Nuclear Physics B271 (1986) 653–680
North-Holland, Amsterdam

THE CONSTRAINT EFFECTIVE POTENTIAL

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Received 19 December 1985

Because of the non-perturbative nature of the conventional effective potential $\Gamma(\Omega,\bar{\varphi})$ (for classical Higgs potentials and volume Ω) and because of the inconvenience of a Legendre transform for numerical computations, it is proposed to replace $\Gamma(\Omega,\bar{\varphi})$ by a "constraint" effective potential $U(\Omega,\bar{\varphi})$, which has a direct intuitive meaning, which is very convenient for lattice computations, and from which $\Gamma(\Omega,\bar{\varphi})$ can immediately be recovered (as the convex hull). In particular, $\Gamma(\infty,\bar{\varphi})=U(\infty,\bar{\varphi})$. Various properties of $U(\Omega,\bar{\varphi})$, such as convexity properties, upper and lower bounds and volume dependence are established. It is computed directly for zero dimensions and by Monte Carlo simulations in one and four dimensions, with up to 160 and 8^4 lattice sites, respectively.

1. Introduction

A widely used method to study the radiative corrections in a (continuum or lattice) quantum field theory is to use the effective potential $\Gamma(\Omega,\bar{\varphi})$ [1], defined conventionally as the Legendre transform of the Schwinger function, i.e.

$$\Gamma(\Omega,\bar{\varphi})=\sup_j\left(j\bar{\varphi}-W(\Omega,j)\right), \tag{1.1}$$

where

$$\exp(\Omega W(\Omega,j))=\int \mathscr{D}\varphi \exp\left\{-S[\varphi]+j\int_\Omega \varphi(x)\,\mathrm{d}^d x\right\},$$

where Ω is the total volume, j is a constant external current, and $S[\varphi]=\int_\Omega \mathscr{L}(\varphi)\,\mathrm{d}^d x$ is the classical action. It is well-known that $\Gamma(\Omega,\bar{\varphi})$ is convex [2] (whether or not the classical potential $V(\varphi)$ which generates $S[\varphi]$ is convex), and it has the property that if its minimum occurs at a unique point $\bar{\varphi}=\mathring{\varphi}$, the point $\mathring{\varphi}$ defines the vacuum state of the theory, and the loop expansion around $\mathring{\varphi}$ generates the one-particle-irreducible Feynman graphs [3]. The minimum is unique if either the volume is finite, or the classical potential is convex (or both). When the classical potential is not convex, as happens in particular for spontaneously broken potentials, the minimal points $\mathring{\varphi}$ of

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$\Gamma(\bar{\varphi}) = \Gamma(\infty, \bar{\varphi})$ are not unique but lie on a plane in $\bar{\varphi}$-space. In this case the vacuum is not determined by $\Gamma(\bar{\varphi})$ but by $\Gamma(\bar{\varphi})$ plus the direction from which a "trigger current" j approaches the value zero (see sect. 2). Furthermore, in this case the loop expansion breaks down and must be replaced by some alternative approximation [4]. Since for $\Omega = \infty$, V non-convex, the loop expansion has problems, a computational approach is more desirable, and in that case Γ may not be the best quantity to consider. A much more suitable quantity is the effective potential introduced by Fukuda and Kyriakopoulos [5]. This is defined by

$$\exp(-\Omega U(\Omega, \bar{\varphi})) = \int \mathscr{D}\varphi\, \delta\left(\frac{1}{\Omega}\int \varphi - \bar{\varphi}\right) \exp(-S[\varphi]) . \tag{1.2}$$

Since the delta-function introduced into the functional integral in (1.2) constrains the average value of the field φ to be $\bar{\varphi}$, we shall call $U(\Omega, \bar{\varphi})$ the constraint effective potential, and denote it by $U(\Omega, \bar{\varphi})$ throughout. In any case, one sees that nothing is lost by considering $U(\Omega, \bar{\varphi})$, because from (1.1) and (1.2) we have

$$\exp(\Omega W(\Omega, j)) = \int \mathrm{d}\bar{\varphi} \exp\{\Omega(j\bar{\varphi} - U(\Omega, \bar{\varphi}))\} , \tag{1.3}$$

which means that $W(\Omega, j)$ and $\Gamma(\Omega, \bar{\varphi})$ can always be recovered from $U(\Omega, \bar{\varphi})$ (and conversely). However, there are certain gains from using $U(\Omega, \bar{\varphi})$. First, one sees that (1.3) reduces (1.1) to a zero-dimensional (single-integral) analogue, with effective "classical" potential $U(\Omega, \bar{\varphi})$ and this corresponds to the usual intuitive treatment of $W(\Omega, j)$ and $\Gamma(\Omega, \bar{\varphi})$ in terms of single integrals. But more importantly, $\exp(-\Omega U(\Omega, \bar{\varphi}))$ relates to similar definitions in statistical mechanics and spin systems [6] and $\exp(-\Omega U(\Omega, \bar{\varphi}))/\int \mathrm{d}\bar{\varphi} \exp(-\Omega U(\Omega, \bar{\varphi}))$ can be interpreted as the probability density for the system to be in a state of "magnetization" $\bar{\varphi}$. Note that the probability for the occurrence of a state whose averaged field is not a minimum of $U(\Omega, \bar{\varphi})$ then becomes less and less as $\Omega \to \infty$ and thus $\langle \varphi(x) \rangle_\Omega \to \bar{\varphi}_\mathrm{m}$ as $\Omega \to \infty$, where $\bar{\varphi}_\mathrm{m}$ is some minimum point of $U(\Omega, \bar{\varphi})$ (not necessarily unique). Thirdly, $U(\Omega, \bar{\varphi})$ is a more direct quantity to compute with in Monte Carlo simulations, since an external current need not be introduced.

The formal expressions in the right-hand side of (1.1) and (1.2) must, of course, be regularized in some standard manner in order to remove the divergences. The natural regularization for our purpose will be the lattice regularization, since all our computations will be on the lattice, and, as explained in sect. 8, the lattice regularization ensures that the convexity properties of $\Gamma(\infty, \bar{\varphi})$ and $U(\infty, \bar{\varphi})$ are valid for all values of the lattice constant a, and in particular, are preserved in the continuum limit.

For brevity we shall use the notation $\Gamma(\bar{\varphi})$ and $U(\bar{\varphi})$ for the infinite-volume limits of $\Gamma(\Omega, \bar{\varphi})$ and $U(\Omega, \bar{\varphi})$ respectively, i.e.

$$\Gamma(\bar{\varphi}) \equiv \Gamma(\infty, \bar{\varphi}), \qquad U(\bar{\varphi}) \equiv U(\infty, \bar{\varphi}) .$$

The main purposes of the present paper are:

(i) To find the relationships between the conventional and constraint potentials $\Gamma(\Omega, \bar{\varphi})$ and $U(\Omega, \bar{\varphi})$.

(ii) To investigate the convex properties of $U(\Omega, \bar{\varphi})$.

(iii) To obtain upper and lower bounds for $U(\bar{\varphi})$.

(iv) To carry out lattice computations for $U(\Omega, \bar{\varphi})$.

The main results are:

(a) $\Gamma(\bar{\varphi})$ is the double Legendre transform of $U(\bar{\varphi})$ and is thus the convex hull of $U(\bar{\varphi})$ in the infinite-volume limit.

(b) $U(\Omega, \bar{\varphi})$ is not necessarily convex for finite Ω, but becomes convex as $\Omega \to \infty$.

(c) As an immediate consequence of (a) and (b), the two potentials become identical as $\Omega \to \infty$, i.e.

$$U(\bar{\varphi}) = \Gamma(\bar{\varphi}). \tag{1.4}$$

(d) In zero dimensions, or equivalently in the absence of kinetic terms in any number of dimensions, numerical integration shows that $U(\Omega, \bar{\varphi})$ becomes convex very rapidly as Ω increases (for typical models it is already convex for $5 \sim 7$ lattice sites!).

(e) In the quantum mechanical (QM) case, with non-convex classical potential, Monte Carlo (MC) simulations show that $U(\Omega, \bar{\varphi})$ is not convex for small volumes but quickly becomes convex as Ω increases.

(f) In four dimensions, MC simulations show that $U(\Omega, \bar{\varphi})$ becomes convex relatively slowly as $\Omega \to \infty$ (it is still non-convex for 8^4 lattice sites). For clarity these three results, (d), (e), (f), are summarized in the form of a table at the end of sect. 7.

(g) Reasonably good upper and lower bounds for $U(\bar{\varphi})$ can be found in terms of incoherent models, i.e., classical actions $S[\varphi]$ with no kinetic terms but modified parameters.

The development of the paper is as follows: in sect. 2 the relevant properties of the conventional effective potential $\Gamma(\Omega, \bar{\varphi})$ are recalled. In sect. 3 the constraint effective potential $U(\Omega, \bar{\varphi})$ is introduced and its properties are discussed. Incoherent models, i.e. models without kinetic terms, are introduced in sect. 4. The convexity of $U(\bar{\varphi})$ is established in sect. 5 and in sect. 6 bounds for $U(\bar{\varphi})$ are found. The results of the Monte Carlo simulations are presented in sect. 7. In sect. 8, the effects of renormalization on convexity are discussed.

2. Conventional effective potential $\Gamma(\bar{\varphi})$ and convexity

Consider a field theory described by a lagrangian density $\mathscr{L}(\varphi(x))$, where $\varphi(x)$ is a Higgs field which generally transforms non-trivially under the action of a symmetry group G.

$$\varphi(x) \to U(g)\varphi(x). \tag{2.1}$$

The classical vacuum is defined by the minimum of the classical action

$$S[\varphi]=\int\mathscr{L}(\varphi(x))\,\mathrm{d}^dx$$

$$=\int\left\{\tfrac{1}{2}\partial_i\varphi(x)\,\partial_i\varphi(x)+V(\varphi(x))\right\}\mathrm{d}^dx \tag{2.2}$$

and thus it is given by a constant field which minimizes the classical potential $V(\varphi)$. This value is not necessarily the VEV of the quantum field $\langle\varphi(x)\rangle$.

