of b. From this point of view, eq. (10) provides a test also for the validity of some reasonable but still unproven assumptions hidden behind the TBA.

The theoretical inputs required to compute b are

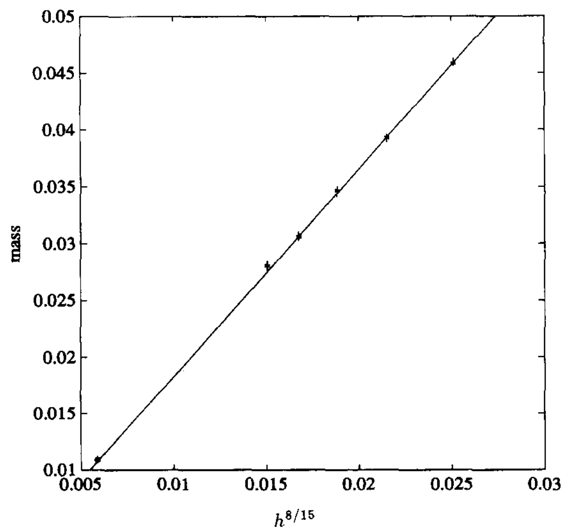


Fig. 2. The inverse correlation length as a function of $h^{8/15}$.

the S-matrix, the specific properties of the grand-canonical ensemble of a PEST and the fundamental symmetry of euclidean functional integrals under the exchange of space and time. By definition, the various different particles of the E_8 minimal PEST are conserved in number and their scattering processes are factorized and completely diagonal. The grand-canonical (infinite space volume) thermodynamics can then be formulated much like in non-relativistic quantum statistical mechanics, and the minimization of the thermodynamic free energy leads to a set of coupled non-linear integral equations for the statistical distributions of each species of particles at equilibrium. These are the so-called TBA equations [8], in which the original S-matrix uniquely fixes the integration kernels. The free energy F at the minimum point is a function of the temperature T alone and can be explicitly computed in terms of the solution of the TBA equations. By construction, $F(T)$ vanishes at $T=0$, since then no particle at all can be present. On the other hand, since we expect this scattering theory to correspond to a QFT, the free energy can be expressed as the logarithm of some euclidean functional integral over fields defined on a cylinder with circumference $1/T$. By euclidean symmetry, the same functional integral defines the ground state energy $E_0(L)$ on a circle of length $L=1/T$. Hence we are led to the identification

$$E_0(L)=F(1/L)+fL\,, \tag{11}$$

where the term linear in L should be present on general grounds, since $F(0)=0$. Notice that f in (11) is exactly the bulk specific free energy previously introduced. Now recall that the model at hand corresponds to a massive perturbation of the critical Ising field theory. On a cylinder it is then possible to apply conformal perturbation theory to the study of the above-mentioned functional integral. One can then show, provided the conformal dimension d of the perturbing field is less than one ($d=\frac{1}{8}$ in our case), that the perturbation series for the ground state energy $E_0(L)$ organizes itself in integer powers of the dimensionless coupling λL^{2-d}, where λ is a dimensionful coupling constant. The crucial fact for our purposes is that *no term linear in L* is then present in the small L behavior of $E_0(L)$. It follows that the specific free energy f can be calculated from the small L limit of the TBA free energy $F(1/L)$, that is for very large temperatures T. In refs. [8,6] this idea was applied to several classes of PCFT models, including the Ising model with external field. The general expression for f implied by a (rather heuristic) treatment of the large T limit of the TBA equations was found to be

$$f=-\frac{m_1^2}{2\phi_{11}^{(1)}}\,, \tag{12}$$

where the quantity in the denominator is related to the large energy limit of the scattering of two lightest particles. It depends on the complete bootstrap solution of the scattering problem. For instance, in the Ising case, Zamolodchikov's analysis implies that the 1–1 scattering must have poles corresponding to at least three more particles. Then the smallest bootstrap closes on a set of eight particles, with all relative 36 two-body scatterings completely determined up to CDD ambiguities (absent in the so-called minimal choice). Our numerical experiments can thus be regarded as a mean to support this full multiparticle picture (and in particular the minimal choice) and not just the existence of two particles with a golden mass ratio.

