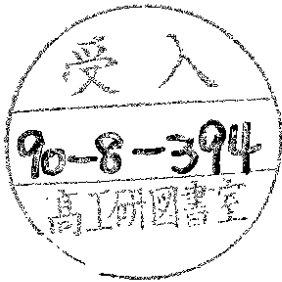


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# Finite size scaling analysis of the constraint effective potential computed from Multigrid Monte Carlo

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### Abstract

In lattice  $\phi^4$  - theory close to the critical line, finite size effects can be computed by renormalized loop expansions if the renormalized mass and coupling constant are known. Using this fact, we are able to extract results for renormalized masses and coupling constants from Multigrid Monte Carlo data of Mack and Meyer for the constraint effective potential close to the critical line, and compare them with the analytical results of Lüscher and Weisz. Perfect agreement is found.

### 1 Introduction

The constraint effective potential contains a great deal of information about a lattice field theory. It was introduced by Fukuda and Kyriakoulou<sup>[1]</sup> and further analysed by O'Raifeartaigh, Wipf and Yoneyama<sup>[2]</sup>. It is a not necessarily convex function of the magnetization. It determines the free energy as a function of the magnetization, and becomes equal to it in the large volume limit, provided one divides by the volume. Knowledge of the effective potential locates phase transitions and determines their order, it also determines renormalized masses and coupling constants<sup>[3]</sup>, surface tension etc. . . Therefore it is important to have methods to compute and analyse the effective potential for various models.

In this paper single component  $\phi^4$ -theory is considered with bare mass  $m_0^2$  and bare coupling constant  $g_0$  on a lattice of lattice spacing  $a$  set equal to 1. This model has a critical line where the renormalized mass vanishes.

It is known<sup>[4]</sup> that the renormalized coupling constant  $g_R$  is always rather small near the critical line, whatever the values of the bare parameters are, with a maximal value of about

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2/3 of the tree unitarity bound. This is true whenever the UV-cut-off is bigger than twice the renormalized mass (scaling region). Also, since the Callan Symanzik  $\beta$ -function is positive, the renormalization group equation drives  $g_R$  to smaller values as  $m_R$  decreases. Therefore the renormalized perturbation theory becomes an even better approximation as the system goes to the critical line. In conclusion, the renormalized loop expansion can be expected to describe very accurately the low energy properties of the theory; at least in the scaling region where the UV-cut-off is high enough.

This observation does not amount to a complete solution of the model near the critical line yet. The renormalized loop expansion requires knowledge of the renormalized parameters (mass and coupling constant), and there remains the highly nontrivial problem of finding the renormalized parameters as functions of the bare parameters  $m_0^2$  and  $g_0$ . Lüscher and Weisz<sup>4</sup> were able to solve this problem by an ingenious combination of high temperature expansions and standard perturbation theory. They published also estimates of errors of their calculation. These errors are generally very small.

In this paper, a comparison of this calculation with numerical results for constraint effective potentials is reported. The numerical results were obtained by Mack and Meyer<sup>5</sup>, using a Multigrid Monte Carlo method (MGMC). They computed the constraint effective potential on a  $12^4$  lattice for fixed bare coupling constant and 3 values of the bare mass very near to the critical line and on both sides of it. In this way the crossover of the constraint effective potential from single well shape to a double well behaviour in the vicinity of the second order phase transition could be studied.

The multigrid Monte Carlo method was designed to beat critical slowing down and this was indeed essential for the success of their numerical calculation. Critical slowing down gives rise to a divergent autocorrelation time  $\tau$  as the critical point is approached,  $\tau \sim \xi^z$  where  $\xi$  is the autocorrelation length and  $z$  is a dynamical critical exponent that is roughly 2 for most of the systems<sup>6</sup>. This implies that the time needed to equilibrate the system (generate statistically independent configurations) becomes exceeding large.<sup>7</sup> Several methods have been proposed to beat this phenomenon<sup>8</sup>. The particular multigrid method of Meyer and Mack has the additional advantage that it permits very convenient calculation of the constraint effective potential<sup>9</sup> (see Appendix).

Ordinarily, physical results can be extracted from numerical data only if the lattice size is large compared to the correlation length. This condition was not fulfilled in the computation of Mack and Meyer. However, because the renormalized loop expansion is expected to converge well near criticality, one can compute the constraint effective potential for arbitrary finite volume as a function of the renormalized coupling constant, and fit the result to the numerical data for the constraint effective potential. In this way the renormalized mass and coupling constant for the infinite volume theory can be extracted from the numerical data on a finite volume. Comparing with the result of Lüscher and Weisz gives a meaningful test of that part of their calculation that transcends perturbation theory.

Perfect agreement is found. The "numerical" values of the renormalized parameters agree with those of Lüscher and Weisz within the errors quoted by these authors (see table in section 4).

The paper is organized as follows: after the introduction, chapter 2 gives a detailed descrip-

tion of the expansion for the constraint effective potential as a function of the renormalized quantities  $m_R$  and  $g_R$ . Chapter 3 examines the finite size effects. Finally, the results are presented and conclusions are discussed in Chapter 4.

We expect also that our finite size effects analysis is also reliable for other models, such as Higgs models with dynamical gauge fields, at least when they are weakly interacting. We hope to come back to such applications elsewhere.

## 2 Loop Expansion for the constraint effective potential

We recall the definition of the constraint effective potential introduced by Fukuda and Kynakoulou<sup>10</sup>:

$$\exp\left(-\frac{v}{h}U_v(\phi)\right) = \int D\phi \delta(\phi - av\phi) \exp\left(-\frac{S}{h}[\phi]\right) \quad (2.1)$$

where:  $v$  is the total volume of the system  
 $av\phi = \frac{1}{v} \int_v \phi$  is the average of  $\phi$  in  $v$  and  
 $S[\phi]$  is the action of the system.

Since the delta function introduced into the functional integral in (2.1) constrains the average value of the field  $\phi$  to be  $\phi$ , one calls  $U_v(\phi)$  the constraint effective potential, which is not necessarily convex for finite  $v$ , but becomes convex as  $v$  goes to infinity.

Also the conventional effective potential  $\Gamma_v(\phi)$  used to study the radiative corrections in a quantum field theory<sup>10</sup>, can be recovered as its convex hull<sup>11</sup>, so that no information is lost. In fact, one sees that the generating functional  $W[j]$  (Schwinger functional for constant external source  $j$ ) is given through the integral:

$$\exp\left(\frac{v}{h}W[j]\right) = \int D\phi \exp\left\{\frac{v}{h}(j\phi - U_v(\phi))\right\} \quad (2.2)$$

Through its Legendre transformation, one gets the effective potential

$$\Gamma_v(\phi) = \sup_j (j\phi - W[j]) \quad (2.3)$$

which is always convex and whose expansion generates the one-particle irreducible n-points vertex functions.

We will now consider the lattice action for the  $\phi^4$ -theory defined by:

$$S = \sum_x \left\{ \frac{1}{2} \sum_{\mu=0}^3 (D_\mu \phi(x))^2 + \frac{1}{2} m_0^2 \phi^2(x) + \frac{\lambda_0}{4!} \phi^4(x) \right\} \quad (2.4)$$

where:  $\phi(x)$  is a real valued field defined on the hypercubic lattice with  $x \in Z^4$   
 $m_0, \lambda_0$  are the bare mass and coupling constant respectively  
 $D_\mu \phi(x)$  is the lattice derivative.