To study the quantum corrections to the classical value one introduces effective potentials. Most approaches to this subject begin with the partition function

$$Z(j)=\int\mathscr{D}\varphi\exp\left(-S[\varphi]+j\int\varphi(x)\right) \tag{2.3}$$

in the presence of a constant external current j. The external current is chosen constant so as to preserve the translational invariance of $Z(j)$ and thus corresponds to the constant effective field limit which is conventionally used to obtain the effective potential from the effective action. (For finite volumes Ω, translational invariance is understood to be with respect to periodic boundary conditions.) The Schwinger function

$$W(j)=\frac{1}{\Omega}\log Z(j) \tag{2.4}$$

is strictly convex since its second derivative

$$\frac{\mathrm{d}^2W}{\mathrm{d}j^2}=\Omega\left\langle\left(M-\langle M\rangle_j\right)^2\right\rangle_j, \tag{2.5}$$

where $M=(1/\Omega)\int\varphi(x)\,\mathrm{d}^dx$, is manifestly positive. Here we adopted the notation

$$\langle O\rangle_j=\frac{\int\mathscr{D}\varphi\,O[\varphi]\exp(-S[\varphi]+j\int\varphi)}{\int\mathscr{D}\varphi\exp(-S[\varphi]+j\int\varphi)} \tag{2.6}$$

for the expectation value of the observable O in the presence of an external current. $W(j)$ allows one to compute the effective field, defined as

$$\langle\varphi(x)\rangle_j=\frac{\mathrm{d}W}{\mathrm{d}j}. \tag{2.7}$$

In the ordinary approach one now defines the effective potential $\Gamma(\bar{\varphi})$ as the Legendre transform of the Schwinger function. It may be worth mentioning that one

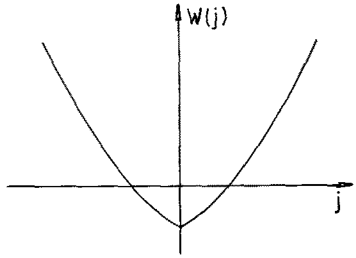

Fig. 1. In the infinite-volume limit, W may have a singular point at $j=0$.

must be cautious in defining the Legendre transform. In cases where the derivative of $W(j)$ is not continuous as shown in fig. 1, the commonly used transformation

$$\Gamma(\bar{\varphi}) = j\bar{\varphi} - W(j),$$

where j solves $\bar{\varphi} = \mathrm{d}W/\mathrm{d}j$, fails to be applicable. This happens typically when the classical potential that generates $S[\varphi]$ is not convex and the volume is infinite.
In order to handle the general case we use the sup-inf definition of the Legendre transformation [7], namely

$$\Gamma(\bar{\varphi}) = (LW)(\bar{\varphi}) = \sup_j \{ j\bar{\varphi} - W(j) \}. \tag{2.8}$$

This definition coincides with the one given above for a differentiable W.

Before discussing the various features of Γ we mention some properties of L in order to prepare the ground for the following sections.

First of all, for $(Lf)(y) = \sup_x (xy - f(x))$ to be well-defined, it is only necessary that $f(x)$ be strictly convex for large $|x|$, not necessarily for all x. For such f's the transformed function is always convex and the double Legendre transform $L^2 f$ is the convex hull of f [7]. In particular $L^2 f = f$ for any convex f, or in other words $L = L^{-1}$ is invertible on convex functions. Note that the definition (2.8) can be extended at once to vectors x, y by letting xy be the inner product (x, y).

Let us illustrate these properties by means of the constant field approximation $\partial_i \varphi = 0$ in which case the functional integral reduces to a single ordinary integral over constant fields $\exp(\Omega W(\Omega, j)) = \int \mathrm{d}\varphi \exp(\Omega(j\varphi - V(\varphi))$, with a potential of the general form

$$V(\varphi) \geqslant 0 \qquad \text{for } |\varphi| \leqslant c,$$

$$V(\varphi) = (|\varphi| - c)^2 \qquad \text{for } |\varphi| \geqslant c,$$

as illustrated in fig. 2a. One sees at once that

$$W(j) = \lim_{\Omega \to \infty} W(\Omega, j) = (LV)(j) = c|j| + \tfrac{1}{4} j^2$$

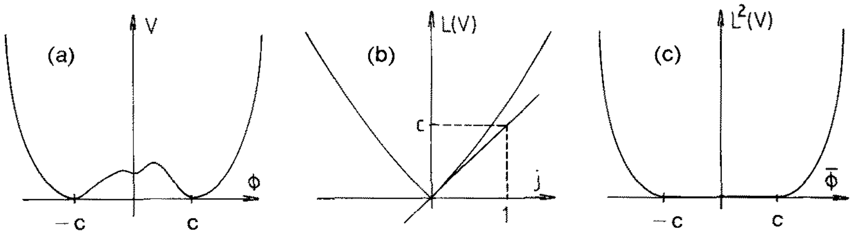

Fig. 2. LV and L^2V for a non-convex function.

has a discontinuous derivative at $j=0$ as shown in fig. 2b, and that the double transform

$$\Gamma(\bar{\varphi}) = (LW)(\bar{\varphi}) = (L^2V)(\bar{\varphi}) = \begin{cases} V(\bar{\varphi}) & \text{for } |\bar{\varphi}| \geqslant c \\ 0 & \text{for } |\bar{\varphi}| \leqslant c \end{cases}$$

is linear in the interval $-c \leqslant \bar{\varphi} \leqslant c$. Note that the discontinuity $2c$ in the derivative of LV is equal to the length of the linear interval $[-c, c]$. It is a general feature that when V is not strictly convex the derivative of LV is discontinuous and L^2V is piecewise linear, the length of the linear intervals being equal to the discontinuities in the derivative of LV.

In order to consider the more relevant case of a field theory it will be convenient to restrict ourselves to the case in which the action S, the measure $\mathscr{D}\varphi$ and the inner product (j, φ) are invariant with respect to some non-trivial group, i.e. with respect to transformations of the form $\varphi \to U(g)\varphi$ where $U(g)$ is a unitary representation of the group G. Then $W(j)$ is also group-invariant, and since

$$\Gamma(U\bar{\varphi}) = \sup_j \{(j, U\bar{\varphi}) - W(j)\} = \sup_{\tilde{j}} \{\tilde{j}\bar{\varphi} - W(U\tilde{j})\} = \Gamma(\bar{\varphi}),$$

the effective potential is invariant as well.

If we assume that the group leaves only the origin invariant, i.e. $U(g)j = j$ for all $g \in \mathrm{G}$ is only possible for $j=0$, then the strict convexity of W implies that $j=0$ is the unique minimum of the Schwinger function. The same reasoning can be applied to $\Gamma(\bar{\varphi})$ in the cases where it is strictly convex, but in the cases that it is only convex, but not strictly so, the argument fails, and although $\bar{\varphi}=0$ is a minimum of $\Gamma(\bar{\varphi})$ it is not the unique minimum. This happens in the example of fig. 2 where the minimum of $\Gamma(\bar{\varphi})$ lies in the whole linear interval $[-c, c]$ and it happens in the field theoretic case in the following way:

For group-invariant non-convex classical potentials $V(\varphi) \geqslant 0$ and $j \simeq 0$, the steepest-descent approximation yields not a single point $\mathring{\varphi}$ for which $\partial\mathring{\varphi}/\partial x = 0$, $V(\mathring{\varphi}) = 0$, but one or more group orbits G/H of such points, where H is the little group of any such $\mathring{\varphi}$. In this approximation

$$e^{\Omega W(j)} = \int d\sigma(\varphi) e^{\Omega(j,\varphi)}, \tag{2.9}$$

where the measure $d\sigma(\varphi)$ is over the orbits (usually only one) which minimize $V(\varphi)$, and

$$\bar{\varphi} = \int d\sigma(\varphi) e^{\Omega(j,\varphi)} \varphi \Big/ \int d\sigma(\varphi) e^{\Omega(j,\varphi)}. \tag{2.10}$$

For example for the reflection-invariant potential in one-variable $V(\varphi) = V(-\varphi) = (\varphi^2 - a^2)^2$, the formulae (2.9) and (2.10) become

$$e^{\Omega W(j)} = 2\cosh j\Omega a, \qquad \bar{\varphi} = a \tanh j\Omega a,$$

respectively, as discussed in detail in [4], and for the same potential but with φ and j in the n-dimensional fundamental representation of SO(n), one sees at once that the formulae become

$$e^{\Omega W(j)} = \text{const}\, B_0(|j|\Omega a),$$

$$\bar{\varphi} = \frac{aj}{|j|} B_0'(|j|\Omega a)/B_0(|j|\Omega a),$$

respectively, where B_0 is the Bessel function of order zero. From these examples one sees that the direction of j determines the direction of $\bar{\varphi}$, but that as the norm $|j|$ of j ranges over the small interval $0 \leqslant |j| \leqslant O(a^{-1}\Omega^{-1})$ the norm of $\bar{\varphi}$ ranges over the large interval $0 \leqslant |\bar{\varphi}| \leqslant a + O(\Omega^{-1})$. In the limit of $\Omega \to \infty$, therefore, the whole sphere $0 \leqslant |\bar{\varphi}| \leqslant a$ corresponds to $j = 0$ and thus within this sphere $\Gamma(\bar{\varphi}) = \Gamma(0)$. This sphere is the analogue of the interval $[-c, c]$ in the simple example above.

In the above examples the direction of $\bar{\varphi}$ is actually parallel to j, but this is because the potential depends only on the second-order invariant $I_2 = (\varphi, \varphi)$. More generally, one can only say that the direction of j determines that of $\bar{\varphi}$. For example, if $V(\varphi)$ and hence $W(j)$ depends on a cubic invariant $I_3(j)$, then

$$\bar{\varphi} = \frac{dW}{dj} = 2\frac{\partial W}{\partial I_2} j + \frac{\partial W}{\partial I_3}\frac{\partial I_3}{\partial j}$$

and it is well-known [8] that $\partial I_3/\partial j$ is not necessarily parallel to j. Similarly, in making the large-volume approximation to (2.10) one sees that the dominant value of φ is that for which (φ, j) is maximal, and since φ is constrained to lie on the minimizing orbits this φ is not necessarily parallel to j. We hope to give a more detailed discussion of these points in a subsequent publication.

To sum up, therefore, when $\Gamma(\bar{\varphi})$ is not strictly convex the vacuum state is not intrinsically determined by the system, but by the system plus the trigger. The direction of $\bar{\varphi}$ is fixed by an external current j which acts as a trigger provided that limits $\Omega \to \infty$, $j \to 0$ are taken in that order (or equivalently $\mathrm{Lt}_{\Omega j=\infty}$, $\mathrm{Lt}_{j=0}$). Since the vacuum state $\bar{\varphi}$ is not determined intrinsically, it is not surprising that the conventional loop expansion fails, as pointed out in [4]. What one then has to do is to make a loop expansion for each point $\mathring{\varphi}$ on the minimizing orbit(s) in (2.3) and integrate around the orbit(s). The result is the generalization of the "interpolated" loop expansion discussed in [4] for the reflexion group.