Now, comparing eqs. (12) and (7), we obtain

$$b=\frac{1}{2\phi_{11}^{(1)}}=\frac{1}{8\sqrt{3}\cos(\frac{1}{30}\pi)\sin(\frac{1}{5}\pi)}\,, \tag{13}$$

where use has been made of the explicit form of the minimal 1–1 scattering [1]. Then the theoretical prediction for the universal ratio A/C^2 reads

$$G\equiv\frac{A}{C^2}=0.298823568\,. \tag{14}$$

We now describe our numerical results. We implemented the original Swendsen–Wang algorithm on a scalar machine (a UNIX workstation) and on a parallel machine (a CM-2 with 8K processors). The total independence of the two codes and their final perfect agreement was a reassuring check that everything was right. We measured the magnetization as a function of the external field at $\beta=\beta_c$ by allowing the lattice size to grow as $h^{-8/15}$, in order to keep finite-size effects uniform. This is not a logical loop, since from other runs we check that indeed the correlation length scales according to eq. (4). The scalar code makes use of "improved estimators" for the magnetization and for the susceptibility (an extension to non-vanishing field of Niedermayer's formulae [9]). The formulae we apply are the following:

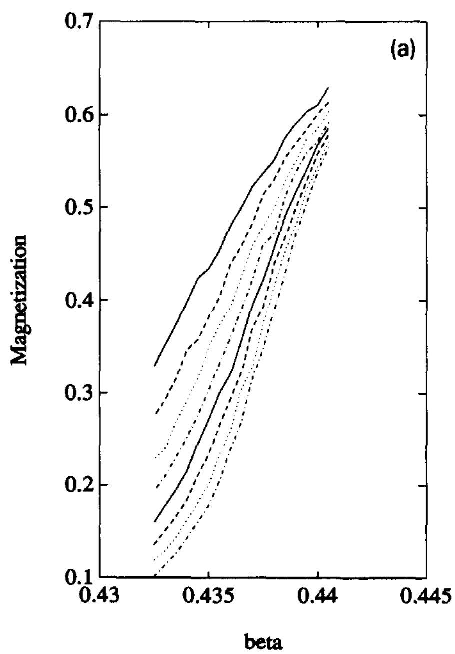
$$\langle\sigma\rangle=\langle\tanh(\beta h N_{\mathscr{C}})\rangle\,, \tag{15}$$

$$\langle\sigma_x\sigma_y\rangle_{\rm conn}=\left\langle\frac{\delta_{\mathscr{C}_x\mathscr{C}_y}}{\cosh^2(\beta h N_{\mathscr{C}_x})}\right\rangle + \langle\tanh(\beta h N_{\mathscr{C}_x})\tanh(\beta h N_{\mathscr{C}_y})\rangle_{\rm conn}\,, \tag{16}$$

$$\chi=\frac{\beta}{V}\left[\left\langle\sum_{\mathscr{C}}\frac{N_{\mathscr{C}}^2}{\cosh^2(\beta h N_{\mathscr{C}})}\right\rangle + \left\langle\left(\sum_{\mathscr{C}}\tanh(\beta h N_{\mathscr{C}})\right)^2\right\rangle_{\rm conn}\right], \tag{17}$$

where χ is the susceptibility, $V=N^2$ is the total number of sites, and $N_{\mathscr{C}}$ is the size of the cluster $\mathscr{C}$. Their validity is based on the idea of a multihit procedure: for each sweep on the link variables we may think to execute many updates of the spins. Since clusters' updates are independent, the average on the spin updates is easy to calculate. We estimate that in the critical region statistical fluctuations are only reduced by a factor of two, hence this trick is useless for large lattices (larger than 200×200) because it makes averaging over translations too costly.

