Application of a modified mean-field method to a gauge-invariant variational calculation

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A previously described variational approach turns a gauge problem into a global-symmetric equivalent model. The use in the latter of a mean-field method with an effective dimensionality is shown to give agreement with the low- and high-temperature expansions. We apply this method to the $Z(2)$ gauge and matter field model in any dimension finding in particular that it quantitatively improves the results for the $(2+1)$-dimensional case.

I. INTRODUCTION

There has recently been interest in mean-field[1,2] and variational[3–5] approaches to gauge theories, which have provided results in fair agreement with those of Monte Carlo simulations. As far as the variational method is concerned, the gauge invariance of the trial state has been shown[6] to be crucial to obtain the correct features of the phase diagram of the $Z(2)$ gauge and matter field model. The use of the same state for every link (or site) leads, through gauge symmetrization, to an equivalent Ising model with external field in one less dimension that can be analyzed either by low- and high-temperature expansions[4] or with a method which consists in replacing the variables of sites outside a volume of exactly calculated configurations by a mean-field boundary condition.[6,7] The latter method is easier to apply but, as is shown in this paper, fails to reproduce the low-temperature (LT) and high-temperature (HT) expansions in the proper limits, beyond the terms corresponding to graphs which may be drawn in the exactly computed volume. We note that a change in the effective dimensionality for the determination of the mean field ranging from $d-\frac{1}{2}$ for $T\rightarrow\infty$ to $d-1$ for $T\rightarrow 0$ gives the exact subsequent terms in the corresponding expansions and the correct orders and signs of the rest. The implementation of this modified mean-field method is shown to improve slightly the $(3+1)$-dimensional model and significantly the $(2+1)$-dimensional case in the region where it can be compared with renormalization-group techniques.[8]

II. VARIATIONAL APPROACH TO THE Z(2) MODEL

We study the $Z(2)$ gauge and matter field theory in $d+1$ dimensions using the Hamiltonian formalism[9]

$$H=-\sum_{\text{links}}\sigma_1-\lambda\sum_{\text{plaquettes}}\sigma_3\sigma_3\sigma_3\sigma_3 -\sum_{\text{sites}}\tau_1-\omega\sum_{\text{links}}\tau_3\sigma_3\tau_3\ , \tag{1}$$

where σ_i are Pauli matrices corresponding to gauge variables which live on the links l and τ_i are Pauli matrices for matter variables lying on the sites x of a d-dimensional lattice. This Hamiltonian has the local invariance

$$G_x H G_x{}^{-1} = H, \quad G_x = \tau_1(x) \prod_{l \in x} \sigma_1(l) \ . \tag{2}$$

Following Ref. 4 we introduce a gauge-non-invariant state for the vacuum

$$|0\rangle = \prod_l \begin{bmatrix} \cos\theta/2 \\ \sin\theta/2 \end{bmatrix}_l \prod_x \begin{bmatrix} \cos\phi/2 \\ \sin\phi/2 \end{bmatrix}_x , \tag{3}$$

depending on one link parameter θ and one site parameter ϕ, and we symmetrize it through all possible gauge transformations giving the variational ground state

$$|\emptyset\rangle = \prod_x \tfrac{1}{2}(1+G)_x |0\rangle \ . \tag{4}$$

The norm turns out to be equivalent to the partition function of a d-dimensional Ising model in an external field

$$\langle \emptyset | \emptyset \rangle \propto \sum_{\{\mu\}} \exp\left[\beta \sum_{\langle xx' \rangle} \mu\mu' + h \sum_x \mu\right] , \tag{5}$$

where $\mu = \mp 1$ denotes the action of G_x or of the identity in Eq. (4), and the inverse temperature and external field are defined by

$$e^{-2\beta} = \sin\theta, \quad e^{-2h} = \sin\phi \ . \tag{6}$$

It is straightforward to show that the expectation value per unit link of the Hamiltonian equation (1) in the state of Eq. (4) is