Much of the foregoing discussion can be nicely illustrated by the following zero-dimensional toy-model

$$e^{\Omega W(j)} = \int_{-\infty}^{\infty} d\varphi \, e^{\Omega(j\varphi - V(\varphi))},$$

where $V(\varphi)$ is the classical symmetric potential

$$V(\varphi) = h(|\varphi| - 1)\mathrm{sgn}(|\varphi| - 1), \qquad h > 0$$

depicted in fig. 3 and the volume is mimicked by Ω. Since $V(\varphi)$ increases only linearly as $|\varphi| \to \infty$, the model can only be used for $|j| < h$ but this region is sufficient for the previous discussion. The advantage of the model is that $W(j)$ can be computed explicitly and one finds

$$W(j) = \frac{1}{\Omega}\log\{2\cosh \Omega j - e^{-h\Omega}\} + \frac{1}{\Omega}\frac{2h}{\log\{\Omega(h^2 - j^2)\}},$$

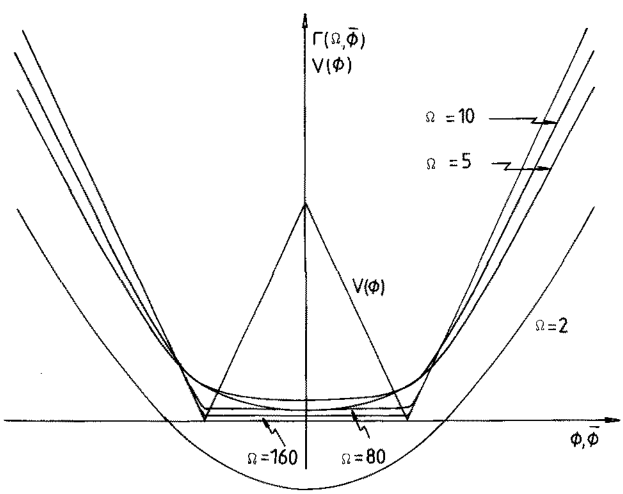

Fig. 3. Volume dependence of $\Gamma(\Omega, \bar{\varphi})$ for the W-well classical potential.

where the second term on the right is just a multiplying factor for $2\cosh \Omega j - \exp(-h\Omega)$ and carries the singularity that must appear as $|j| \to h$. The factor $2\cosh \Omega j - \exp(-h\Omega)$ is the interesting one. The term $2\cosh \Omega j$ is exactly the interpolated loop expansion [4] and $\exp(-h\Omega)$ the correction to it. This correction vanishes exponentially as $\Omega \to \infty$ as one might expect and decreases with the height h of the central peak.

Furthermore, since $W'(j) = \tanh \Omega j + O(1/\Omega)$ converges to the signature function in the limit $\Omega \to \infty$, the graph of the effective potential $\Gamma(\bar{\varphi}) = \sup_j(j\bar{\varphi} - W(j))$ contains a horizontal line between $\bar{\varphi} = -1$ and $\bar{\varphi} = 1$. Fig. 3 shows the "volume" dependence of $\Gamma(\bar{\varphi})$ for $h = 1$. As expected, Γ converges to the convex hull of the classical potential.

3. The constraint effective potential

In this section we introduce the constraint effective potential discussed in the introduction. One way to motivate its introduction is to consider the order parameter, which is defined as vacuum expectation value (VEV) of some functional $O[\varphi]$ of the fields

$$\langle O[\varphi]\rangle = N^{-1}\int O[\varphi]\mathrm{e}^{-S[\varphi]}. \tag{3.1}$$

This suggests introducing a constraint that fixes the functional $O[\varphi]$ which corresponds to the order parameter, i.e. to write

$$Z(\bar{O}) = \int \mathscr{D}\varphi\, \delta(O[\varphi] - \bar{\varphi})\mathrm{e}^{-S[\varphi]} \tag{3.2}$$

and this leads one to define alternative effective potentials as

$$U(\bar{O}) = -\frac{1}{\Omega}\log Z(\bar{O}). \tag{3.3}$$

One sees at once that

$$\langle O[\varphi]\rangle = N^{-1}\int \mathrm{d}\bar{O}\,\bar{O}\,\mathrm{e}^{-\Omega U(\bar{O})}, \tag{3.4}$$

where $N = \int \mathrm{e}^{-\Omega U(\bar{O})}\mathrm{d}\bar{O}$. We shall confine ourselves to the order parameter $O[\varphi] = (1/\Omega)\int \varphi(x)$, since its expectation value decides whether the system exhibits a spontaneous symmetry breakdown. The potential $U(\bar{\varphi})$ is then defined as

$$\mathrm{e}^{-\Omega U(\bar{\varphi})} = \int \mathscr{D}\varphi\, \delta(M - \bar{\varphi})\mathrm{e}^{-S[\varphi]}, \qquad M = \frac{1}{\Omega}\int_\Omega \varphi(x) \tag{3.5}$$

and this is the potential which we shall call the *constraint* effective potential (CEP).

Note that from the definition (3.5) and the translational invariance of the system, $N^{-1}\exp(-\Omega U(\bar{\varphi}))\Delta\bar{\varphi}$ is the probability of finding a value of the Higgs field at a point x, $\varphi(x)$, between $\bar{\varphi}$ and $\bar{\varphi}+\Delta\bar{\varphi}$. This property gives a very intuitive interpretation of $U(\bar{\varphi})$. We shall now discuss some further properties of $U(\bar{\varphi})$. These will be useful not only from a theoretical but also from a computational point of view.

Properties of U. In what follows we shall be interested not only in the infinite-volume limit $\Omega \to \infty$ but also in the volume dependence of the various potentials. So we keep the Ω explicit to emphasize that $W(\Omega, j)$, $U(\Omega, \bar{\varphi})$ and $\Gamma(\Omega, \bar{\varphi})$ are volume dependent.

First we establish the relation between the functions $W(\Omega, j)$, $U(\Omega, \bar{\varphi})$ and $\Gamma(\Omega, \bar{\varphi})$. Multiplying both sides of (3.5) by $\exp(\Omega j\bar{\varphi})$ and integrating over $\bar{\varphi}$, yields

$$\int e^{\Omega(j\bar{\varphi}-U(\Omega,\bar{\varphi}))}\,d\bar{\varphi} = e^{\Omega W(\Omega, j)}. \tag{3.6}$$

Hence $W(\Omega, j)$ is related to $U(\Omega, \bar{\varphi})$ by a Laplace transformation. Note that since $\Gamma = \mathrm{LW}$, the function $\Gamma(\Omega, \bar{\varphi})$ is uniquely determined by $U(\Omega, \bar{\varphi})$. Conversely, $W = L\Gamma$ so $U(\Omega, \bar{\varphi})$ can be recovered from $\Gamma(\Omega, \bar{\varphi})$ by an inverse Laplace transformation. Thus there is a one-to-one correspondence between the potentials $U(\Omega, \bar{\varphi})$ and $\Gamma(\Omega, \bar{\varphi})$.

Now let us discuss what happens in the infinite-volume limit $\Omega \to \infty$. For $\Omega \to \infty$ the saddle-point approximation to the integral in (3.6), $\int \exp\{j\bar{\varphi} - U(\Omega, \bar{\varphi})\}\,d\bar{\varphi} \sim \exp\{\Omega \sup_{\bar{\varphi}}(j\bar{\varphi} - U(\Omega, \bar{\varphi}))\}$ becomes exact. Then

$$W(j) = (LU)(j) = \sup_{\bar{\varphi}}\{j\bar{\varphi} - U(\bar{\varphi})\}, \tag{3.7}$$

where $W(j) = \lim_{\Omega\to\infty} W(\Omega, j)$ etc. It follows that $\Gamma = LW = L^2U$. Thus Γ *is the convex hull of* U. In sect. 5 we will prove that U is convex and then

$$\Gamma(\bar{\varphi}) = U(\bar{\varphi}). \tag{3.8}$$

Thus in the infinite-volume limit the two potentials actually become identical. However, in a finite volume the two potentials are not identical and $U(\Omega, \bar{\varphi})$ need not necessarily be convex. For example, in a zero-dimensional field theory, $U(\bar{\varphi})$ is actually the classical potential $U(\bar{\varphi}) = V(\bar{\varphi})$, which need not, of course, be convex. From the formula (3.5) one sees at once that a G-symmetric action defines a G-symmetric potential $U(\Omega, \bar{\varphi})$. Hence when the classical action is G-invariant all three quantities, $W(\Omega, j)$, $U(\Omega, \bar{\varphi})$ and $\Gamma(\Omega, \bar{\varphi})$ are G-invariant.

This remark completes the comparison of the three potentials. The results are summarized in the following fig. 4 which shows the qualitative shape of the various potentials for a SO(2) symmetric theory which exhibits a spontaneous symmetry breakdown.

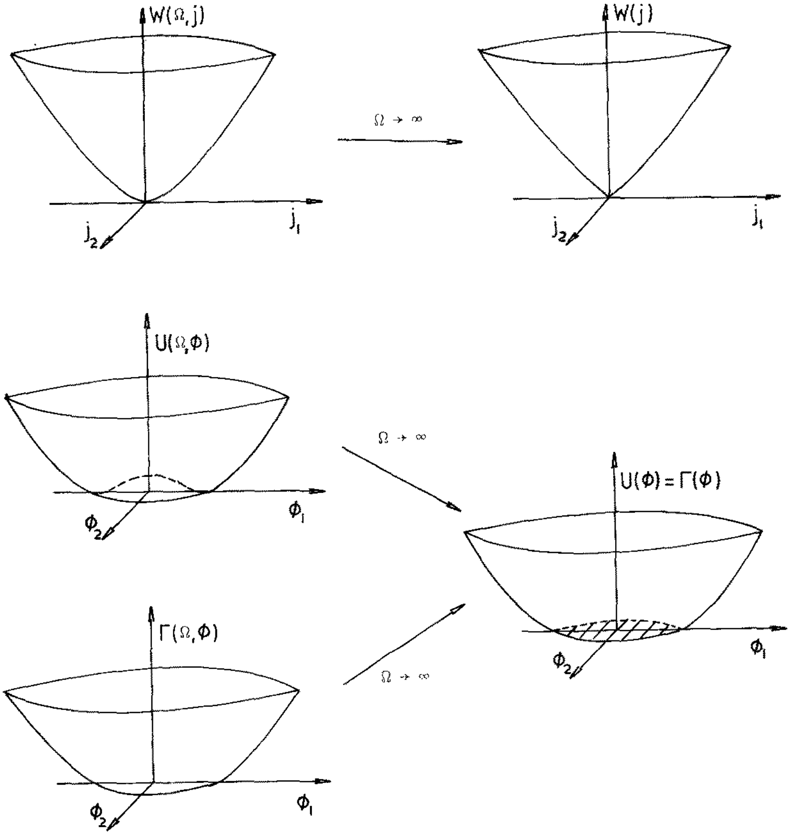

Fig. 4. $W(\Omega, j)$ and "Mexican-hat" type of $U(\Omega, \bar{\varphi})$ for a SO(2) model. As $\Omega \to \infty$, W becomes singular at $j = 0$, and U develops a flat region.

