Higher order coupled cluster approximation to the vacuum of Φ^4 field theory in 1 + 1 dimensions

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(Received 15 July 1993)

The S_6 approximation of the coupled cluster method is applied to the vacuum state, energy, and field expectation value of Φ^4 field theory in 1+1 dimensions. Depending on the quantities considered the results show good to excellent convergence.

PACS number(s): 11.10.Lm, 03.70.+k

I. INTRODUCTION

In a series of papers the coupled cluster method (CCM) has been applied to Φ^4 field theory in 1+1 dimensions (Φ^4) [1–3]. Another paper [4] deals with the various theories with both Φ^4 and Φ^6 coupling. They all are based on the "S_4 approximation." In this scheme all terms with more than four virtual particles in the exponent operator $S = \Sigma S_n$ for the vacuum state have been omitted, and the remaining equations for S_1, S_2, S_3, and S_4 have been solved exactly. It turned out that, except for a certain "critical region" around second-order phase transitions, this method works quite well, both for the ground state (= vacuum) as well as for the one and two meson states [3,4]. This is quite in line with the great success of the method in quantum chemistry or, more generally, in QED of many electron systems [5]. In these cases there is no doubt that higher orders will contribute very little. This is also true for the anharmonic oscillator [6]. Here a direct comparison with exact results and those from some other methods can be made. It exhibits a much higher accuracy of the CCM as compared, for instance, to the Lanczos method [7]. In quantum field theory so far the quality of the approximation was not well under control because no higher orders have ever been computed. Ideally, a check of the ground state should be performed by solving the equation for the next higher S_n's. Thus, in the present paper the "S_6 approximation" will be described in which also both S_5 and S_6 have been fully taken into account. This then allows one to draw conclusions about the quality of the various approximations.

Recently there have been many discussions on the meaning and structure of field theoretical vacua. From them there emerged the insight that it is indeed a nontrivial object (i.e., not a bare vacuum), regardless of whether one is using the equal time or light front dynamics [8,9]. Indeed, the origins of this insight are quite old [10]. Thus, it certainly makes sense to construct explicitly such a vacuum. The vacuum energy by itself has no physical meaning. But it is needed to redefine the Hamiltonian such that the vacuum state becomes an eigenstate with eigenvalue zero, as required by symmetry arguments.

For applications of the CCM to lattice versions of field theories see Refs. [11,12] and the literature quoted therein.

This paper is organized as follows. In Sec. II the model with the application of the (standard) CCM to the vacuum, whereas in Sec. III techniques for computing expectation values, will be described, followed in Sec. IV by some remarks on numerical techniques and problems. Finally the results and conclusions will be presented in Sec. V.

II. HAMILTONIAN AND ITS VACUUM

The model is given by the Hamiltonian

$$\mathcal{H} = \int dx H \tag{2.1}$$

with

$$H = N_m \left[\frac{1}{2}(\nabla\Phi)^2 + \frac{1}{2}\Pi^2 + \frac{m}{2}\Phi^2 + \frac{\lambda}{4}\Phi^4 \right] . \tag{2.2}$$

Here N_m means normal ordering with respect to the mass parameter m. It has been introduced to remove ultraviolet divergences generating an irrelevant infinite constant. The recipes for performing the transition from non-normal ordering to normal ordering are standard [13], and thus we shall not write down the non-normal ordered Hamiltonian. Spatial integrations extend over a normalization volume $L \to \infty$.

There are some properties specific to the Φ^4_{1+1} field theory which have to be taken into account for a proper approximation (truncation) scheme. The model has two phases (or Hilbert space sectors): the "symmetric sector" (with field expectation value $\langle\Phi\rangle = 0$), and the "condensed" phase (field expectation value different from zero, the "symmetry breaking" or "$\langle\Phi\rangle \neq 0$ sector"). The phase transition is of second order [14].

Expanding as usual

$$\Phi = \int dk \frac{1}{\sqrt{4\pi\omega_k}} (a_k e^{ikx} + a_k^\dagger e^{-ikx}),$$
$$\omega_k = \sqrt{m^2 + k^2} \tag{2.3}$$

the Bogolubov transformation

$$a_k = \frac{\omega_k + \epsilon_k}{2\sqrt{\omega_k \epsilon_k}} b_k + \frac{\omega_k - \epsilon_k}{2\sqrt{\omega_k \epsilon_k}} b^\dagger_{-k} + \sqrt{\pi\omega_0}\, t\delta(k) \qquad (2.4)$$