$$\begin{aligned} E_\emptyset = &-\langle \exp(-2\beta\mu_1\mu_2)\rangle - \lambda \tfrac{1}{2}(d-1)\cos^4\theta \langle \delta_{\mu_1 m_2}\delta_{\mu_2\mu_3}\delta_{\mu_3\mu_4}\delta_{\mu_4\mu_1}\rangle - d^{-1}\langle \exp(-2h\mu_1)\rangle \\ &-\omega\cos^2\phi\cos\theta \langle \delta_{\mu_1 1}\delta_{\mu_2 1}\rangle , \end{aligned} \tag{7}$$

where sites 1 and 2 form a link and 1, 2, 3, and 4 build a plaquette. The problem consists now in calculating the statistical averages of Eq. (7) and finding the minimum of $E_\emptyset$ as a function of β and h.

III. LOW- AND HIGH-TEMPERATURE EXPANSIONS

One possibility of analysis is to perform the usual $\beta \to 0$ (HT) and $\beta \to \infty$ (LT) expansions.[10] Denoting $c = 2d$ and S, L_G, L_M, and P as the site, gauge link, matter link, and plaquette statistical averages which appear in Eq. (7) one has the following two cases.

(i) HT expansions. Defining $y = \tanh\beta$ and $\eta = \tanh h$, we obtain

$$\begin{aligned} S = &\langle \exp(-2h\mu_1)\rangle \\ \simeq &1 - 2cy\eta^2 - 2c(c-1)y^2\eta^2 + 2c(2c-1)y^2\eta^4 - 2c(c-1)^2y^3\eta^2 \\ &+ \left\{-2\left[\begin{bmatrix} c \\ 3 \end{bmatrix} + c\begin{bmatrix} c-1 \\ 2 \end{bmatrix}\right] + 2c\left[(c-1)(3c-2) + 2(c-1)^2 + 2\begin{bmatrix} c-1 \\ 2 \end{bmatrix} + 2(c-1)\right]\right\} y^3\eta^4 \\ &- 2c[(2c-1)^2 + (c-1)^2]y^3\eta^6 , \end{aligned} \tag{8a}$$

$$\begin{aligned} L_G = &\langle \exp(-2\beta\mu_1\mu_2)\rangle \\ \simeq &1 - 2y\eta^2 - 4(c-1)y^2\eta^2 + 2(2c-1)y^2\eta^4 - 6(c-1)^2y^3\eta^2 \\ &+ 4[(c-1)(3c-2) + (c-1)^2 + c - 1]y^3\eta^4 - 2[(2c-1)^2 + (c-1)^2]y^3\eta^6 , \end{aligned} \tag{8b}$$

$$\begin{aligned} L_M = &\cos\theta\cos^2\phi \langle \delta_{\mu_1 1}\delta_{\mu_2 1}\rangle \\ \simeq &2y^{1/2}\eta\{1 + 2(c-1)y\eta - (2c-1)y\eta^2 + 2(c-1)^2y^2\eta - [(c-1)^2 + 2(c-1)]y^2\eta^2 \\ &- 2(c-1)(3c-2)y^2\eta^3 + [(2c-1)^2 + (c-1)^2]y^2\eta^4\} , \end{aligned} \tag{8c}$$

$$\begin{aligned} P = &\cos^4\theta \langle \delta_{\mu_1\mu_2}\delta_{\mu_2\mu_3}\delta_{\mu_3\mu_4}\delta_{\mu_4\mu_1}\rangle \\ \simeq &2y^2\{1 + 6\eta^2 + \eta^4 + 4[4(c-2) - (c-1)]y\eta^2 - 4[6(c-1) - 4(c-2)]y\eta^4 - 4(c-1)y\eta^6\} \ . \end{aligned} \tag{8d}$$

In the above expressions, to keep the same approximation in y we have included diagrams up to the three-link order for S, L_G, and L_M and up to one-link order for P, apart from links on the plaquette (see Fig. 1 for typical examples).