The lattice  $\phi^4$ -theory is known to exist in two phases, one where the reflection symmetry

$\phi \rightarrow -\phi$  is spontaneously broken and the other where it is not. Therefore, in order to expand around the true minimum of the theory, we will shift the fundamental field  $\phi$ :

$$\phi(x) = \tilde{\phi} + \varphi(x) \quad (2.5)$$

and the field  $\varphi(x)$  is required to satisfy the requirement that its zero Fourier component  $\varphi_F$  vanishes:

$$\int_V \varphi = 0 \Rightarrow \varphi_F(0) = 0 \quad (2.6)$$

## 2.1 General expansion

Now we substitute the action (2.4) into the Eq.(2.1) and, expressing it as function of the field  $\varphi$ , we get:

$$\exp\left(-\frac{v}{\hbar}U_c(\tilde{\phi})\right) = \exp\left(-\frac{v}{\hbar}U_c(\tilde{\phi})\right) \int D\varphi \exp\left(-\frac{1}{\hbar}\sum_{xy}\varphi(x)M(x,y)\varphi(y)\right) \times \quad (2.7)$$

$$\exp\left(-\frac{\lambda_0}{4\hbar}\sum_x\left(4\tilde{\phi}\varphi^3(x) + \varphi^4(x)\right)\right)$$

where:

$$U_c(\tilde{\phi}) = \frac{m_0^2}{2!}\tilde{\phi}^2 + \frac{\lambda}{4!}\tilde{\phi}^4 \quad (2.8)$$

is the classical potential and

$$S_0(\varphi) = \sum_{xy}\varphi(x)\frac{1}{2}\{D^\mu D_\mu + m_c^2 + \frac{\lambda_0}{2}\tilde{\phi}^2\}\delta_{xy}\varphi(y) = \sum_{xy}\varphi(x)M(xy)\varphi(y) \quad (2.9)$$

is the whole quadratic contribution to the free theory. We make a Taylor expansion of the last term of Eq.(2.7):

$$\exp\left(-\frac{v}{\hbar}U_v(\tilde{\phi})\right) = \exp\left(-\frac{v}{\hbar}U_c(\tilde{\phi})\right) \int D\varphi \exp\left(-\frac{1}{\hbar}\sum_{xy}\varphi(x)M(x,y)\varphi(y)\right) \left\{1 - \frac{\lambda_0}{4\hbar}\sum_x\left(4\varphi^3(x)\tilde{\phi} + \varphi^4(x)\right) + \dots\right\} \quad (2.10)$$

Using the formula:

$$\int D\phi \exp\left(\frac{1}{\hbar}\sum_{xy}\phi(x)M(x,y)\phi(y)\right) \sum_z \phi^{2n}(z) = \frac{(2n-1)!!}{2^n} \left(\det\left(\frac{M}{\pi\hbar}\right)\right)^{-1/2} \hbar^n \quad (2.11)$$

we conclude that one can factorize the contributions to  $U_v(\tilde{\phi})$  in terms of growing powers of Planck's constant  $\hbar$ . This produces the loop expansion<sup>[11]</sup>. Thus, we can write the expansion (2.10) as:

$$U_v(\tilde{\phi}) = U_c(\tilde{\phi}) + \hbar U_v^{(1)}(\tilde{\phi}) + \hbar^2 U_v^{(2)}(\tilde{\phi}) + \dots \quad (2.12)$$

## 2.2 One loop contribution

We need to evaluate the Gaussian integral of the first term in Eq.(2.10). Using the trace representation for the determinant of a linear operator, we get:

$$\exp\left(-\frac{v}{\hbar}U_v^{(1)}(\tilde{\phi})\right) = (\det M/\pi\hbar)^{-1/2} = (\text{const}) \exp\left(-\frac{1}{2}\text{Tr}(lnM)\right) \quad (2.13)$$

We can express the operator  $M$  of Eq.(2.9) in the Fourier space as:

$$M(\tilde{k}) = \frac{1}{2}\left(\tilde{k}^2 + m_0^2 + \frac{\lambda_0}{2}\tilde{\phi}^2\right) \quad (2.14)$$

which corresponds to the inverse of the propagator in the real space:

$$M_{\tilde{\phi}}^{-1}(x,y) = \Delta_{\tilde{\phi}}(x,y) \equiv \langle \varphi(x)\varphi(y) \rangle = \frac{1}{v} \sum_{\tilde{k} \neq 0} \exp(-i\tilde{k}(x-y)) \frac{\hbar}{\tilde{k}^2 + m_0^2 + \frac{\lambda_0}{2}\tilde{\phi}^2} \quad (2.15)$$

where the lattice momentum vector  $\tilde{k}_\mu$  is given by:

$$\tilde{k}_\mu = 2\sin(k_\mu/2) \quad (2.16)$$

$$\text{with } \tilde{k}^2 = 4\sum_{\mu=0}^4 \sin^2(k_\mu/2)$$

The momentum components  $k_\mu$  are constrained to be in the Brillouin zone

$$k_\mu = \frac{2\pi}{L}n_\mu - \pi \quad n_\mu = 1, \dots, L \quad (2.17)$$

Substituting (2.14) into Eq.(2.13), we get:

$$U_v^{(1)}(\tilde{\phi}) = \frac{1}{2^v} \sum_{\tilde{k} \neq 0} \ln \left[ \frac{1}{2} \left( \tilde{k}^2 + m_0^2 + \frac{\lambda_0}{2}\tilde{\phi}^2 \right) \right] \quad (2.18)$$

which agrees with reference<sup>[12]</sup> for the 1 component case  $N = 1$ . Expanding in Taylor series  $\ln(1+x)$ , we obtain a sum of the graphs:

$$\frac{1}{2} \left( \text{circle with two vertices} \right) - \frac{1}{4} \left( \text{circle with two vertices and a loop} \right) + \frac{1}{6} \left( \text{circle with two vertices and two loops} \right) - \dots \quad (2.19)$$

where we used the following Feynman rules:

PROPAGATOR  =  $\frac{1}{k}$

VERTEX  =  +  (2.20)

$m_0^2$    $\frac{\lambda}{2} \phi^2$

Up to a constant, the diagrammatic representation of  $U_0^{(1)}(\phi)$  of Eq.(2.18) is given by the sum of the one-particle irreducible diagrams at zero external momentum, where the factors  $1/2n$  are combinatorial factors, which can be computed from symmetry considerations. In fact, from the diagrammatic expansion, we see that there are  $(2n)!$  ways to distribute  $2n$  particles to the external lines of a  $n$ -vertex diagram, but from them  $2^n n$  are dependent, connected through reflections, rotations of  $n$  vertices on the ring and interchange of any two external legs at a given vertex. So the combinatorial factor is  $(2n)!/2^n 2^n (2n)! = 1/2^n 2^n$ , where  $1/2^n$  is responsible for the factor  $1/2$  in the numerator of the argument of logarithm, and  $1/2^n$  is its Taylor's coefficient<sup>[13]</sup>.