We spanned a whole region of β around β_c to study the behavior of the susceptibility at non-vanishing external field. The results are reported in fig. 3. The magnetization data are less noisy at low field because this corresponds to larger lattices. We observe the migration of the susceptibility peak toward β_c (fig. 3b). Obviously we are still rather far from the critical behavior, where the magnetization should be nearly zero on the left of β_c; it is also obvious that owing to the tiny exponent $\frac{1}{15}$ it will not be possible to improve this in a substantial way (going to a magnetization of 0.25 at β_c would involve an increase of lattice size of six orders of magnitude). However, we knew from the work of ref. [4] that a precocious scaling actually sets in even at rather large fields. This is indeed checked in our data which refer to fields as low as 2.0×10^{-5} (fig. 1). The measure of the correlation length ξ was also done using improved estimators (on small lattices); on larger lattices it is faster to measure $\langle\sigma_x\sigma_{x+n}\rangle$ and average on x. We take the projec-



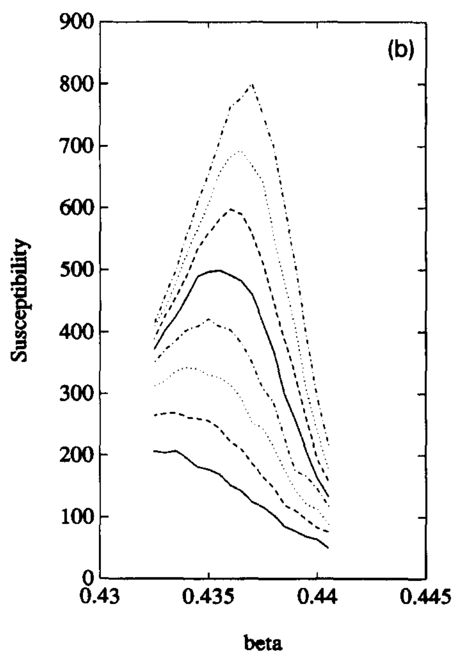


Fig. 3. The magnetization (a) and the susceptibility (b) as a function of β at $h=0.001$, 0.00075, 0.00058, 0.000468, 0.000384, 0.000321, 0.000273, 0.000235.

tion on zero transverse momentum to clean up the correlation function from power factors. We find that the values of ξ are strongly dependent of β in the neighborhood of β_c as expected. In particular the *best* values are taken at the peak of the susceptibility. We would like to argue that this is the right place to look for precocious scaling in the infrared sensitive observables like ξ. Indeed the values for m_1 obtained at the peaks scale as expected (eq. (5)) and finally yield

$$G=0.299\pm0.002\,, \tag{18}$$

in very good agreement with the theoretical prediction equation (14).

There are admittedly several sources of systematic errors which could be easily reduced with some additional work. The determination of the susceptibility peak, for instance, can be improved using the "histogram" technique [10]. This will be attempted to improve the data on the CM-2, where it proved to be too expensive to scan a whole region around β_c in search of the (very narrow) peak.

What we *did not* check is the spectrum of masses predicted by the theory. We tried several ways to extract a second mass from the correlation data, including spin–energy and energy–energy correlation, but two-masses fits are still too unstable to be reliable. Our opinion is that the amplitude of the second mass exponential is too small to be detected. Work is in progress to calculate the ratio $\langle 0|\sigma|m_1\rangle/\langle 0|\sigma|m_2\rangle$ within the perturbed CFT.

Finally some technical detail: we made a total of 64K sweeps for each value of the field on lattices ranging from 160^2 to 400^2 on a UNIX workstation; the CM-2 data are limited to 8K sweeps on a 1024^2 lattice. We observe an autocorrelation time of five sweeps in the worst case. The cluster algorithm for the parallel code was developed by two of us [11] – it is *not* a multigrid scheme and it works at a $\log(N)^2$ rate.

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