(ii) LT expansions. Defining $x=\sin\theta$, $\xi=\sin\phi$, we have

$$S\simeq \xi+x^{c}(1-\xi^2)+cx^{2c-2}\xi(1-\xi^2)-(c+1)x^{2c}\xi(1-\xi^2)+\left[c(c-1)+\begin{bmatrix} c\\ 2\end{bmatrix}\right]x^{3c-4}\xi^2(1-\xi^2)$$
$$-k_1x^{3c-2}\xi^2(1-\xi^2)+k_2x^{3c}\xi^2(1-\xi^2)\,, \tag{9a}$$

$$L_G=x\left\{1+2x^{c-2}(1-x^2)\xi+2(c-1)x^{2c-4}(1-x^2)\xi^2-2(c+1)x^{2c-2}(1-x^2)\xi^2\right.$$
$$\left.+2\left[(c-1)^2+\begin{bmatrix} c-1\\ 2\end{bmatrix}\right]x^{3c-6}(1-x^2)\xi^3-k_3x^{3c-4}(1-x^2)\xi^3+k_4x^{3c-2}(1-x^2)\xi^3\right\}, \tag{9b}$$

$$L_M=(1-x^2)^{1/2}(1-\xi^2)\left\{1-2x^{c}\xi-(2c-1)x^{2c-2}\xi^2+2(c+1)x^{2c}\xi^2\right.$$
$$\left.-2\left[(c-1)^2+\begin{bmatrix} c-1\\ 2\end{bmatrix}+c-1\right]x^{3c-4}\xi^3+k_5x^{3c-2}\xi^3-k_6x^{3c}\xi^3\right\}, \tag{9c}$$

$$P=(1-x^2)^2\left\{1-4x^{c}\xi-4(c-1)x^{2c-2}\xi^2+2(2c+3)x^{2c}\xi^2\right.$$
$$\left.-4\left[(c-2)(c-1)+\begin{bmatrix} c-2\\ 2\end{bmatrix}+2(c-2)+1\right]x^{3c-4}\xi^3+k_7x^{3c-2}\xi^3-k_8x^{3c}\xi^3\right\}. \tag{9d}$$

In Eq. (9) we have kept terms up to three spin flips (see Fig. 2) and all the coefficients k_i turn out to be positive.

These LT and HT expansions are useful to determine some features of the phase diagrams of Figs. 3 and 4. For $\lambda\rightarrow\infty$ the Ising second-order transition appears at $\omega=0.5/d$ (which is expected to be better for $d=3$ than for $d=2$) using the LT expansion. For $\lambda\approx 0$ and ω small the HT expansion is quickly convergent and the variational energy is a function of $y^{1/2}\eta$ producing a degeneracy in the separate parameters y and η. Increasing ω, the minimum of $E_\emptyset$ corresponds to slowly rising values of y (whereas η increases faster). For $\omega\simeq 1$ the HT expansion is no longer convergent but before this occurs the minimum of $E_\emptyset$ and the parameters y and η join smoothly with those resulting from the LT expansion, appropriate thereafter, giving therefore no sign of phase transition along the axis $\lambda=0$. For $\omega=0$ the use of Padé approximants has shown[4] the presence of a first-order phase transition at $\lambda=0.94$ for $d=3$ and a second-order one at $\lambda=2.22$ for $d=2$. However, the central part of the λ-ω plane is difficult to analyze by means of the HT and LT series whereas the modified mean-field method described below becomes much more practical[6] and allows one to draw the diagrams shown in Figs. 3 and 4.

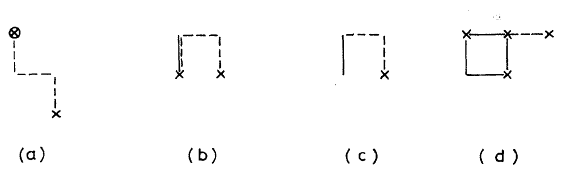

FIG. 1. Examples of HT diagrams for S, L_G, L_M, and P. Dashed segments denote finite-temperature perturbations and crosses external-field corrections. Open dot and solid segments indicate site, link, and plaquette of the averaged operators.

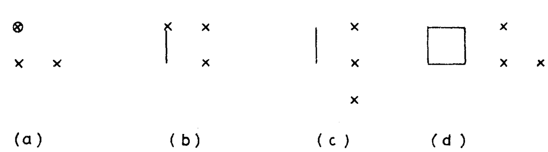

FIG. 2. Examples of LT diagrams. Crosses denote flipped spins.