### 2.3 Two-loop contribution

Keeping the terms proportional to  $\hbar$  in the expansion (2.10), one obtains:

$$\int D\varphi \exp\left(-\frac{1}{\hbar} S_0(\varphi)\right) \left[ -\frac{\lambda}{4! \hbar} \sum_x \varphi^4(x) + \frac{\lambda^2 \phi^2}{72 \hbar^2} \sum_{xy} \varphi^3(x) \varphi^3(y) \right] \quad (2.21)$$

Using the Wick's theorem, we obtain:

$$\left\langle -\frac{\lambda}{4! \hbar} \sum_x \varphi^4(x) \right\rangle = -\frac{\hbar \lambda}{8} \sum_x \Delta_{xx}^2(\phi) = -\frac{\lambda \hbar}{8v} \sum_{k_1, k_2 \neq 0} \Delta_\phi(k_1) \Delta_\phi(k_2) \quad (2.22)$$

$$\begin{aligned} \left\langle \frac{\lambda^2 \phi^2}{72 \hbar^2} \sum_{xy} \varphi^3(x) \varphi^3(y) \right\rangle &= \frac{\lambda^2 \phi^2}{12} \sum_{xy} \left\{ 3 \Delta_\phi(x, x) \Delta_\phi(x, y) \Delta_\phi(y, y) + 3! \Delta_\phi(x, y) \right\} \\ &= \frac{\lambda^2 \hbar \phi^2}{12v^3} \sum_{k_1, k_2, k_3 \neq 0} \left\{ v^2 \delta_{k_2, 0} + v \delta_{k_1+k_2+k_3, 0} \right\} \Delta_\phi(k_1) \Delta_\phi(k_2) \Delta_\phi(k_3) \end{aligned} \quad (2.23)$$

where  $\Delta_\phi(k)$  is the Fourier transformation of the propagator  $\Delta_\phi(x, y)$ , and the expectation value is defined as:

$$\langle O(\varphi) \rangle = \frac{\int D\varphi \exp\left(-\frac{1}{\hbar} S_0(\varphi)\right) O(\varphi)}{\int D\varphi \exp\left(-\frac{1}{\hbar} S_0(\varphi)\right)} \quad (2.24)$$

The two loop contributions of Eq.(2.22) and (2.23) correspond to the Feynman graphs a), b) and c) of Fig. 1 respectively.

From (2.23) we see explicitly that the term corresponding to the diagram b) drops out

because the zero momentum component of  $\varphi_F$  vanishes according to Eq.(2.6). Consequently, we obtain up to two loops:

$$U_1(\phi) = U_c(\phi) + \frac{\hbar}{2v} \sum_{k \neq 0} \ln(k^2 + m_\phi^2) + \frac{\lambda^2 \lambda}{8v^2} \sum_{k_1, k_2 \neq 0} \frac{1}{k_1^2 + m_\phi^2 + \frac{\lambda}{2} \phi^2} \frac{1}{k_2^2 + m_\phi^2 + \frac{\lambda}{2} \phi^2} - \frac{\lambda^2 \hbar^2}{12v^3} \sum_{k_1, k_2, k_3 \neq 0} \frac{\delta_{k_1+k_2+k_3, 0}}{(k_1^2 + m_\phi^2 + \frac{\lambda}{2} \phi^2)(k_2^2 + m_\phi^2 + \frac{\lambda}{2} \phi^2)(k_3^2 + m_\phi^2 + \frac{\lambda}{2} \phi^2)} \quad (2.25)$$

In the infinite volume limit, this expression agrees with the two loop computation of ref.[11] for the effective potential according to the discussion of section 2 (see Eq.(2.2) for instance).

### 2.4 Expansion strategy

Because the Monte Carlo simulation was performed in a region of the bare parameter  $(m_0^2, \lambda_0)$  where the loop expansion in bare parameters is not convergent (the convergent region is given by  $0 < m_0^2 + \frac{\lambda}{2} \phi^2$  in lattice units), we have to look for convergent expansion in terms of running coupling constants.

In fact, it can be proved that the constraint effective potential becomes complex for some values of  $\phi$  if the classical potential is non-convex, but this apparent complexity is due to the failure of the loop expansion. This was pointed out by Fujimoto et al.[14]. We observe from Eq.(2.10) that the gaussian integral is well defined only if the matrix  $M(x, y)$  is positive definite or equivalently if the second derivative of the classical potential is positive. Therefore, the loop expansion make sense as an asymptotic serie only up to the inflexion points of the classical potential.

The fundamental observation is this: due to the proximity of the system to the critical line  $m_0^2(\lambda_0)$ , the renormalized mass  $m_R$  and the self coupling  $\lambda_R$  are small and go to zero as the system approaches the critical line (triviality of the lattice  $\phi^4$ -theory). Therefore it is a good idea to expand in  $\lambda_R$  and  $m_R$ . This can be done by manipulating the bare expansion. Instead of adding counterterms per hand to the tree level, we will define the renormalized quantities through the  $n$ -points vertex functions and compute them up to  $m$  loop consistent with the  $m$  loops expansion of  $U_0(\phi)$ . Then, inverting this relations, we will obtain the bare quantities as a function of the renormalized ones and shall finally substitute them into the expansion of the constraint effective potential to obtain the desired expansion in terms of  $\lambda_R, m_R$ .

The fundamental philosophy of the renormalization theory implies that one shall obtain a finite expression without ultraviolet divergences in the limit when the cutoff is removed. This is the renormalized  $m$  loop expansion of  $U_0(\phi)$ .

It is expected that one obtains in this way an expression for physical quantities like the constraint effective potential which is accurate when  $m_R$  and  $\lambda_R$  are small, in spite of the fact that the expressions for the bare parameters (and other cutoff dependent quantities) are not trustworthy. For a discussion of related issues, see Lüscher and Weisz[6].

## 2.5 Renormalization

The definition of the renormalized quantities  $m_R^2, \lambda_R$  and  $Z_\phi$  is to some extent arbitrary. (Some different definitions are related through the renormalization group equations). We will use the same definition as Lüscher and Weisz to make it possible to compare our numerical results with them. From here on  $\hbar$  will be set to 1.

### 2.5.1 Symmetric phase

We introduce a wave function renormalization constant  $Z_\phi$ , a renormalized mass parameter  $m_R$  and a renormalized coupling  $\lambda_R$  through the two and four-point vertex functions:

$$\gamma^{(2,0)}(\vec{p}, -\vec{p}) = -Z_R^{-1} \{m_R^2 + \vec{p}^2 + O(\vec{p}^4)\} \quad (2.26)$$

$$\gamma^{(4,0)}(0, 0, 0) = -Z_R^{-2} \lambda_R \quad (2.27)$$

Note that  $m_R$  and  $\lambda_R$  are not exactly equal to the physical mass  $m$  and coupling  $\lambda$ , which are defined as the pole of the propagator in the complex energy-plane and the on-shell four-point vertex functions respectively.

The lattice action corresponding to the lattice field  $\varphi(x)$  is:

$$S[\varphi] = \sum_x \left\{ \frac{1}{2} \sum_\mu (D_\mu \varphi(x))^2 + \frac{1}{2} (m_0^2 + \frac{\lambda_0}{2} \phi^2) \varphi^2(x) + \frac{\lambda_0}{6} \phi \varphi^3(x) + \frac{\lambda_0}{4!} \varphi^4(x) \right\} \quad (2.28)$$

and thus the Feynman rules are based on the elements:

$$\text{PROPAGATOR} \quad \text{---} \quad \Delta(\vec{p}) = \frac{1}{\vec{p}^2 + m_0^2} \quad (2.29)$$

$$\text{VERTICES} \quad \text{---} (\lambda \phi) \quad \text{---} (\lambda) \quad (2.30)$$