The potential $U(\Omega, \bar{\varphi})$ is also useful for extracting information directly about the gross properties of the system, such as whether it suffers a spontaneous breakdown or whether it has a finite correlation length. To see this one notes that

$$\frac{\int \bar{\varphi}^l e^{\Omega(j\bar{\varphi} - U(\Omega, \bar{\varphi}))} d\bar{\varphi}}{\int e^{\Omega(j\bar{\varphi} - U(\Omega, \bar{\varphi}))} d\bar{\varphi}} = \Omega^{-l} \int d^d x_1 \ldots d^d x_l \langle \varphi(x_1) \ldots \varphi(x_l) \rangle_j^\Omega , \tag{3.9}$$

i.e. that the moments of $N^{-1}\exp\{\Omega(j\bar{\varphi} - U(\Omega, \bar{\varphi}))\}$ are the averaged Schwinger functions in the presence of an external current. For $l = 1$ (3.9) gives the vacuum expectation value

$$\langle \varphi(x) \rangle_j^\Omega = N^{-1} \int \bar{\varphi} e^{\Omega(j\bar{\varphi} - U(\Omega, \bar{\varphi}))} d\bar{\varphi} . \tag{3.10}$$

For any finite volume the symmetry of U leads to $\langle \varphi(x) \rangle_0^\Omega = 0$. To get a non-trivial result one must keep a trigger current, and only after the infinite-volume limit has been taken can the trigger be removed, as has already been discussed in sect. 2 for the potential $\Gamma(\Omega, \bar{\varphi})$. For any non-vanishing j the saddle-point approximation to the integral in (3.10) picks the unique point $\bar{\varphi}$ on the G-invariant minimum set of U which has the maximal inner product with j, and if this point is not zero there is a spontaneous symmetry breakdown. For $l=2$ and $j=0$ the formula (3.9) reads

$$N^{-1}\int \bar{\varphi}^2 \mathrm{e}^{-\Omega U(\Omega,\bar{\varphi})}\mathrm{d}\bar{\varphi} = \Omega^{-2}\int \mathrm{d}^d x_1\, \mathrm{d}^d x_2 \langle \varphi(x_1)\varphi(x_2)\rangle_0^{\Omega}.$$

The expectation value on the r.h.s. is the 2-point Schwinger function $S_2(x_1 - x_2)$ which only depends on $x_1 - x_2$ because of translational invariance. So we end up with

$$\chi = \Omega \frac{\int \bar{\varphi}^2 \mathrm{e}^{-\Omega U(\Omega,\bar{\varphi})}\mathrm{d}\bar{\varphi}}{\int \mathrm{e}^{-\Omega U(\Omega,\bar{\varphi})}\mathrm{d}\bar{\varphi}} = \int S_2(x)\,\mathrm{d}^d x. \tag{3.11}$$

(For spin systems χ would be the susceptibility.) In the infinite-volume limit the saddle-point approximation becomes valid and one sees that

$$\chi \to \infty \qquad \text{if, and only if } \left.\frac{\partial^2 U}{\partial \bar{\varphi}^2}\right|_0 \overset{\Omega\to\infty}{\to} 0.$$

On the other hand, from (3.11) and the known asymptotic properties of $S(x)$, namely $S(x) \sim \exp(-|x|/\xi)$ as $|x| \to \infty$ one sees that $\chi \to \infty$ implies that $\xi \to \infty$, i.e. that the correlation length is infinite.

4. Lattice theory and incoherent models

A precise definition of "sum over all fields" must be given to the functional integrals in the previous two sections to make sense. One way to proceed is to introduce a d-dimensional space-time lattice discretizing the euclidean space-time by a hypercubic lattice with lattice spacing a. The action (2.2) becomes

$$S[\varphi] = \sum_{\langle ij\rangle} a^{d-2}\tfrac{1}{2}(\varphi_i - \varphi_j)^2 + \sum_i a^d V(\varphi_i), \tag{4.1}$$

where $\varphi_i = \varphi(x_i)$ $(i = 1,2,\dots, N = \Omega/a^d)$ and $\Sigma_{\langle ij\rangle}$ is the sum over all nearest-neighbour pairs. We take periodic boundary conditions.

By introducing a dimensionless lattice field $\varphi^{\mathrm{L}} = a^{d/2-1}\varphi$, (4.1) can be rewritten as

$$S[\varphi] = S^{\mathrm{L}}[\varphi^{\mathrm{L}}] = \sum_{\langle ij\rangle} \tfrac{1}{2}\left(\varphi_i^{\mathrm{L}} - \varphi_j^{\mathrm{L}}\right)^2 + \sum_i V^{\mathrm{L}}\left(\varphi_i^{\mathrm{L}}\right), \tag{4.2}$$

where the lattice potential V^{L} is equal to the classical potential, but with rescaled parameters. The masses and coupling constants are rescaled according to their dimensions, e.g. $m_{\mathrm{L}} = a^2 m$ etc. By using the lattice field as a new integration variable in the lattice version of (3.5) one easily finds

$$\Omega U(\Omega, \bar{\varphi}) = N U^{\mathrm{L}}(N, \bar{\varphi}^{\mathrm{L}}) + \mathrm{const}(a), \tag{4.3}$$

where $\bar{\varphi}^{\mathrm{L}} = a^{d/2-1}\bar{\varphi}$ is dimensionless and

$$\mathrm{e}^{-NU^{\mathrm{L}}(N, \bar{\varphi}^{\mathrm{L}})} = \int \prod \mathrm{d}\varphi_i^{\mathrm{L}}\, \delta\left(\frac{1}{N}\sum \varphi_i^{\mathrm{L}} - \bar{\varphi}^{\mathrm{L}}\right) \mathrm{e}^{-S^{\mathrm{L}}[\varphi^{\mathrm{L}}]}. \tag{4.4}$$

For any finite a one recovers $U(\Omega, \bar{\varphi})$ from $U^{\mathrm{L}}(N, \bar{\varphi}^{\mathrm{L}})$ by a trivial rescaling of U^{L} and $\bar{\varphi}^{\mathrm{L}}$. We will use the formula (4.3) for the constraint effective potential in the following sections. In what follows the subscript L will mostly be dropped. Note also, that in terms of dimensionless quantities the theory is defined only on a unit lattice of size N.

For a fixed lattice constant a the volume is proportional to N. Hence, studying the volume dependence of $U(\Omega, \bar{\varphi})$ is equivalent to studying the N dependence of $U^{\mathrm{L}}(N, \bar{\varphi}^{\mathrm{L}})$.

Let us first consider models in which there are no kinetic terms, which we shall call *incoherent models* since the lattice points then behave independently. At first sight these models may appear to be trivial, but there are some very good reasons for studying them. First, they show properties which we will meet again in the full theory, e.g. the convergence of $U(N, \bar{\varphi})$ to a convex function. Secondly, we can extract the influence of the kinetic term on the effective potentials by comparing the incoherent models with those of the full theory. Lastly, the incoherent models deliver upper and lower bounds for the true effective potential, as will be shown in sect. 6.

In order to factorize the functional integral (4.4) for the incoherent models we replace the constraint $\delta(M - \bar{\varphi})$ by $(2\pi)^{-1}\int \mathrm{d}p \exp(-ip(\mathrm{M} - \bar{\varphi}))$. As a consequence

$$\mathrm{e}^{-NU^0(N, \bar{\varphi})} = \frac{N}{2\pi} \int \mathrm{d}p\, \mathrm{e}^{N(ip\bar{\varphi} + \log f(p))}, \tag{4.5}$$

where $f(p) = \int \exp(-ip\varphi - V(\varphi))\mathrm{d}\varphi$. For large N this integral approaches its saddle-point value. The saddle point of $ip\bar{\varphi} + \log f(p)$ in the complex p-plane is the point $p = i \cdot j$, where j is a solution of $\bar{\varphi} = \mathrm{d}W^0/\mathrm{d}j$ and $\exp(W^0(j)) = \int \mathrm{d}\varphi \exp(j\varphi - V(\varphi))$. Hence we find that in the limit $N \to \infty$

$$U^0(\bar{\varphi}) = (LW^0)(\bar{\varphi}), \tag{4.6}$$

where W^0 is the Schwinger function of the zero-dimensional theory with potential V, i.e.

$$\mathrm{e}^{W^0(j)} = \int \mathrm{e}^{j\varphi - V(\varphi)}\mathrm{d}\varphi. \tag{4.7}$$

Since W^0 is not only strictly convex but also analytic in this case the constraint potential $U^0(\bar{\varphi})$ is strictly convex as well.

In order to obtain an intuitive feeling for the manner in which $U^0(N, \bar{\varphi})$ converges to the convex $U^0(\bar{\varphi})$ as $N \to \infty$, we compute $U^0(N, \bar{\varphi})$ for the toy model [9]

$$V(\varphi) = \varphi^2 - \log(1 + \lambda\varphi^2). \tag{4.8}$$

This potential is non-convex for $\lambda > 1$. After a tedious but straightforward calculation one obtains for $U^0(N, \bar{\varphi})$ the explicit expression

$$U^0(N, \bar{\varphi}) = \bar{\varphi}^2 - \frac{1}{N}\log P_N(\bar{\varphi}^2) + C, \tag{4.9}$$

where P_N is the polynomial of degree N,

$$P_N(\bar{\varphi}^2) = \sum_{k=0}^{N} \left\{ \sum_{q=0}^{N-k} \binom{k+q}{k} \binom{N}{k+q} (2k+2q-1)!! \left(\frac{\lambda}{(2+\lambda)N} \right)^q \right\} \times \left(\frac{2\lambda\bar{\varphi}^2}{2+\lambda} \right)^k \frac{1}{(2k-1)!!} \tag{4.10}$$

and C is the constant

$$C = -\log\left\{ \left(1 + \tfrac{1}{2}\lambda\right)\sqrt{\pi} \left(\frac{N}{\pi} \right)^{1/(2N)} \right\}. \tag{4.11}$$

On the other hand, the limiting potential U^0 is derived by (4.6) through the formula (4.7) which yields

$$W^0(j) = \tfrac{1}{4}j^2 + \log\left\{1 + \tfrac{1}{2}\lambda + \tfrac{1}{4}\lambda j^2\right\} + \tfrac{1}{2}\log\pi. \tag{4.12}$$

In fig. 5 we show the potentials $U^0(N, \bar{\varphi})$ for different numbers of lattice sites and the limiting function $U^0(\bar{\varphi})$. It is remarkable how fast the potentials converge to U^0.