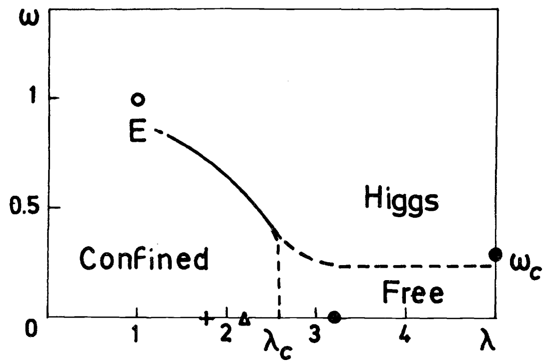

FIG. 3. Phase diagram for $d+1=3$ obtained with Eqs. (10) and (11) and $c_e(\beta)$. The solid (dashed) line indicated first- (second-) order transition and the ending point E is a second-order one. The open dot denotes a self-dual point, solid dots the renormalization-group critical coupling (Refs. 8 and 14), the cross is the critical pure gauge coupling (Ref. 6) from normal mean field with $c_e=2d$, and the triangle the result with Padé treatment of HT and LT expansions (Ref. 4).

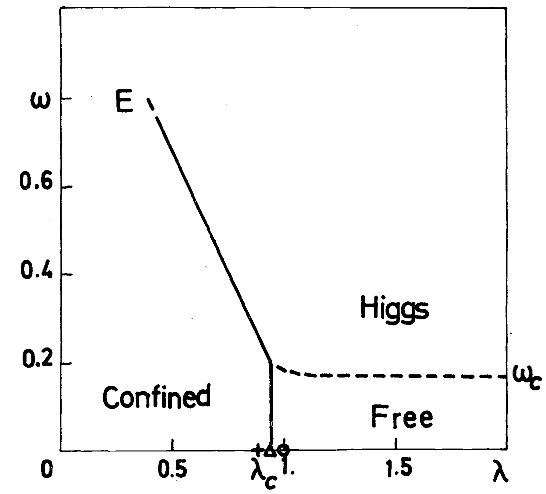

FIG. 4. Phase diagram for $d+1=4$ obtained with Eqs. (10) and (11). The open dot denotes the self-dual pure gauge point, the cross the critical coupling obtained (Ref. 6) with $c_e=2d$, and the triangle the Padé result (Ref. 4).

IV. MODIFIED MEAN-FIELD TREATMENT

An alternative method for the evaluation of the averages in Eq. (7) is obtained by exactly taking into account, in the spirit of the Bethe-Peierls approximation,[11] the configurations of variables in a volume containing at least the sites on which the operators are defined. The effect of the outer part is represented by a mean field m determined by a self-consistency condition.

Considering as a first approximation the exact configurations of the minimal volume, i.e., one site for S, one link for L_G and L_M, and one plaquette for P (see Fig. 5) we obtain

$$S=[\cosh(c\beta m-h)]/[\cosh(c\beta m+h)]\ , \tag{10a}$$

$$L_G=\frac{1+\exp(-2\beta)\cosh\{2[(c-1)\beta m+h]\}}{\cosh\{2[(c-1)\beta m+h]\}+\exp(-2\beta)}\ , \tag{10b}$$

$$L_M=\tfrac{1}{2}\cos\theta\cos^2\phi\frac{\exp\{2[(c-1)\beta m+h]\}}{\cosh\{2[(c-1)\beta m+h]\}+\exp(-2\beta)}\ , \tag{10c}$$

$$P=\cos^4\theta\frac{\exp(4\beta)\cosh\{4[(c-2)\beta m+h]\}}{\exp(4\beta)\cosh\{4[(c-2)\beta m+h]\}+4\cosh\{2[(c-2)\beta m+h]\}+\exp(-4\beta)+2}\ , \tag{10d}$$

together with the consistency condition for the mean-field value

$$m=\tanh(c_e\beta m+h)\ , \tag{11}$$

where c_e is an effective coordination number whose determination will be shown below.