Up to one loop, we find:

$$\begin{aligned} \gamma^{(2,0)}(\vec{p}, -\vec{p}) &= \frac{1}{2} \text{---} \text{---} + \frac{1}{2} \text{---} \text{---} + \frac{1}{2} \text{---} \text{---} \\ &= \frac{\lambda_0}{2} \left( -1 + \frac{\lambda_0 \phi^2}{m_0^2} \right) j_1(m_0) + \frac{1}{2} \lambda_0^2 \phi I_2(\vec{p}, -\vec{p}; m_0) \end{aligned} \quad (2.30)$$

$$\begin{aligned} \gamma^{(4,0)}(\vec{p}, -\vec{p}) &= \frac{1}{2} \left\{ \begin{array}{c} \vec{p}_4 \\ \text{---} \text{---} \text{---} \text{---} \\ \vec{p}_3 \end{array} \right\} + \begin{array}{c} \vec{p}_4 \\ \text{---} \text{---} \text{---} \text{---} \\ \vec{p}_2 \end{array} + \begin{array}{c} \vec{p}_4 \\ \text{---} \text{---} \text{---} \text{---} \\ \vec{p}_1 \end{array} \\ &= \frac{1}{2} \lambda_0^2 \left\{ A(\vec{p}_1 + \vec{p}_2; m_0^2) + A(\vec{p}_1 + \vec{p}_3; m_0^2) + A(\vec{p}_1 + \vec{p}_4; m_0^2) \right\} \end{aligned} \quad (2.31)$$

where:

$$\begin{aligned} j_p(m) &= \frac{1}{v} \sum_{\vec{k} \neq 0} (m^2 + \vec{k}^2)^{-p} \\ A(q) &= \frac{1}{v} \sum_{\vec{k} \neq 0} \frac{1}{m_0^2 + \vec{k}^2} \frac{1}{m_0^2 + (q + \vec{k})^2} \end{aligned} \quad (2.32)$$

$$I_2(\vec{p}_1, \vec{p}_2; m) = \frac{1}{v} \sum_{\vec{k} \neq 0} \frac{1}{m^2 + (\vec{k} + \vec{p}_1)^2} \frac{1}{m^2 + (\vec{k} + (q_1 + q_2))^2}$$

and the sums are over the Brillouin zone (2.16) with  $\vec{k}^2 \neq 0$ . After some algebra, we get:

$$\begin{aligned} Z_\phi &= 1 + O(\lambda_0^2) \\ \lambda_R &= \lambda_0 \left[ 1 - \frac{3}{2} \lambda_0 j_2(m_0) \right] + O(\lambda_0^3) \end{aligned} \quad (2.33)$$

$$m_R^2 = m_0^2 \left[ 1 + \frac{\lambda_0}{2m_0^2} j_1(m_0) \right] + O(\lambda_0^2)$$

And therefore we obtain the renormalized one-loop expansion by inserting (2.33) into (2.18):

$$U_v(\vec{\phi}_R) = U_v(\vec{\phi}_R) + \frac{1}{2v} \sum_{\vec{k} \neq 0} \ln \left\{ 1 + \frac{\lambda_R \vec{\phi}_R^2 / 2}{\vec{k}^2 + m_R^2} \right\} - \frac{\lambda_R}{4} j_1(m_R) \phi_R^2 + \frac{1}{16} \lambda_R^2 j_2(m_R) \phi_R^4 \quad (2.34)$$

which is in fact finite in the limit when we remove the UV cutoff ( $\Lambda = 1/a \rightarrow \infty$ ).

### 2.5.2 Broken phase

We define the renormalized mass  $m_R$  and the wave function renormalization constant  $Z_\phi$  through the limit  $\vec{p}^2 \rightarrow 0$  (if  $L$  is large enough in units of lattice spacing) of the two points vertex function in the same way as in the symmetric phase:

$$\gamma^{(2,0)}(\vec{p}, -\vec{p}) = -Z_\phi^{-1} \{m_R^2 + \vec{p}^2 + O(\vec{p}^4)\} \quad (2.35)$$

The self-coupling constant  $\lambda_R$  is now defined through the tree level relation:

$$\lambda_R = 3 m_R^2 / v_R^2 \quad (2.36)$$

where  $v_R$  is the vacuum expectation value (V.E.V.) of the field  $\phi_R = Z_\phi^{-1/2} \phi$ . This definition implies that the four-point vertex at zero momentum is a non-trivial function of  $\lambda_R$  and only approximately equal to  $\lambda_R$ . One finds in an analogous way up to one loop:

$$\begin{aligned} Z_\phi &= 1 + \frac{\lambda_0 m_0^2}{16} j_2(m_0) - (8 + m_0^2) j_3(m_0) \\ m_R^2 &= m_0^2 \left\{ 1 - \frac{\lambda_0}{m_0^2} j_1(m_0) - \frac{3}{2} \lambda_0 j_2(m_0) - \frac{\lambda_0 m_0^2}{16} [j_2(m_0) - (8 + m_0^2) j_3(m_0)] \right\} \\ v_R &= \left( \frac{3m_0^2}{\lambda_0} \right)^{1/2} \left\{ 1 - \frac{\lambda_0}{2m_0^2} j_1(m_0) - \frac{\lambda_0 m_0^2}{32} [j_2(m_0) - (8 + m_0^2) j_3(m_0)] \right\} \\ \lambda_R &= \lambda_0 \left\{ 1 - \frac{3}{2} \lambda_0 j_2(m_0) + \frac{\lambda_0 m_0^2}{8} [j_2(m_0) - (8 + m_0^2) j_3(m_0)] \right\} \end{aligned} \quad (2.37)$$

After shifting the field to the true minimum (correct up to one loop) and inserting Eq.(2.37) into (2.18), we get:

$$U_v(\phi_R) = U_v(\phi_R) + \frac{1}{2} \sum_k \ln \left\{ 1 + \frac{\lambda_R v_R \phi_R + \lambda_R \phi_R^2 / 2}{k^2 + m_R^2} \right\} - \frac{1}{2} v_R \lambda_R j_1(m_R) \phi_R - \left\{ \frac{\lambda_R}{4} j_1(m_R) - \frac{v_R \lambda_R}{4} j_2(m_R) \right\} \phi_R^2 + \frac{1}{4} \lambda_R^2 v_R j_2(m_R) \phi_R^3 + \frac{\lambda_R^2}{16} j_2(m_R) \phi_R^4 \quad (2.38)$$

which is again finite in the limite when we remove the UV cutoff ( $\Lambda \rightarrow \infty$ ).

### 3 Finite size scaling analysis

The quantities computed in section 2 depend on the scale  $L = v^{1/4}$ . For example in the sums  $j_p(m)$  appearing in the loop expansion (see Eq.(2.34)-(2.38)) for  $U_v(\phi)$  the lattice momentum is restricted to discrete values given by (2.17).

Again, the fundamental observation for our finite size scaling analysis is based on the fact that the  $\phi^4$ -theory is weakly interacting in the scaling region ( $\Lambda \geq 2m_R$ ) in both phases. Therefore, one can compute the deviation of the renormalized quantity  $X(L)$  for finite  $L$  from its infinite volume limit by loop expansion:

$$\delta X(L) = X(L) - X(\infty) = \sum_{\nu=0}^{\infty} C_\nu(L) \lambda_R^\nu \quad (3.1)$$

where the coefficients  $C_\nu(L)$  may depend on  $m_R^{[15]}$ .

The advantage of this procedure is that one is not restricted to the consideration of side length  $L$  which is large compared to the correlation length, and no unknown constant appears.

#### 3.1 Symmetric phase

We recall that the renormalized mass  $m_R(L)$  and the coupling constant  $\lambda_R(L)$  for a finite lattice of side length  $L$  was defined as the zero momentum limit of the two and four-point vertex functions respectively (see Eq.(2.26) - (2.27)).

The one-loop calculation for these quantities yields (Eq. 2.33):

$$m_R^2(L) = m^2 + \frac{3}{2} j_1(m) + (C.T.)_1 \quad (3.2)$$

$$\lambda_R(L) = \lambda - \frac{3}{4} \lambda^2 j_2(m) + (C.T.)_2$$

where  $(C.T.)_1$  and  $(C.T.)_2$  are  $L$ -independent counterterms which define the renormalization scheme.

The parameters  $m$  and  $\lambda$  are determined by the bare parameters of the theory, and we will chose them to equal the renormalized mass and coupling constant in the infinite volume limit. By definition, the quantities  $j_1(m), j_2(m)$  are  $L$ -dependent (Eq. 2.32) and  $m$  and  $\lambda$  do not

depend on the volume. Therefore, we obtain:

$$\delta m_R^2 = m_R^2(L) - m_R^2(\infty) = \frac{\lambda_R}{2} \{j_1(m_R) - I_1(m_R)\} + 0(\lambda_R^2)$$

$$\delta \lambda_R = \lambda_R(L) - \lambda_R(\infty) = -\frac{3}{2} \lambda_R^2 \{j_2(m_R) - I_2(m_R)\} + 0(\lambda_R^3) \quad (3.3)$$

where:

$$I_p(m) = \int \frac{d^4 k}{(2\pi)^4} (k^2 + m^2)^{-p} \quad (3.4)$$

is the infinite volume limit of  $j_p(m)$ .