In passing, it may be of interest to note that the functional integral for the toy model (4.8) may be written as

$$\int \mathscr{D}\varphi \exp\left(- \int \tfrac{1}{2}(\nabla\varphi)^2 + \varphi^2 + \log(1 + \lambda\varphi^2) \right)$$

$$= \int \mathrm{d}\varphi\, \mathrm{d}\psi\, \mathrm{d}\bar{\psi} \exp\left(- \int \tfrac{1}{2}(\nabla\varphi)^2 + \varphi^2 + \bar{\psi}(1 + \lambda\varphi^2)\psi \right),$$

which shows that the logarithmic potential (4.8) for the bosonic variable φ may be

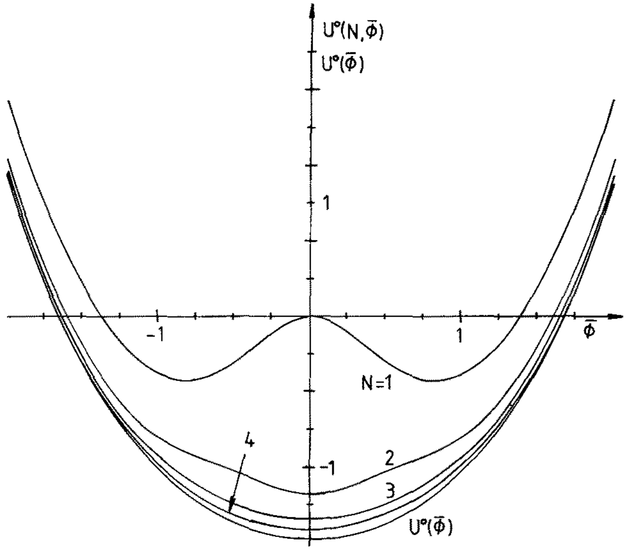

Fig. 5. Volume (N) dependence of the incoherent constraint effective potential $U^0(N, \bar{\varphi})$ for the classical potential (4.8).

derived from a Yukawa-like interaction of the boson field with a fermion field (in the limit when the fermion field is constant, $\partial_\mu \psi = 0$). This derivation of the logarithmic potential (4.8) is rather similar to the derivation of the well-known Coleman-Weinberg potential [10].

5. Convexity of the constraint potential in the infinite-volume limit

We now return to the realistic models with kinetic terms. In this section we will show that in the infinite-volume limit the constraint effective potential must be convex, i.e. that

$$U(\bar{\varphi}) \leqslant \mu U(\bar{\varphi}_A) + (1-\mu) U(\bar{\varphi}_B), \tag{5.1}$$

or equivalently

$$\mathrm{e}^{-NU(\bar{\varphi})} \geqslant \mathrm{e}^{-\mu N U(\bar{\varphi}_A)} \mathrm{e}^{-(1-\mu) N U(\bar{\varphi}_B)}, \tag{5.2}$$

where

$$\bar{\varphi} = \mu \bar{\varphi}_A + (1-\mu) \bar{\varphi}_B, \qquad 0 \leqslant \mu \leqslant 1. \tag{5.3}$$

For that purpose we divide a lattice with N sites into two sub-lattices, say A and B, with $NA = \mu N$ and $NB = (1-\mu)N$ sites, respectively. Let IA (IB) denote the sites

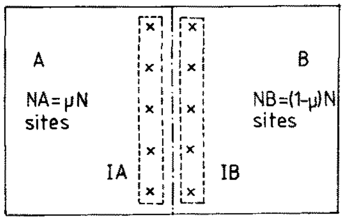

Fig. 6. A lattice with N sites is divided into two sub-lattices A and B with $NA = \mu N$ and $NB = (1-\mu)N$ sites, respectively. IA and IB denote the sites in A and B, respectively on the boundary between A and B.

in A (B) nearest to the interface I between A and B (fig. 6).

By applying the inequalities

$$0 \leqslant \tfrac{1}{2}(\varphi_i - \varphi_j)^2 \leqslant \varphi_i^2 + \varphi_j^2 \tag{5.4}$$

to the kinetic energy of the nearest neighbour pairs whose connecting line intercepts I, one obtains

$$\begin{aligned} S_{NA}[\varphi_A] + S_{NB}[\varphi_B] &\leqslant S_N[\varphi] \\ &\leqslant S_{NA}[\varphi_A] + S_{NB}[\varphi_B] + \sum_{IA}\varphi_i^2 + \sum_{IB}\varphi_i^2 , \end{aligned} \tag{5.5}$$

where φ_A (φ_B) stands for the restriction of the configuration φ to the sub-lattice A (B). With $M_A = (1/NA)\Sigma_A\varphi_i$, $M_B = (1/NB)\Sigma_B\varphi_i$ and therefore $\mu M_A + (1-\mu)M_B = M$, one sees at once that

$$\delta(M - \bar{\varphi}) = \int \mathrm{d}\alpha\, \delta(M_A - \bar{\varphi} + (1-\mu)\alpha)\,\delta(M_B - \bar{\varphi} - \mu\alpha) \tag{5.6}$$

and hence

$$\begin{aligned} &\int \mathrm{d}\alpha \exp(-N\tilde{U}(N, \mu, \alpha, \bar{\varphi})) \\ &\quad \geqslant \exp(-NU(N, \bar{\varphi})) \\ &\quad \geqslant \int \mathrm{d}\alpha \left\{ \int \prod_A \mathrm{d}\varphi_i\, \delta(M_A - \bar{\varphi} + (1-\mu)\alpha) \exp\left(-S_{NA}[\varphi_A] - \sum_{IA}\varphi_i^2 \right) \right. \\ &\qquad\qquad \left. \times \int \prod_B \mathrm{d}\varphi_j\, \delta(M_B - \bar{\varphi} - \mu\alpha) \exp\left(-S_{NB}[\varphi_B] - \sum_{IB}\varphi_j^2 \right) \right\}, \end{aligned}$$

where

$$\tilde{U}(N, \mu, \alpha, \bar{\varphi}) = \mu U(NA, \bar{\varphi} - (1-\mu)\alpha) + (1-\mu)U(NB, \bar{\varphi} + \mu\alpha) .$$

To get rid of the boundary terms $\Sigma_{IA}\varphi_i^2$ and $\Sigma_{IB}\varphi_j^2$ we use Jensen's inequality $\int d\mu \exp(f) \geqslant \exp\{\int d\mu\, f/\int d\mu\}\int d\mu$ with $f = -\Sigma\varphi_i^2$ and $d\mu = \prod d\varphi_i\, \delta(\cdot)\exp(-S)$ and find

$$\int d\alpha \exp(-N\tilde{U}(N,\mu,\alpha,\bar{\varphi})) \geqslant \exp(-NU(N,\bar{\varphi}))$$

$$\geqslant \int d\alpha \exp(-N\{\tilde{U}(N,\mu,\alpha,\bar{\varphi}) + B(N,\mu,\alpha,\bar{\varphi}\}) . \tag{5.7}$$

The boundary term $B(N,\mu,\alpha,\bar{\varphi}) = (1/N)\Sigma_{IA}\langle\varphi_i^2\rangle_A + (1/N)\Sigma_{IB}\langle\varphi_j^2\rangle_B$ is of order $O(N^{-1/d})$, since by translational invariance

$$B(N,\mu,\alpha,\bar{\varphi}) = \frac{|IA|}{N}\langle\varphi_i^2\rangle_A + \frac{|IB|}{N}\langle\varphi_j^2\rangle_B = O(cN^{-1/d}) ,$$

where $|IA|$ ($|IB|$) denotes the number of sites of IA (IB). Hence, for large N we may neglect the boundary term in the r.h.s. of (5.7) and then the upper and lower bounds become the same. In the limit $N \to \infty$ the integral is equal to its saddle-point value and for $U(N,\bar{\varphi})$, $U(NA,\bar{\varphi})$, $U(NB,\bar{\varphi}) \overset{N\to\infty}{\to} U(\bar{\varphi})$ one therefore has

$$U(\bar{\varphi}) = \inf_{\substack{\alpha \\ 0\leqslant\mu\leqslant 1}} \{\mu U(\bar{\varphi} - (1-\mu)\alpha) + (1-\mu)U(\bar{\varphi} + \mu\alpha)\} . \tag{5.8}$$

In particular, for $\alpha = \bar{\varphi}_B - \bar{\varphi}_A$ one finds

$$U(\bar{\varphi}) \leqslant \mu U(\bar{\varphi}_A) + (1-\mu)U(\bar{\varphi}_B) ,$$

which establishes the convexity of the constraint potential in the infinite-volume limit, as required*. The quantity on the r.h.s. of (5.8) is actually the convex hull of U (see appendix) so that (5.8) could be written as $U(\bar{\varphi}) = (L^2U)(\bar{\varphi})$.

6. Properties of $U(\bar{\varphi})$ useful for computations

Before proceeding to compute $U(\bar{\varphi})$ it will be convenient to obtain some of its general properties that are useful for computations. These take the form of lower and upper bounds, and of a differential (Ehrenfest) equation for $U(\bar{\varphi})$. The lower bound is fairly trivial as it is obtained by simply neglecting the kinetic terms to obtain

$$U(\bar{\varphi}) \geqslant U^0(\bar{\varphi}) , \tag{6.1}$$

* For a qualitative discussion of the convexity of U, see [11].

where $U^0(\bar{\varphi})$ is the constraint effective potential (CEP) for the corresponding incoherent model. Next we derive an upper bound for U. With (5.4) one finds

$$T[\varphi] = \tfrac{1}{2} \sum_{\langle ij \rangle} (\varphi_i - \varphi_j)^2 = T[\varphi - \bar{\varphi}] \leqslant 2d \sum \varphi_i^2 - 4d\bar{\varphi} \sum \varphi_i + 2dN\bar{\varphi}^2 ,$$

where we have taken into account that in d dimensions every site has $2d$ nearest neighbours. By inserting this inequality into (4.4) one obtains

$$e^{-NU(N,\bar{\varphi})} \geqslant e^{2dN\bar{\varphi}^2} \int \delta(M - \bar{\varphi}) e^{-V^d[\varphi]} ,$$

where $V^d[\varphi] = 2d\Sigma\varphi_i^2 + \Sigma_i V(\varphi_i)$. This yields the upper bound

$$U(\bar{\varphi}) \leqslant -2d\bar{\varphi}^2 + U^d(\bar{\varphi}) , \tag{6.2}$$

where $U^d(\bar{\varphi})$ is the incoherent CEP which corresponds to $V^d[\varphi]$. However since $U(\bar{\varphi})$ is known to be convex, (6.2) actually implies that

$$U(\bar{\varphi}) \leqslant L^2(-2d\bar{\varphi}^2 + U^d(\bar{\varphi})) , \tag{6.3}$$

where $L^2(-2d\bar{\varphi}^2 + U^d(\bar{\varphi}))$ is the convex hull of $-2d\bar{\varphi}^2 + U^d(\bar{\varphi})$. Eq. (6.3) is the required upper bound.

In fig. 7 we show these bounds for the Higgs model

$$V(\varphi) = \lambda(\varphi^2 - \sigma^2)^2 \tag{6.4}$$

in various dimensions using the values $\lambda = 10$ and $\sigma^2 = 0.375$ for the parameters. It is remarkable that the upper bound in (6.3) is much better than those given in (6.2) in the dimensions $d = 3, 4$, for which one expects to have spontaneous symmetry breakdown. In sect. 7 we will compare these bounds with the results obtained by Monte Carlo (MC) simulations.