When confronted with the HT approach, the expansions of Eqs. (10) and (11) in powers of y coincide up to the first order for S, up to the second for L_G, and up to the linear terms in the curly brackets of L_M and P of Eq. (8). There it is only

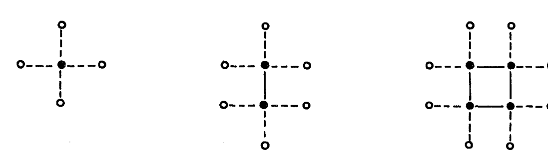

FIG. 5. Mean-field method of Eqs. (10) and (11). Dashed links indicate interactions between exactly considered variables (solid dots) and mean-field ones (open dots). HT diagrams (a), (b), and (c) of Fig. 1 and LT graphs of Fig. 2 are not reproduced with $c_e=2d$ but appear using the effective $c_e(\beta)$.

necessary to use the zero order for $m \simeq \tanh h = \eta$. This is consistent with the fact that the considered volume allows for the corresponding HT diagrams where the mean-field sites are also included. If we wish to compare the expansions of S, L_G, and L_M up to the next order, the β linear corrections for m must be taken into account and the agreement is obtained with

$$c_e \underset{\beta \to 0}{=} c-1 \ .$$

This effective coordination number can be intuitively understood by the fact that our computation combines the HT diagrams for an operator with the one for m so that the joining link is counted twice unless it is suppressed from the calculation of m. In a similar way, to obtain the right third order of the HT expansion of S an order-β correction must be included in c_e, i.e., $c_e \simeq c-1-\beta/3$, showing that c_e must decrease for increasing β in agreement with what will be discussed for the LT limit. The same results are obtained by calculating m with exact nearest-neighbor variables instead of the simplest formula Eq. (11). To see the consistency of our approach, we have verified that the correct third-order HT term of S is also obtained by expanding the volume around the site to include either the nearest neighbors (and using the linear approximation for m with $c_e = c-1$) or the next to nearest neighbors (and taking simply $m = \eta$) as indicated in Fig. 6.

Now performing the comparison with the LT expansions [Eqs. (9)], the one-flip corrections are correctly given by the mean-field formulas [Eqs. (10)] whose evaluation at this order involves only the extreme value $m = 1$. It is interesting to observe that all the powers of x and the signs of the coefficients which appear in Eqs. (9) are reproduced if the effective coordination number is

$$c_e \underset{\beta \to \infty}{=} c-2 \ .$$

This can be understood since joining the expansions of the operators with that of m, two neighboring flips imply a factor x^{-2}. In more detail, the LT behavior

$$c_e = c-2+[\ln(4\beta)]/(2\beta)$$

gives for every case of Eq. (10) agreement with the leading terms of Eq. (9) corresponding to two flips. In analogy with the previous HT analysis, the exact variable computation either of nearest neighbors or also of next to nearest neighbors (see Fig. 6) gives agreement with the two-flip and three-flip terms, respectively, with $m = 1$.

Summarizing, the use of a definite volume inside which all the configurations are exactly computed is consistent with the HT expansion up to diagrams connecting the most external considered site with the outer mean field (and broken diagrams of the same order) and with the LT expansion up to neighboring flips on the exact sites (and nonadjacent flips of the same order), using $m = \eta$ and $m = 1$, respectively. To extend the agreement to the next order using the same exact volume, one must include the β dependence of m with $c_e = c-1$ and $c_e = c-2$ for HT and LT, respectively.

It must be noted that a similar Bethe-Peierls approximation has been applied to the Lagrangian formalism of gauge theories to improve the mean-field results.[12]

V. RESULTS AND COMMENTS

To obtain the phase diagrams of Figs. 3 and 4 we have used Eqs. (10) together with the mean field m which has been determined from $m = \tanh[(c-2)\beta m]$ for $\omega = 0$, and for $\omega > 0$ by an interpolation between the LT and HT expansions of Eq. (11) (which in the limits correspond to $c_e = c-1$ and $c_e = c-2$, respectively). Although there is a certain degree of arbitrariness in this interpolation, the main features of the phase diagrams are not affected.