Eq.(3.3) is the desired relation for the finite volume shift of the renormalized mass and coupling constant, giving their values in the infinite volume limit.

We can solve Eq.(3.3) (by relaxation for instance) to obtain the infinite volume limit for the renormalized parameters  $m_R(L)$  and  $\lambda_R(L)$ .

#### 3.2 Broken phase

Using the same strategy as in the symmetric phase, we obtain from (2.37):

$$\delta m_R^2 = m_R^2 \left\{ \frac{\lambda_R}{m_R} [I_1(m_R) - j_1(m_R)] + \frac{3}{2} \lambda_R [I_2(m_R) - j_2(m_R)] - \frac{\lambda_R m_R^2}{16} [|I_2(m_R) - j_2(m_R)| - (c + m_R^2) |I_3(m_R) - j_3(m_R)|] \right\}$$

$$\delta \lambda_R = \lambda_R \left\{ \frac{3}{2} \lambda_R [I_2(m_R) - j_2(m_R)] - \frac{\lambda_R m_R^2}{8} [|I_2(m_R) - j_2(m_R)| - (8 + m_R^2) |I_3(m_R) - j_3(m_R)|] \right\} \quad (3.5)$$

$$\delta Z_\phi = \frac{\lambda_R m_R^2}{16} \{ |I_2(m_R) - j_2(m_R)| - (8 + m_R^2) |I_3(m_R) - j_3(m_R)| \}$$

Again we solve the coupled equations (3.5) by relaxation with tolerance  $10^{-5}$  and obtain the renormalized mass  $m_R$ , the coupling constant  $\lambda_R$  and the wave function renormalization constant  $Z_\phi$  in the infinite volume limit.

It is possible to work out analytically the volume dependence of  $j_p(m)$  for large volume by making an expansion in  $1/L^2$ . This gives<sup>[16]</sup>:

$$j_p(m) = a - \frac{b}{L^2} + \dots \quad (3.6)$$

Then, one computes the coefficients  $a$  and  $b$  for the actual values of  $m$ , provide  $\frac{m^2 L^2}{4\pi} \ll 1$  and, from them, extrapolates the infinite volume limit<sup>[17]</sup>.

However, we do not wish to restrict our attention to large volume and therefore we use an asymptotic expansion for these integrals, which remain accurate for moderate  $L$ .



## 4 Results

We expect that the results of the loop expansion for physical quantities like the effective potential as function of renormalized parameters  $m_R, \lambda_R$  are accurate near the critical line where  $\lambda_R$  (and  $m_R$ ) are small.

Lüscher and Weisz have shown that one can also compute the bare quantities  $m_0, \lambda_0, Z_A$  with a great deal of work. Here we will use numerical data for the constraint effective potential instead, and compare the results with Lüscher and Weisz.

Corresponding to each value of the bare parameter chosen for the Monte Carlo simulation, we make a fitting with the renormalized one loop expansion formula deduced in section 2. We did not use the two-loop formula because the order of magnitude of this contribution is smaller than the error-bars of the Monte Carlo data.

The input values  $\lambda_0 = 16.376$ ,  $m_0^2 = -1.14, -1.15$  and  $-1.16$  were chosen to study the crossover of the constraint effective potential from a single well shape to double well behaviour<sup>[18]</sup>.

Therefore, the first two points must correspond to the symmetric phase in the infinite volume limit and the last to the broken phase. According to Lüscher and Weisz, the critical point associated with the second order phase transition lies at  $m_0^2 = -1.157 \pm 0.006$ <sup>[9]</sup> for  $\lambda_0 = 16.376$ .

The fits are shown in Fig. 2 (a), (b) and (c) for the values  $\lambda_0 = 16.376$ ;  $m_0^2 = -1.14, -1.15$  and  $-1.16$  respectively. The error-bars on the numerical data were computed using the standard deviation formula for the available independent Monte Carlo simulation data set for each value of the bare parameters.

The errors for the fitted values and their infinite volume limits were also estimated using a standard deviation formula.

From these fits, we can obtain immediately the renormalized quantities, as it was explained in section 2. The result is shown in the following table both for finite volume,  $L = 12$  lattice spacings and for the infinite volume limit. For comparison, the infinite volume results of Lüscher and Weisz are listed in the last two columns.

	$m_R(L)$	$\lambda_R(L)$	$m_R(\infty)$	$\lambda_R(\infty)$	$m_R^{LW}$	$\lambda_R^{LW}$
$m_0^2 = -1.14$	$0.055 \pm 0.005$	$8.8 \pm 0.8$	$0.079 \pm 0.003$	$7.5 \pm 0.6$	$0.08$	$7.4 \pm 0.2$
$m_0^2 = -1.15$	$0.10 \pm 0.003$	$8.8 \pm 0.1$	$0.06 \pm 0.005$	$7.1 \pm 0.1$	$0.06$	$7.2 \pm 0.2$
$m_0^2 = -1.16$	$0.16 \pm 0.003$	$8.9 \pm 0.1$	$0.13 \pm 0.008$	$7.8 \pm 0.1$	$0.13$	$7.6 \pm 0.2$

We see that they agree within the error quoted by Lüscher and Weisz.

## A Appendix

In this appendix, we recall the Multigrid Monte Carlo method of Meyer and Mack<sup>[9]</sup> and present one criteria for its performance to beat critical slowing down (CSD). In order to define the algorithm, we must specify the following elements.

### i) Multigrid

A multigrid  $\Lambda = \Lambda_0 + \Lambda_1 + \dots + \Lambda_N$  is introduced which consists of a sequence of coarse-grids  $\Lambda_j$ , called layers, of decreasing lattice spacing  $a_j = L^{N-j} a_N$  where  $L$  is some integer  $\geq 2$ .  $\Lambda_N$  (called base) is the fundamental lattice of spacing  $a_N$ , where the field theory is defined. The points  $x \in \Lambda_j$  of the  $j^{\text{th}}$  layer may be identified with hypercubes of side length  $a_j$  in the base space. If  $z$  is a point of the hypercube  $y \in \Lambda_j$ , then we write  $z \in y$ . Also if the point  $x \in \Lambda_j$  is contained in the block  $y \in \Lambda_k$  with  $k < j$ , then we write  $x \in y$ .

### ii) Block spin fields

A sequence of block spins  $\Phi^j(x)$  is defined with  $x \in \Lambda_j$  as the block averages:

$$\Phi^j(x) = av_{z \in x} \phi(z) = C^j \phi(x) \quad \text{for } z \in \Lambda_N \quad (\text{A.1})$$

This definition of the block spins is particularly simple because the average of an average is again an average:

$$av_{x \in x'} \phi(x) = av_{x'' \in x'} av_{x \in x''} \phi(x) \quad (\text{A.2})$$

This is very convenient for an iterative procedure (Multigrid).

### iii) Linear decomposition

The fundamental field  $\phi(z)$  is split into a term called "background field", which is determined by the block spin  $\Phi^j$  and a "fluctuation field"  $\zeta^j$ , which has vanishing block averages:

$$\phi(z) = a_j^d \sum_{x \in \Lambda_j} A^j(z, x) \Phi^j(x) + \zeta^j(z) \quad (\text{A.3})$$

where  $d$  is the dimension of the base space  $\Lambda_N$ .