We conclude this section by deriving for $U(\bar{\varphi})$ an Ehrenfest equation which turns out to be very useful for MC simulations. For that purpose we return to (3.5) and in that equation shift the field by a constant, $\varphi(x) \to \varphi(x) + \bar{\varphi}$. Because of the translational invariance of the measure $\mathscr{D}\varphi$ we obtain

$$e^{-\Omega U(\bar{\varphi})} = \int \mathscr{D}\varphi \, \delta(M) e^{-S[\varphi + \bar{\varphi}]} .$$

Since only the potential term in S is affected by the shift, one then obtains

$$\frac{d}{d\bar{\varphi}} U(\bar{\varphi}) = \frac{1}{\Omega} \langle V'[\varphi] \rangle_{\bar{\varphi}} , \tag{6.5}$$

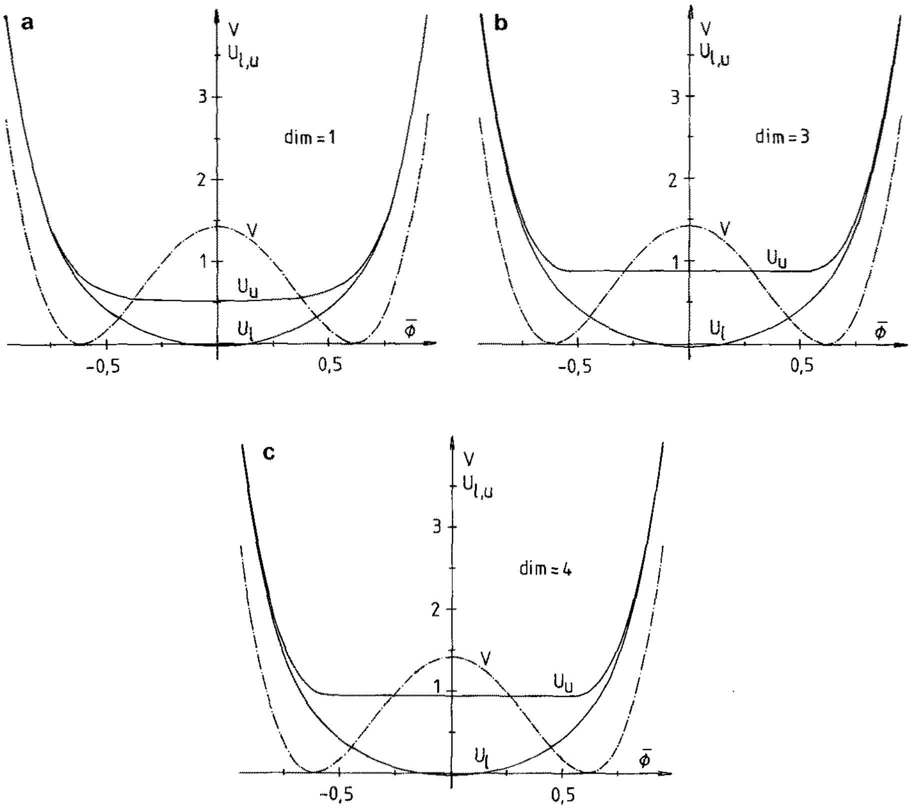

Fig. 7. Upper and lower bounds, U_u, U_ℓ for U in dimensions $d=1$ (a), $d=3$ (b) and $d=4$ (c). V is the classical potential; $V(\varphi)=\lambda(\varphi^2-\sigma^2)^2$ with $\lambda=10$ and $\sigma^2=0.375$.

where $\langle O[\varphi]\rangle_{\bar{\varphi}} = N^{-1}\int \mathscr{D}\varphi\, \delta(M-\bar{\varphi})O[\varphi]\mathrm{e}^{-S[\varphi]}$. This is the required Ehrenfest equation. To obtain a feeling for its content let us apply it to two simple models, namely the free model, with potential $V(\varphi)=\frac{1}{2}m^2\varphi^2$ and the Higgs model (6.4). For the free model (6.5) reduces to $U'(\bar{\varphi}) = m^2\langle M\rangle_{\bar{\varphi}} = m^2\bar{\varphi}$. Hence the CEP becomes

$$U(\bar{\varphi}) = \tfrac{1}{2}m^2\bar{\varphi}^2 + \text{const}. \tag{6.6}$$

Of course the constant is not determined. We can use the bounds in (6.1) and (6.3) to limit its possible values. For the free model

$$U^d(N,\bar{\varphi}) = \tfrac{1}{2}(m^2+4d)\bar{\varphi}^2 - \frac{N-1}{2N}\log\frac{2\pi}{m^2+4d} + \frac{1}{2N}\log N \tag{6.7}$$

and therefore

$$\tfrac{1}{2}m^2\bar{\varphi}^2 + \tfrac{1}{2}\log\frac{m^2}{2\pi} \leqslant U(\bar{\varphi}) \leqslant \tfrac{1}{2}m^2\bar{\varphi}^2 + \tfrac{1}{2}\log\frac{m^2+4d}{2\pi}\,.$$

For the Higgs model (6.4) eq. (6.5) reads

$$U'(\bar{\varphi}) = 4\lambda\left\{\langle\varphi^3(x)\rangle_{\bar{\varphi}} - \sigma^2\bar{\varphi}\right\}, \tag{6.8}$$

where we have used the translational invariance, i.e. $\langle \int\varphi^3\rangle_{\bar{\varphi}} = \Omega\langle\varphi^3(x)\rangle_{\bar{\varphi}}$. For the Higgs model equation (6.8) actually serves as a starting point for the MC simulations (see next section), and in general turns out to be an extremely useful equation in making MC simulations for the constraint effective potential.

7. Monte Carlo simulations

From the discussion of the previous sections we know that the conventional effective potential $\Gamma(\Omega, \bar{\varphi})$ is convex for any volume and that in the spontaneously broken case it develops a range R of $\bar{\varphi}$ for which it is flat (constant) in the infinite volume limit, i.e., with suitable normalization $\Gamma(\infty, \bar{\varphi}) = 0$ for $\bar{\varphi} \in$ R. We also know that the CEP $U(\Omega, \bar{\varphi})$ is not necessarily convex for finite Ω, but that as $\Omega \to \infty$, $U(\Omega, \bar{\varphi}) \to \Gamma(\bar{\varphi})$, and therefore $U(\Omega, \bar{\varphi})$ becomes convex for all $\bar{\varphi}$ (and in the spontaneously broken case flat for $\bar{\varphi} \in$ R) in the infinite-volume limit. It is therefore interesting to study $U(\Omega, \bar{\varphi})$ for finite volumes, to see for example for which volume it is not convex, and how it approaches $\Gamma(\bar{\varphi})$ in the infinite-volume limit.

As is well known, the Monte Carlo (MC) simulations are very useful in the computation of various non-perturbative quantities in statistical physics and field theories [12]. Hence to study $U(\Omega, \bar{\varphi})$ for finite volumes we shall carry out the MC simulations for a quantum mechanical (QM) system and a four-dimensional scalar field theory with the non-convex classical potential. From the computational point of view, the advantage of computing U rather than Γ is that it is more direct [13]. It is not necessary to introduce external currents j and to construct Legendre transforms. It is enough to simulate the system just by taking the constraint into account. In practice we take the constraint into account by integrating over one of the site variables, say the Nth one φ_N to get rid of the constraint.

The effective theory we obtain is then

$$e^{-NU(N,\bar{\varphi})} = \int \prod_1^{N-1} d\varphi_i \exp\left\{ -\tfrac{1}{2} \sum_{i \in \text{nn of } N} (\varphi_i - \varphi_N)^2 - V(\varphi_N) \right.$$
$$\left. -\tfrac{1}{2} \sum_{\langle ij\rangle}{}' (\varphi_i - \varphi_j)^2 - \sum_1^{N-1} V(\varphi_i) \right\}, \tag{7.1}$$

where $\varphi_N = N\bar{\varphi} - \Sigma_1^{N-1}\varphi_i$ and $\Sigma'_{\langle i,j\rangle}$ is the sum over all nearest-neighbour pairs except those which contain φ_N. The Metropolis algorithm is then applied to this theory. The trial variable φ_i in the updating process is taken to be

$$\varphi_i' = \varphi_i + \delta, \tag{7.2}$$

where φ_i is the variable of the old configuration, and δ is a random number between $-\Delta$ and Δ, i.e. $\delta = \{2 \cdot (\text{uniform random number}) - 1\} \cdot \Delta$. The factor Δ is adjusted so that the acceptance rate in the procedure becomes reasonable (about 50%). The updating hits the sites successively from $i = 1$ to $N-1$. This induces at the same time the updating of the Nth site

$$\varphi'_N = \varphi_N - \delta, \tag{7.3}$$

i.e., the two site variables φ_i and φ_N are updated by the same amount but with different signs. The total sum $\Sigma_1^N \varphi_i$ is thus kept at $N\bar{\varphi}$. This procedure is carried out until only the last pair $(\varphi_{N-1}, \varphi_N)$ is left. Then the sweep is finished and the next sweep starts again with φ_1. Actually we take 5 updatings per sweep for each pair (φ_i, φ_N) to obtain a faster convergence to the equilibrium state.

The Ehrenfest differential equation (6.5) derived in the previous section is very useful for computing $U(\bar{\varphi})$ since $\langle V'[\varphi]\rangle_{\bar{\varphi}}$ of the right-hand-side is an expectation value of a local quantity. For the potential of a form $V(\varphi) = \lambda(\varphi^2 - \sigma^2)^2$, the differential equation is given in (6.8), from which one sees that it is sufficient to compute the expectation value $\langle \varphi^3 \rangle_{\bar{\varphi}}$ of φ^3 to obtain $U(\bar{\varphi})$. Fig. 8 shows how fast $\langle \varphi^3 \rangle_{\bar{\varphi}}$ converges to its equilibrium value in the four-dimensional scalar field theory, starting from the ordered initial configuration, i.e. $\varphi_i = \bar{\varphi}$ for all i with the parameters $\lambda = 10$, $\sigma^2 = 0.375$ and $\bar{\varphi} = 0.2$. The expectation value $\langle \varphi^3 \rangle_{\bar{\varphi}}$ is computed using

$$\langle \varphi^3 \rangle_{\bar{\varphi}} = \frac{1}{\frac{1}{2} It} \sum_{l = It/2+1}^{It} \langle \varphi^3 \rangle_{\bar{\varphi}}^{(l)}, \tag{7.4}$$

where $\langle \varphi^3 \rangle_{\bar{\varphi}}^{(l)} = (1/N)\Sigma_1^N (\varphi_i^{(l)})^3$ is the arithmetic mean of $\{\varphi_i^3\}$ in the lth sweep

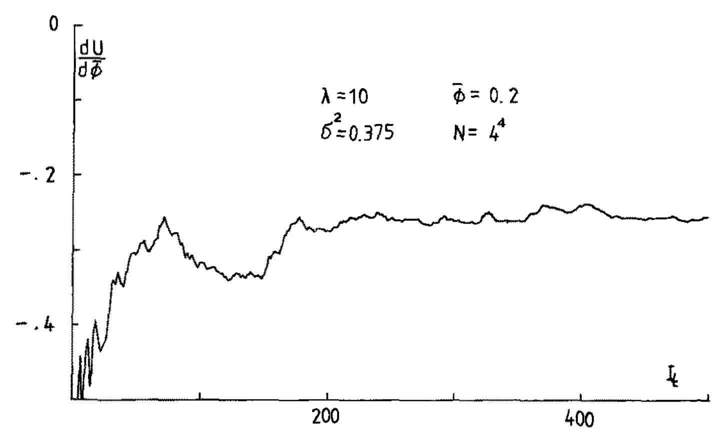

Fig. 8. Plot of $\mathrm{d}U/\mathrm{d}\bar{\varphi}$ versus number of sweeps I_t for a 4^4 lattice at $\bar{\varphi} = 0.2$.