Following the minimum of the variational energy we have obtained that along the axis $\lambda = 0$ there is no phase transition and, in agreement with the LT and HT results, the values of the parameters

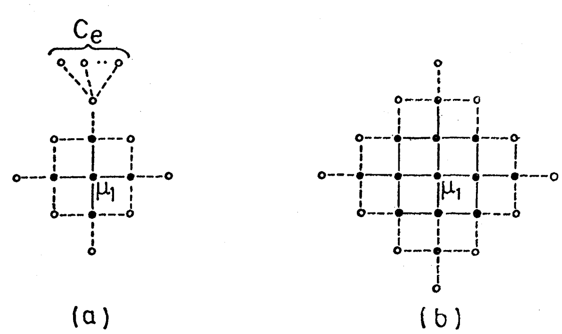

FIG. 6. Alternative choices to obtain all three-leg HT diagrams and three-flip LT ones for the site term. (a) Nearest neighbors are exactly treated and coupled to mean fields (open dots) which are determined by c_e interactions ($c_e = c-1$, $c-2$ for HT and LT, respectively). (b) Also next to nearest neighbors are included exactly and coupled to mean fields $m = \eta, 1$ for HT and LT, respectively.

which start from $x=\xi=1$ for $\omega=0$ decrease slowly for the former and faster for the latter when ω increases. At fixed $\omega<\omega_c$, the minimum very quickly approaches $\xi=1$ and $x_c=\exp[-2/(c-2)]$. For $\lambda>\lambda_c$, ξ reaches exactly 1 and x starts moving faster toward lower values for $d=2$ (defining a second-order line) or jumps discontinuously to another minimum for $d=3$ (showing a first-order transition). If we now keep λ fixed in the free phase and increase ω, ξ remains equal to 1 up to ω_c beyond which ξ decreases with continuity defining the Ising second-order line in agreement with the LT expansion. Repeating the description for $\omega>\omega_c$, but smaller than that of point E, x again decreases toward x_c and ξ increases toward 1 when one increases λ. But since in the Higgs sector there is another minimum with lower ξ, the minimum on the confining side does not remain as the absolute one up to λ_c so that before this value is reached there is a discontinuous jump defining a first-order transition. When going toward the point E along this first-order line, the modification of the parameters of the left minimum grows faster whereas that of the right one tends to decelerate. As a result, at the point E both minima coincide and the first-order line ends in a second-order point. For values of ω larger than the one of E there is a single minimum which moves with continuity defining a single phase.

Regarding the numerical values, we see from Fig. 3 that for $d=2$ the critical coupling $\lambda_c\simeq2.6$ is considerably better than the one $\lambda_c=1.8$ obtained by the normal mean-field method applied to our variational procedure.[6] It is, however, still lower than the value 3.2 found by renormalization-group techniques[8] consistent with the perturbative[13] and renormalization-group calculations[14] for the dual Ising model. The same happens for our value $\omega_c=0.25$, something lower than the dual critical coupling corresponding to the above results. This excessive tendency to order in our approach is certainly the consequence of the too uniform *Ansatz* [Eq. (3)].

It is clear that if one uses the same *Ansatz* for the dual model the excessive tendency to the dual order will imply a too marked disorder in the direct model. The dual model corresponds to $\lambda\to\omega^{-1}$ and $\omega\to\lambda^{-1}$ so that one obtains with the dual variational approach $\lambda_c=1/0.25=4$ and $\omega_c=1/2.6=0.385$. The correct critical lines are certainly contained in the region bounded by the corresponding curves obtained from the direct and dual approaches.

For $d=3$ the agreement with the self-dual value $\lambda_c=1$ is much better, as it could be expected, our pure gauge transition occurring for the direct model at $\lambda_c=0.95$.