If one requires that

$$av_{z \in y} A^j(z, x) = a_j^{-d} \delta_{xy} \quad \text{for } x, y \in \Lambda_j \quad (\text{A.4})$$

then the decomposition (A.3) is consistent with the block spin choice (A.1).

Following the renormalization group interpretation of the multigrid transform, we iterate the split (A.3) in each layer  $\Lambda_j$ :

$$\Phi^j(x) = \int_{z \in \Lambda_{j-1}} A^j(x, x') \Phi^{j-1}(x') - \varphi^j(x) \quad (\text{A.5})$$

with

$$av_{x \in x'} \varphi^k(x) = 0 \quad \forall x' \in \Lambda_{k-1}, k = 1, \dots, N \quad (\text{A.6})$$

Inserting this into Eq. (A.3), one finds:

$$\phi(z) = \int_{x \in \Lambda_j} A(z, x) \Phi^j(x) + \zeta^j(z) \quad (\text{A.7})$$

$$\zeta^j = \sum_{k=j+1}^N \int_{x \in \Lambda_k} A(z, x) \varphi^k(x)$$

The kernel  $A(z, x)$  for  $x \in \Lambda_j$  is defined by induction as the convolution of  $A(z, y)$  with the kernel  $A(y, x)$  with  $y \in \Lambda_{j+1}$ , which appeared in the decomposition of  $\Phi^{j+1}$ :

$$A(z, x) = \int_{y \in \Lambda_{j+1}} A^{j+1}(z, y) A(y, x) \quad x \in \Lambda_j, z \in \Lambda_N \quad (\text{A.8})$$

The kernel obeys to the condition (A.4) which ensures the validity of (A.1). One introduces a multigrad field  $\varphi \in \Lambda$  by setting:

$$\begin{aligned} \varphi^0 &= \Phi^0 \\ \varphi(x) &= \varphi^j(x) \quad \text{if } x \in \Lambda_j, j = 0, \dots, N \end{aligned} \quad (\text{A.9})$$

In terms of this field, one can reexpress  $\phi$  as:

$$\phi(z) = \int_{x \in \Lambda} A(z, x) \varphi(x) \equiv \sum_{j=0}^N a_j^z \sum_{x \in \Lambda_j} A(z, x) \varphi(x) \quad (\text{A.10})$$

The field  $\varphi$  obeys to the constraints (A.6) for all layers except  $j = 0$ . These constraints determine  $\varphi(x)$  at block centers  $x = z_c \in \Lambda_j$  in terms of the other variables (for simplicity, one chooses  $L$  odd).

Then, there are as many independent variables  $\varphi(x)$  as  $\phi(z)$ , or equivalently  $\varphi$  is uniquely determined by  $\phi$ . Thus, its probability distribution is determined by the probability distribution of  $\phi$ . The idea is to map a (nearly) critical lattice field theory on base with hamiltonian  $H(\phi)$  into a theory on  $\Lambda$  with hamiltonian  $H(\varphi)$  which is hopefully not critical.

To reach this aim, we have to solve the important problem how to choose the kernel  $A$  (coarse-grid operator) properly.

#### iv) Coarse-grid operator

The fundamental issue to beat critical slowing down is to choose  $A$  in such way that the different layers  $\Lambda_j$  decouple as much as possible. In fact, if the kernel  $A^j(z, x)$  are chosen to decay exponentially in the distance  $|z - x|$  of  $z$  from the hypercube  $x$ , with decay length  $a_j$ , they introduce a non-locality in the horizontal direction over distances  $a_j$  only. But the number of point  $y \in \Lambda_k$  within the hypercube  $x \in \Lambda_j$  increases exponentially with  $k - j$  like  $L^d |k - j|$ . Therefore the coupling between layers  $\Lambda_j$  and  $\Lambda_k$  ( $k > j$ ) could induce correlations in  $\Lambda_k$  over distances of order  $L^{k-j}$  lattice spacings.

This shows that non criticality of the multigrad theory can only be achieved if the correlation between the low frequency field  $\varphi^j$  and the high frequency fields  $\varphi^k$  decay fast enough with  $k - j$ .

For weakly coupled models without spontaneous symmetry breaking, K. Gawedzki and A. Kupiainen<sup>[19]</sup> showed that the polymer representation of the theory on the multigrad admits

convergent cluster expansions, and therefore is essentially non critical if one chooses the  $A$  kernel so that:

$$-\Delta_z A^j(z, x) = \text{const.} \quad (\text{A.11})$$

as a function of  $z$  on cubes  $x \in \Lambda_j$ .

In fact, with these selections for  $A^j(z, x)$  it can be proved that<sup>[20]</sup>:

$$\langle \varphi^j(x) \varphi^k(y) \rangle > 0 = \nu^j(x, z) \delta_{jk} \quad \text{for } x \in \Lambda_j, y \in \Lambda_k \quad (\text{A.12})$$

where  $\nu^j$  is the propagator on the layer  $\Lambda_j$ . The expectation value is defined according to the free theory:

$$\langle A(\varphi) \rangle > 0 = \int d\mu_{\nu_0}(\varphi) \exp(-H_0(\varphi)) A(\varphi) / \int d\mu_{\nu_0}(\varphi) \exp(-H_0(\varphi)) \quad (\text{A.13})$$

That is, there is no correlation between different layers  $\Lambda_j \neq \Lambda_k$  in the free theory. Therefore, for weak coupling constant, one may follow the proposal of this rigorous analytical work based on renormalization group and cluster expansions and choose  $A^j(z, x)$  as:

$$A^j(z, x) = v C^j U_j^{-1} \quad (\text{A.14})$$

where  $v$  is the free propagator on  $\Lambda_N$

$U_j$  the block spin propagator

$C^j$  the dual operator of  $G^j$

The decomposition of the fundamental field  $\phi$  induces a decomposition of the free propagator  $v(z_1, z_2) = \langle \phi(z_1) \phi(z_2) \rangle > 0$ .

According to (A.7), it takes the form:

$$v(z_1, z_2) = \sum_{j=0}^N \iint_{x_1, x_2 \in \Lambda_j} A(z_1, x_j) v^j(x_j, y_j) A(z_2, y_j) \quad z_1, z_2 \in \Lambda_N \quad (\text{A.15})$$

These kernels  $A^j(z, x)$  have in fact the properties of exponential decay in  $|z - x|$  over distances  $a_j$  and satisfies the constraints (A.4).

#### v) Effective Hamiltonian

Inserting the decomposition (A.7) into the free action  $H_0 = \frac{1}{2}(\phi, -\Delta\phi)$ , one obtains:

$$\begin{aligned} H_0 &= -\frac{1}{2} \int_{x \in \Lambda_N} \int_{y \in \Lambda_N} A(z, x_j) \Phi^j(x_j) \Delta_x A(z, y_j) \Phi^j(y_j) \\ &\quad - \frac{1}{2} \sum_{k=j+1}^N \sum_{i=j+1}^N \int_{x \in \Lambda_N} \int_{y \in \Lambda_k} A(z, x_k) \varphi^k(x_k) \Delta_x A(z, y_i) \varphi_i(y_i) \\ &\quad - \sum_{k=j+1}^N \int_{x \in \Lambda_N} \int_{y \in \Lambda_k} A(z, y_j) \Phi^j(y_j) \Delta_x A(z, x_k) \varphi^k(x_k) \quad j < N \end{aligned} \quad (\text{A.16})$$