($\frac{1}{2}It + 1 \leqslant l \leqslant It$ for even integers It). The first $\frac{1}{2}It$ configurations are discarded. The figure shows that it is reasonable to consider a relaxation "time" $\frac{1}{2}It$ as $100 \sim 150$ sweeps.

Since $U(\bar{\varphi}) = U(-\bar{\varphi})$, one computes U only for positive values of $\bar{\varphi}$. We start the simulations with $\bar{\varphi} = 1$ which is larger than the value of the classical minimum ($\sigma = 0.612$), so that the semiclassical approximation is expected to be valid. In other words, the fluctuations of $\varphi^3(x)$ are expected to be small. After the computation of $\langle \varphi^3 \rangle_{\bar{\varphi}}$ at $\bar{\varphi} = 1$, the final configuration is stored in the memory as the initial configuration for the next run, in which the value $\bar{\varphi}$ is chosen to be slightly smaller than unity, $\bar{\varphi} = 1 - \Delta\bar{\varphi}$. This is justified since the equilibrium states for these two values of $\bar{\varphi}$ are close to each other if $\Delta\bar{\varphi}$ is small enough. In fact we took $\Delta\bar{\varphi} = 0.05$. This procedure is repeated until $\bar{\varphi}$ comes to zero. Finally, of course, the obtained $U'(\bar{\varphi})$ must be integrated to find $U(\bar{\varphi})$.

Quantum mechanics. Let us first study a quantum mechanical system or 1-dimensional scalar theory. It is known that there is no spontaneous symmetry breaking in such a theory. What we then expect is that $U(N, \bar{\varphi})$ converges to $\Gamma(\bar{\varphi})$ which is strictly convex as the volume goes to infinity. The result of the MC simulations shows that $U(N, \bar{\varphi})$ is convex for a finite volume as well. Fig. 9 shows the behaviour of $U(N, \bar{\varphi})$ and that of the corresponding $\Gamma(N, \bar{\varphi})$ for different volumes ($N =$ the number of sites) $N = 20$, 80 and 160. $\Gamma(N, \bar{\varphi})$ is computed using

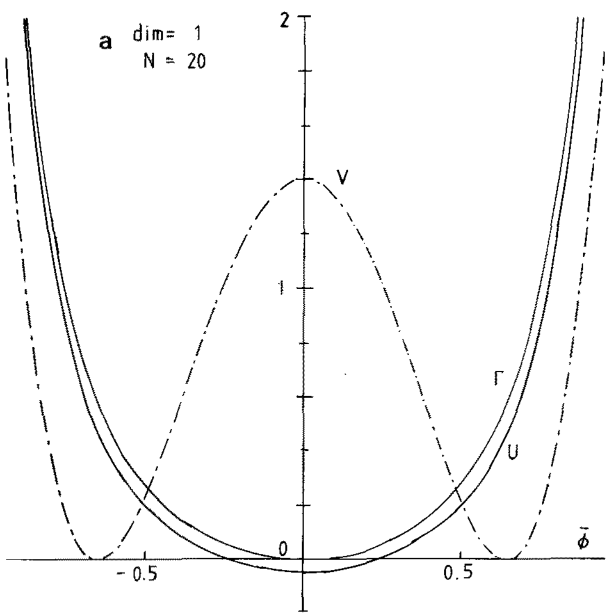

Fig. 9. U and Γ for the classical potential V with the parameters $\lambda = 10$ and $\sigma^2 = 0.375$ for a quantum mechanical system. The number of sites are $N = 20$ (a), 80 (b) and 160 (c). In fig. 9c the upper and lower bounds U_u and U_l for U are also shown. The normalization of U and Γ is fixed in fig. 9c since U_u and U_l approach each other for large values of $|\bar{\varphi}|$.

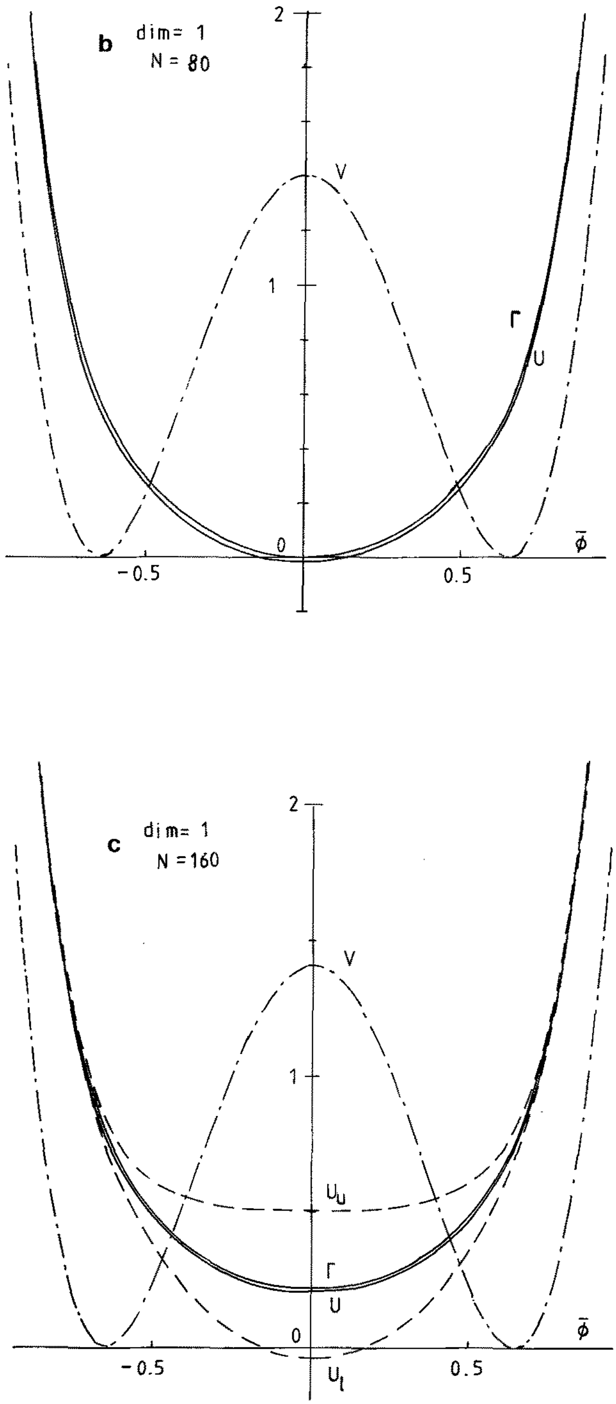

Fig. 9 (continued).

the data of $U(N, \bar{\varphi})$. For its computation we first use the Laplace transform (3.6) to obtain $W(N, j)$ from $U(N, \bar{\varphi})$ and then the Legendre transform (2.8) to obtain $\Gamma(N, \bar{\varphi})$ from $W(N, j)$. These two convex potentials approach each other as N increases. For $N = 80$, they are already almost equal. In Fig. 9c, the lower and upper bounds (6.1) and (6.3) for U are also shown.

4-dimensional scalar theory. We now turn to the more interesting case, the 4-dimensional Higgs scalar theory. We find that $U(N, \bar{\varphi})$ is non-convex for the finite volumes considered in this case. Fig. 10 shows $U(N, \bar{\varphi})$ and the corresponding $\Gamma(N, \bar{\varphi})$ for three different volumes $N = 2^4$, 4^4 and 8^4. $U(N, \bar{\varphi})$ is clearly non-convex, while $\Gamma(N, \bar{\varphi})$ develops the flat region, which signals a SSB.

From the discussion of the previous section, we know that $U(N, \bar{\varphi})$ finally converges to $\Gamma(\bar{\varphi})$. Such a tendency can be seen in the figure, but the rate of the convergence is rather slow compared to the one-dimensional case. This is because in higher dimensions the contributions of the kinetic terms become more important and they slow down the convergence. The slowdown due to the kinetic terms can be exhibited more explicitly by comparing these results with those for the corresponding "incoherent" CEP $U^0(N, \bar{\varphi})$ derived from the same classical action, but without kinetic terms. Fig. 11 shows the behaviour of $U^0(N, \bar{\varphi})$ of the truncated model for different values of N. One sees that $U^0(N, \bar{\varphi})$ converges to its limit $U^0(\bar{\varphi})$ remarkably quickly. We also note that the upper bound (6.3) for U, which is shown in Fig. 10c, is astonishingly good.

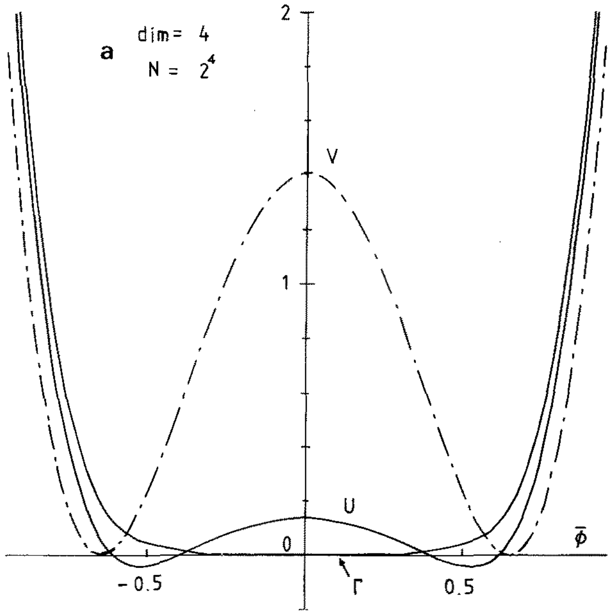

Fig. 10. U, Γ and V for a four dimensional scalar field theory for $N = 2^4$ (a), 4^4 (b) and 8^4 (c). The upper and lower bounds U_u, U_l for U are also shown in fig. 10c, and the normalization of U and Γ are fixed by U_u and U_l in the same way as in the quantum mechanical case.