The parameters x and ξ whose discontinuities reflect the presence of a phase transition are not always easily related to well-defined order parameters. For the case $\omega=0$, the only relevant parameter x of the direct variational approach determines the Wilson loop but unfortunately, as shown in Ref. 4, its change produces a nonanalyticity which does not correspond to a modification of the perimeter law. On the other hand, the use of the variational approach in the dual model for $d=3$ changes the dual low-temperature area behavior for the direct Wilson loop

$$W \underset{\tilde\beta\to\infty}{\simeq} \exp\{A[\ln\tilde x+2\tilde x^4(1+\tilde x^2)]\}$$

to a perimeter dual high-temperature one

$$W \underset{\tilde\beta\to 0}{\simeq} \exp[-2P\tilde y^4(1+16\tilde y^2)]\ .$$

Since in the dual low-temperature limit the magnetization is given by $\tilde m\simeq1-2\tilde x^6$ one may obtain in this region an expression of the string tension in terms of $\tilde m$. For $d=2$ a simpler analysis shows that in the confining phase the Wilson loop is $W=(1-\tilde m^2)^{A/2}$. Therefore, we may assert that an area behavior for the Wilson loop is related in our approximation to the presence of dual magnetization in the equivalent model.

In the $\lambda\to\infty$ limit it is also clear that the Higgs magnetization is related to the parameter ξ by $m_H=(1-\xi^2)^{1/2}$.

In the interior of the phase diagram, even though both the Higgs magnetization and the string tension vanish as they should our parameters x and ξ change smoothly from the values taken on the axis $\lambda\to\infty$ and $\omega=0$ and are still useful to determine the transitions where they exhibit some nonanalyticity.

On the whole, the qualitatively correct features and the quantitatively fair agreement with some previously well-determined points of the phase diagram obtained by our approach without computational effort show an improvement with respect to other methods[15] applied to the complete Hamiltonian $Z(2)$ gauge and matter problem.

One could think of establishing with greater definiteness the temperature dependence of the effective coordination number which determines the mean field. But this does not seem crucial since our present critical temperature for the equivalent

Ising model $\beta_c{}^{-1}=2d-2$ is almost correct and the numerical results are not sensitive to the details of the interpolation for the equivalent magnetization.

It would certainly be of greater importance to implement variational *Ansätze* with more fluctuations while still keeping the simplicity of the equivalent model.

If one tries to apply the direct variational *Ansatz* to a continuous symmetry gauge theory, e.g., the U(1) Abelian case in $2+1$ dimensions, one must deal with an equivalent XY spin model in two dimensions. One would then face the problem that, while the U(1) gauge theory is known to have only the confining phase in $2+1$ dimensions, the Kosterlitz-Thouless transition would induce some nonanalyticity in the original model through our procedure. On the contrary, the application of the variational approach to the dual of the U(1) gauge theory in $2+1$ dimensions, i.e., the discrete Gaussian spin model, indicates only one ordered phase[16] [and therefore only one disordered phase for the U(1) gauge theory].

The analysis of the U(1) gauge model in $3+1$ dimensions would certainly give a phase transition with the direct approach (through the transition of the equivalent XY spin model in three dimensions). Within the dual model (the discrete Gaussian gauge system) the occurrence of a transition is more subtle, since the equivalent model (the discrete Gaussian in three dimensions) has no transition. However, a numerical analysis[17] of the gauge $Z(N)$ model for $N\rightarrow\infty$ in the low-temperature limit (which is mapped to the discrete Gaussian gauge model) indicates a persistence of a second-order phase transition meaning that the transitions of the original model are not always due to the presence of a transition in the equivalent theory.

In Ref. 3 a variational *Ansatz* uniform on the plaquettes, rather than on the links, was used. When applied to the $(2+1)$-dimensional $Z(2)$ gauge model it produces the variational energy of the dual Ising spin system with its transition at $\lambda=4$. When applied to the $3+1$ case it generates an equivalent gauge theory in three dimensions dual to the three-dimensional Ising spin model. In fact the approach of Ref. 3 corresponds to the method described in this paper applied to the dual model. One expects that in general the correct physical results will fall in between.

It is possible that for the cases where the dual model is not known, e.g., the non-Abelian gauge theories, the variational *Ansatz* based on plaquettes or other nonuniform states could supply useful physical insight.

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