And using (A.4) and (A.6), we find:

$$H_0 = \frac{1}{2}(\Phi^j, -\Delta_{eff}^j \Phi^j) + \sum_{k=j+1}^N \frac{1}{2}(\varphi^k, -\Delta_{eff}^k \varphi^k) = \frac{1}{2} \sum_{k=0}^N (\varphi^k, -\Delta_{eff}^k \varphi^k) \quad (\text{A.17})$$

where  $\Delta_{\epsilon_{ij}}^j(x_j, y_j) = \int_{z \in \Lambda_N} A(z, x_j) \Delta_z A(z, y_j)$   $x_j, y_j \in \Lambda_j$ .  
By definition, the effective Hamiltonian at length scale  $a_j$  is a function of the block spin field  $\Phi^j(x) \in \Lambda_j$  and is given by:

$$\exp(H^j(\Phi^j)) = \int D\phi \prod_{x_j \in \Lambda_j} \delta(\Phi^j(x_j) - a v_{x_j \epsilon_j} \phi(z)) \exp(-H(\phi)) \quad (\text{A.18})$$

Inserting the decomposition (A.7) into the Hamilton function,  $H(\phi) = H_0(\phi) + V(\phi)$  with  $V(\phi) = \int_x v(\phi(z))$ , we get:

$$H^j(\Phi) = H_0^j(\Phi) + v^j(\Phi) \quad (\text{A.19})$$

with:

$$\left\{ \begin{aligned} H_0^j(\Phi) &= \frac{1}{2} (\Phi^j, -\Delta_{\epsilon_{ij}}^j \Phi^j) = -\frac{1}{2} \int_{x_j, y_j \in \Lambda_j} \Phi^j(x_j) \Delta_{\epsilon_{ij}}^j(x_j, y_j) \Phi^j(y_j) \\ \exp(-v^j(\Phi^j)) &= N_j \int \prod_{x \in \Lambda_{\geq j+1}} d\varphi(x) \exp\left(-\sum_{k=j+1}^N H_0^k(\varphi_k)\right) \times \\ &\exp\left[-\int_{x \in \Lambda_N} v\left(\int_{y_j \in \Lambda_j} A(z, y_j) \Phi^j(y_j) + \sum_{k=j+1}^N \int_{y_k \in \Lambda_k} A(z, y_k) \varphi(y_k)\right)\right] \end{aligned} \right. \quad (\text{A.20})$$

$N_j$  is a convenient constant normalization factor,  $\Lambda_{2j} = \Lambda_j + \Lambda_{j+1} + \dots + \Lambda_N$  and the prime on  $\prod d\varphi(x)$  stands to indicate that the fields  $\varphi$  satisfy a constraint (A.6). Therefore, one should integrate over variables attached to sites  $x \in \Lambda_k$  which are not centers of blocks  $x' \in \Lambda_{k-1}$ .

Using this notation the partition function and expectation value for the full theory can be expressed as:

$$\begin{aligned} z &= \int \prod_{x \in \Lambda} d\varphi(x) \exp(-H(A\varphi)) \quad (\text{A.21}) \\ < O > &= z^{-1} \int \prod_{x \in \Lambda} d\varphi(x) O(A\varphi) \exp(-H(A\varphi)) \end{aligned}$$

## vi) Updating

The aim of this procedure is to equilibrate the multigrid field  $\varphi^j$  through the sweeps on  $\Lambda_j$ . Due to the exponential decay of the kernel  $A^j(z, x)$ , the contribution of the field  $\varphi^j$  to  $\phi$  shall represent the contribution from a certain frequency range. Therefore, the conditional probability distribution  $\exp[-H(\varphi)] d\varphi^j$  for  $\varphi^j$ , given the fields  $\varphi^k$  on the other layers  $k \neq j$  is given by an auxiliary theory on  $\Lambda_j$ , with both an ultraviolet cutoff  $a_j^{-1}$  and an infrared cutoff  $a_{j-1}^{-1}$  for  $j \neq 0$ . This auxiliary theory shall have correlation length of order  $a_{j-1}$  and therefore shall be non singular. This affirmation is confirmed by the renormalization group interpretation of the multigrid transformation. For the full theory to be non critical, it is necessary that the coupling between  $\varphi^j$  and the fields  $\varphi^k$  with  $k > j$  (which represent higher frequency ranges) decays fast enough with  $k - j$ .

In fact, for  $k > j$  the number of cubes  $y \in \Lambda_k$  contained in cube  $x$  or within horizontal distance of order  $a_j$  (horizontal non locality introduced by  $A^j(z, x)$ ) increases exponentially with  $k - j$  like  $L^{d(k-j)}$ . Therefore, the coupling between layers  $\Lambda_j$  and  $\Lambda_k$  with  $k > j$  could induce correlations in  $\Lambda_k$  over distances of order  $L^{k-j}$  lattice spacings. In order to equilibrate  $\varphi^j$  through the sweeps on  $\Lambda_j$ , one can use then the fact that the auxiliary system described by the multigrid field  $\varphi$  is not singular and therefore, instead of

update  $\varphi^j$  (which satisfies the constraint (A.6)), one updates the block spin  $\Phi^j(x)$  keeping the fluctuation field  $\xi^j(z)$  fixed. In this way, the dominant and desired effect of update  $\Phi^j$  is to change  $\varphi^j$ , which is the highest frequency part of  $\Phi^j$ , while the lower frequency contributions  $\varphi^k$  with  $k < j$  will change just a little.

From the above-mentioned discussion, if the multigrid method beat critical slowing down completely, then the coupling between the layers must be small enough so that the updating in  $\Lambda_j$  would be nearly non-affected by the layers  $\Lambda_k$  with  $k \gg j$ . This implies that the acceptance probability in  $\Lambda_j$  given by:

$$H_x^j(\Phi, \zeta) = \frac{\delta H}{\delta \Phi^j(x)}(\Phi, \zeta) \quad (\text{A.22})$$

should not depend much on the high frequency contributions coming from  $\zeta^k$  with  $k > j$ . Therefore, the variance of  $H_x^j$ :

$$\sigma(H_x) = < H_x^2(\Phi, \zeta) >_\zeta - < H_x(\Phi, \zeta) >_\zeta^2 \quad (\text{A.23})$$

should have an UV limit or at least does not depend strongly on the UV cutoff.

The notation is as follows:

$$< O(\Phi, \zeta) >_\zeta = \frac{\int d\mu_r(\zeta) O(\Phi, \zeta) \exp(-V(A\Phi + \zeta))}{\int d\mu_r(\zeta) \exp(-V(A\Phi + \zeta))} \quad (\text{A.24})$$

is the average on the high frequency components of the fundamental field  $\phi$ . If one computes  $\sigma(H_x)$  by low order perturbation theory, one finds a quadratically UV divergent expression to lowest order<sup>[21]</sup>. This would indicate that critical slowing down is not completely eliminated. It is not clear how reliable is perturbation theory. Therefore it would be desirable to compute the variance numerically for different lattice sizes.

## vii) Computation of the effective potential and variance $\sigma$ from probabilities considerations

We recall how to extract the effective action  $H_{eff}(\Phi^0)$  its derivatives and explain how to compute  $\sigma(H_x)$  on the last layer  $\Lambda_0$ , which is a single point.

Let us define fluctuation coupling constants  $g_n(\zeta^0)$  by:

$$H(\phi) = H(\Phi^0 + \zeta^0) = \sum_{n=0}^4 \frac{1}{n!} g_n(\zeta^0) (\Phi^0)^n \quad (\text{A.25})$$

We regard the original Hamiltonian  $H$  as a function of the magnetization  $\Phi^0$  and fluctuation field  $\zeta^0(z)$ :

$$\Phi^0 = a v_{z \in \Lambda_N} \phi(z), \quad \zeta^0(z) = \phi(z) - \Phi^0 \quad (\text{A.26})$$

The Monte Carlo procedure produces a sequence of  $N_s$  configurations  $\phi_s$  and, using (A.25), one obtains a sequence of fluctuating fields  $\zeta_s$ .