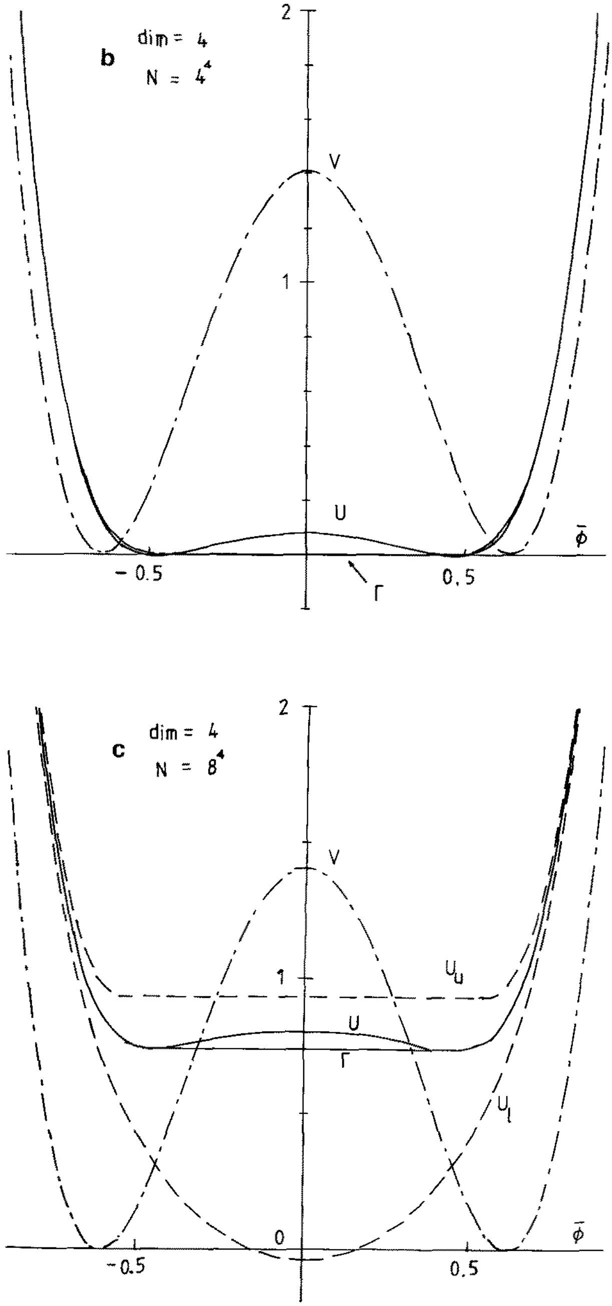

Fig. 10 (continued).

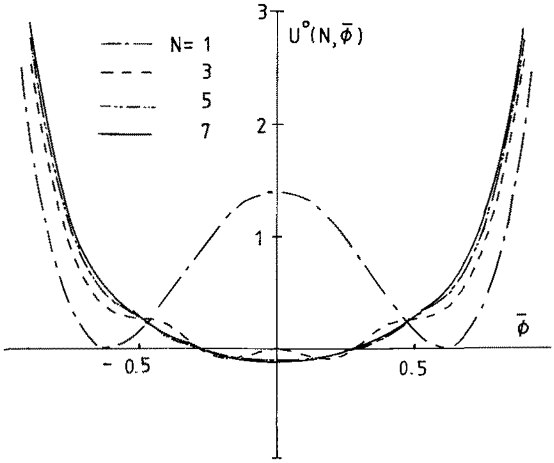

Fig. 11. Volume dependence of $U^0(N,\bar{\varphi})$ for $V=\lambda(\varphi^2-\sigma^2)^2$ with $\lambda=10$ and $\sigma^2=0.375$.

It may be worth remarking that the $\Gamma(N,\bar{\varphi})$'s obtained here are in agreement with that of Creutz-Freedman [14] for the quantum mechanical case and that of Callaway-Maloof [15] for the 4-dimensional scalar field theory ($N=4^4$). Both of these sets of authors carried out the Legendre transform of $W(N,j)$ to obtain $\Gamma(N,\bar{\varphi})$ by introducing the external current j.

It may be convenient to summarize the results of our computations and also of earlier analytical results in the form of a table. First we note that if the classical potential is strictly convex all of the effective potentials considered, $\Gamma(\Omega,\bar{\varphi})$, $U^0(\Omega,\bar{\varphi})$ and $U(\Omega,\bar{\varphi})$ are strictly convex for all Ω including $\Omega=\infty$. Second we note that $U^0(\Omega,\bar{\varphi})$ is actually independent of the space dimensions, because in the absence of a kinetic term there is no distinction between an L^d and an $(L\times L\times\cdots\times L)_d$ lattice. Taking these points into account, we depict the alternatives in the form of a table.

TABLE 1

Summary of convex properties of Γ, U and U^0 for non-convex classical potentials

<table>
<tr><th colspan="2"></th><th>$\Gamma(\Omega,\bar{\varphi})$</th><th>$U(\Omega,\bar{\varphi})$</th><th>$U^0(\Omega,\bar{\varphi})$</th></tr>
<tr><td rowspan="2">V non-convex but no SSB ($d=1$)</td><td>$\Omega<\infty$</td><td rowspan="3">strictly convex</td><td rowspan="2">becomes strictly convex (fairly quickly) as $\Omega\to\infty$</td><td rowspan="4">becomes strictly convex very quickly as $\Omega\to\infty$</td></tr>
<tr><td>$\Omega=\infty$</td></tr>
<tr><td rowspan="2">V non-convex but SSB ($d=4$)</td><td>$\Omega<\infty$</td><td>non-convex</td></tr>
<tr><td>$\Omega=\infty$</td><td colspan="2">convex but not strictly so ($\Gamma=U$)</td></tr>
</table>

8. Preservation of convexity properties under lattice renormalization

In the preceding sections we have not introduced any explicit renormalization, since on a finite lattice this is not necessary for finiteness. However, the bare quantities we have considered have to be related to physical quantities by renormalization and we have to consider whether this renormalization affects the convexity properties. Consider for example the following conventional renormalization scheme. First introduce a dimensionless lattice length ε ($a=\varepsilon\Lambda^{-1}$, where Λ is a scale parameter with a mass dimension) and rescale the various quantities in the manner that is suggested naturally by dimensional considerations, i.e. define

$$U^{\varepsilon}(\bar{\varphi}, m_0, g_0) = \varepsilon^{-d} U^{\varepsilon=1}\big(\varepsilon^{(d-2)/2}\bar{\varphi}, m_0(\varepsilon), g_0(\varepsilon)\big) \tag{8.1}$$

and define a "physical" mass m_{p} and coupling constant g_{p} in terms of U^{ε} by some typical equations such as (for $d=4$)

$$\langle\varphi^2\rangle_{\varepsilon} = \frac{\Lambda^2}{m_{\mathrm{p}}^2}, \qquad \langle\varphi^4\rangle_{\varepsilon} - \langle\varphi^2\rangle_{\varepsilon}^2 = \frac{1}{g_{\mathrm{p}}}, \tag{8.2}$$

where

$$\langle O\rangle_{\varepsilon} = \frac{\int \mathrm{d}\bar{\varphi}\, O(\bar{\varphi})\mathrm{e}^{-U^{\varepsilon}}}{\int \mathrm{d}\bar{\varphi}\, \mathrm{e}^{-U^{\varepsilon}}}. \tag{8.3}$$

Of course, m_{p} and g_{p} as defined in (8.2) will not necessarily be the physical mass and the quartic coupling constant for the φ field, but just some related physical quantities. (Indeed because of its association with $\langle\varphi^2\rangle$ and therefore the width of the classical Higgs potential, m_{p}^2 is more closely associated with the masses of any gauge fields that may interact with φ.)

Now the lattice renormalization consists in letting the bare mass and coupling constant m_0, g_0 depend on ε in such a way that the physical constants $m_{\mathrm{p}}, g_{\mathrm{p}}$ defined in (8.2) do *not* depend on ε. Given the dependence of U^{ε} on ε, m_0, g_0 and given $m_0(1)=m_0$, $g_0(1)=g_0$ the functional dependence $m_0(\varepsilon)$, $g_0(\varepsilon)$ is then determined implicitly by (8.2). In other words the renormalization consists of constructing an ε-dependent map from $(m_{\mathrm{p}}, g_{\mathrm{p}})$ to (m_0, g_0) by means of (8.2). Of course, the domain D (ε, g_{p}, m_{p}) of m_{p} and g_{p} which, for each ε, will produce a real finite $m_0(\varepsilon)$ and a real, finite, positive $g_0(\varepsilon)$, may be limited. In particular, if φ^4 theory in $d=4$ dimensions really is trivial then $g_{\mathrm{p}}\to 0$ as $\varepsilon\to 0$ and D(ε, g_{p}, m_{p}) shrinks to D(0, 0, m_{p}) in this limit. The important point, for us, however, is that for every finite ε each choice of m_{p}, g_{p} in the permitted domain D(ε, m_{p}, g_{p}) defines an acceptable $m_0(\varepsilon)$, $g_0(\varepsilon)$ and since the convexity is with respect to $\bar{\varphi}$ and not the parameters, for this acceptable pair of values corresponding to the physical pair of values m_{p}, g_{p}, the constraint effective potential $U^{\varepsilon}(\bar{\varphi}, m_0, g_0)$ has the convexity properties discussed.

Two of us (A.W. and H.Y.) wish to thank J. Lewis for discussions, L. Chayes and T. Chayes for discussions and for suggesting a method of proof for the convexity of the constraint effective potential. They are also grateful to C.B. Lang for useful conversations on the Monte Carlo simulations. A.W. wishes to thank the Deutsche Forschungsgemeinschaft DFG for partial support.

Appendix

We wish to show that the expression

$$\inf_{\substack{\alpha \\ 0 \leqslant \mu \leqslant 1}} \{\mu f(x-(1-\mu)\alpha)+(1-\mu)f(x+\mu\alpha)\}$$

occurring in (5.8) is the convex hull of $f(x)$ for any function $f(x)$ which is strictly convex as $|x| \to \infty$.

First we recall that the definition of the convex hull of a function $f(x)$ is the boundary of the convex hull of the set of points above $f(x)$, i.e. of all (x, y) such that $y \geqslant f(x)$[16]. Then if we note that such a set is just the set of points

$$(x, y)=(x, \mu f(x-(1-\mu)\alpha)+(1-\mu)f(x+\mu\alpha))$$

for any real α and $0 \leqslant \mu \leqslant 1$, we see that the boundary is just the inf. of the r.h.s., as required.

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