For each of these configurations, one evaluates the fluctuating coupling constants  $g_n = g_n(\zeta_s)$  using (A.24).

With these data, one can compute the power series expansion of  $H_{eff}(\Phi^0)$  around any arbitrary point  $\Phi$  up to any desired order in  $\delta\Phi$ :

$$\delta\Phi = \Phi^0 - \Phi \quad (\text{A.27})$$

In fact, without loss of generality, we assume the normalization  $\int D\phi \exp(-H(\phi)) = 1$ . Then, the probability distribution  $\exp(-H(\phi)) D\phi$  specifies the probability distribution for  $\Phi^0$  viz.  $\exp(-H_{eff}(\Phi^0)) d\Phi^0$  and a probability distribution  $dp(\zeta^0)$  of  $\zeta^0$ . The probability of  $\Phi^0$  is the probability of  $\zeta^0$  times the conditional probability of  $\Phi^0$  given  $\zeta^0$  integrated over  $\zeta^0$ .

$$\exp(-H_{eff}(\Phi + \delta\Phi)) = \int dp(\zeta^0) \times z(\zeta^0)^{-1} \exp(-H(\Phi + \delta\Phi + \zeta^0)) \quad (\text{A.28})$$

where:  $z(\zeta^0) = \int d\Phi^0 \exp(-H(\Phi^0 + \zeta^0))$ .

The Monte Carlo configurations  $\zeta_a$  are distributed with probability  $dp(\zeta)$  so that  $\int dp(\zeta^0) f(\zeta^0) = \frac{1}{N_s} \sum_{a=1}^{N_s} f(\zeta_a)$ . Therefore:

$$\exp(-H(\Phi + \delta\Phi)) = N_s^{-1} \left\{ \sum_{a=1}^{N_s} z(\zeta_a)^{-1} \exp(-H(\Phi + \delta\Phi + \zeta_a)) \right\} \quad (\text{A.29})$$

$$= N_s^{-1} \left\{ \sum_{a=1}^{N_s} z_a^{-1} \exp\left(-\sum_{n=0}^4 \frac{1}{n!} g'_{n,a}(\Phi)(\delta\Phi)^n\right) \right\}$$

where  $\zeta_a$  and  $g'_{n,a}$  are defined by:

$$z_a = \int d\Phi \exp\left(-\sum_{n=0}^4 \frac{1}{n!} g_{n,a} \Phi^n\right) \quad (\text{A.30})$$

$$\sum_{n=0}^4 \frac{1}{n!} g_{n,a} \Phi^n = \sum_{n=0}^4 \frac{1}{n!} g'_{n,a}(\Phi)(\Phi - \Phi)^n$$

Expanding both sides of Eq.(A.29) in a power series in  $\delta\Phi$ , the effective action and its derivatives can be expressed in terms of the fluctuating coupling constant. Analogously, we can compute the variance  $\sigma(H_x^2)$  of Eq.(A.23). The general expression is found to be:

$$\langle O(\Phi, \zeta) \rangle_\zeta = \frac{\sum_{a=1}^{N_s} Z^{-1}(\zeta_a^0) O(\Phi^0, \zeta_a^0) \exp\left(-\sum_{n=0}^4 \frac{1}{n!} g_n(\zeta_a^0)(\Phi^0)^n\right)}{\sum_{a=1}^{N_s} Z^{-1}(\zeta_a^0) \exp\left(-\sum_{n=0}^4 \frac{1}{n!} g_n(\zeta_a^0)(\Phi^0)^n\right)} \quad (\text{A.31})$$

The criteria to know the performance of this Multigrid procedure to beat critical slowing down is thus given by Eq.(A.23) which can be numerically evaluated using Eq.(A.31). If the variance  $\sigma(H_x)$  does not increase with the UV-cut-off, then C.S.D. is eliminated. Otherwise there may be a net gain to reduce the autocorrelation time, but C.S.D. remains.

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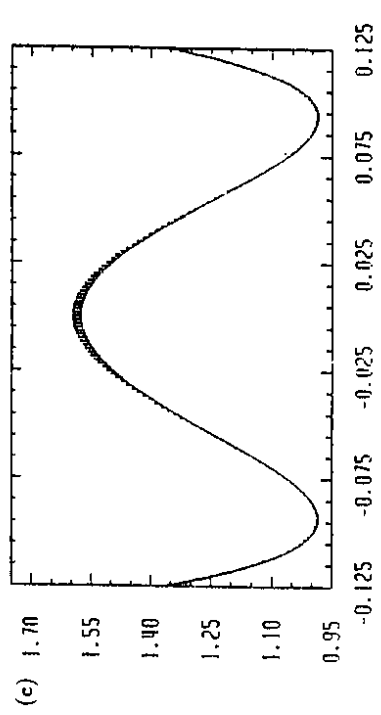
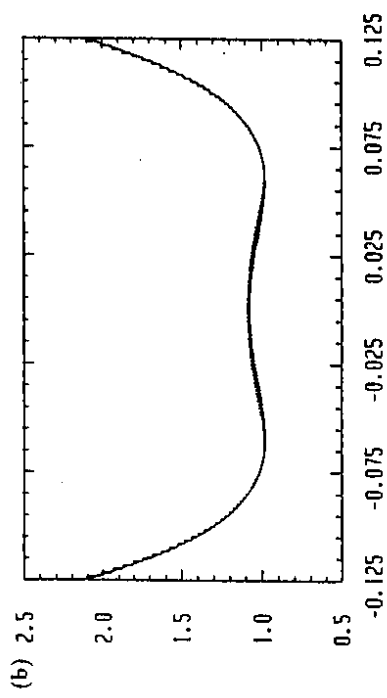
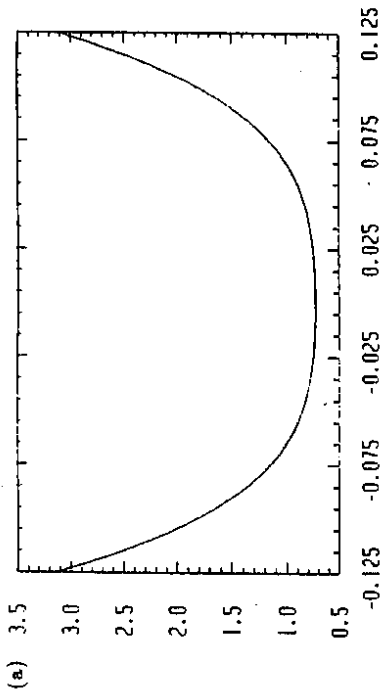


Fig. 2 Multigrid Monte Carlo data with error-bars as a function of the magnetization per site (in lattice units) for  $\lambda_0 = 16.376$  and fitting with the one loop formula of the constraint effective potential for the values of the bare mass: a)  $m_0^2 = -1.14$  b)  $m_0^2 = -1.15$  c)  $m_0^2 = -1.16$

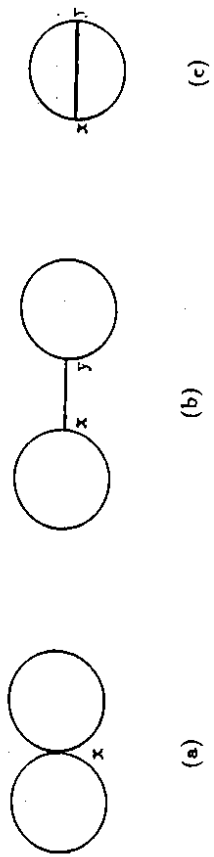


Fig. 1 The three connected diagrams to order  $\hbar^2$  in the expansion of  $U_0(\phi)$ . The diagram (b) drops out because the internal line connecting the bubbles must carry zero momentum due to momentum conservation at vertices and  $\varphi_F$  has no zero momentum component according to Eq.(2.6).