generates new annihilation and creation operators b_k and $b^\dagger_k$ with a new bare vacuum Φ_b defined by $b_k \Phi_b = 0$. t is the wave operator shift introduced to facilitate a nonvanishing field expectation value (i.e., symmetry breaking),

$$\Phi = \Phi_{\text{new}} + t \ , \qquad (2.5)$$

and ϵ_k is a new (theoretical) single particle energy. Varying the energy expectation value $\langle \Phi_b | \mathcal{H} | \Phi_b \rangle$ with respect to t and ϵ_k corresponds to the "Gauss approximation" (Hartree approximation in the language of many body theory) [1,15]. It fixes t and ϵ_k. On the other hand, the "maximum overlap condition" [2] minimizes the overlap $|\langle \Phi_b | \Psi_{\text{vac}} \rangle|$ between the bare vacuum and the exact wave function Ψ_{vac}. It leads to zero amplitudes for one- and two-particle excitations and does not fix t and ϵ_k.

The application of the CCM to the vacuum has been described in much detail in Refs. [1–4]. Thus here only the essentials will be put down without any details. The vacuum state is written in the usual exponential form

$$|\Psi_{\text{vac}}\rangle = \exp(S) |\Phi_b\rangle \qquad (2.6)$$

with

$$S = \sum_n^\infty S_n \ , \qquad (2.7)$$

where S_n creates n virtual particles:

$$S_n = \frac{1}{n!} \int dk_1 \cdots dk_n S_n(k_1 \cdots k_n) b^\dagger_{k_2} \cdots b^\dagger_{k_n} \ . \qquad (2.8)$$

Then the (standard) CCM equations are

$$\begin{aligned} \langle \Phi_b | \exp(-S) \mathcal{H} \exp(S) | \Phi_b \rangle &= E_{\text{vac}} \ , \\ \langle \Phi_{k_1} | \exp(-S) \mathcal{H} \exp(S) | \Phi_b \rangle &= 0 \ , \\ &\vdots \\ \langle \Phi_{k_1 \ldots k_n} | \exp(-S) \mathcal{H} \exp(S) | \Phi_b \rangle &= 0 \ , \\ &\vdots \end{aligned} \qquad (2.9)$$

Here

$$|\Phi_{k_1 \ldots k_n}\rangle = b^\dagger_{k_1} b^\dagger_{k_2} \cdots b^\dagger_{k_n} |\Phi_b\rangle \qquad (2.10)$$

are Fock states of n particles. The S_6 approximation takes all S_n with $n \leq 6$ into account, thus leading to just the first seven equations (2.9), with only up to five dimensions because of momentum conservation. As in Refs. [2] and [4] the maximum overlap condition has been invoked. As noted above, this leads to vanishing S_1 and S_2. The coupled equations (2.9) then determine energy, t, ϵ_k and S_3 to S_6, in this order. More precisely, one has to solve all equations except the first one, and then use the results in the first equation to obtain the energy.

In the symmetric phase only S_n with even n occur, whereas in the condensed one both even and odd n show up [2]. Moreover, in the latter sector there are important cancellations between terms involving even and odd n from their competition in favor of preserving or breaking the symmetry. Thus, an S_5 approximation would not make sense.

Transition from the S_4 to the S_6 approximation means a big step: The number of terms in all equations becomes much larger. And there are 170/660 terms in the S_5/S_6 equations which in the present case have been derived by hand. One just has to exploit commutators and matrix elements via Wick's theorems, which is quite easy for each individual term and cumbersome only because there are so many of them. At present there is work in progress using some of the algebraic computer programs. Once this becomes routine, the CCM hopefully will turn out to be also a very manpower-efficient method to find low-energy states of complex Hamiltonians. In any case, it is not feasible to write down here the explicit equations. Even their graphical representation, a standard in quantum chemistry, being quite extensive and foreign in the realm of quantum field theory, will not be shown here.

III. FIELD EXPECTATION VALUE

The computation of expectation values of operators O is a notoriously difficult task within the standard CCM, because it is hard to utilize fully the exponential. Based on the Feynman-Hellman theorem there is a formally rigorous technique [16]: Replace the Hamiltonian by $\mathcal{H} + \gamma O$. Then the expectation value is

$$\langle O \rangle = \left. \frac{dE_{\text{vac}(\gamma)}}{d\gamma} \right|_{\gamma=0} \ . \qquad (3.1)$$

These derivatives with respect to the new coupling constant γ are difficult to obtain with sufficient accuracy, because they are based on the difference between two large quantities divided by a small one. Thus, in the present work in addition to this more sophisticated method also ordinary low order expansions of the exponentials in

$$\langle O \rangle = \frac{\langle \exp(\Sigma_3^6 S_n) \Phi_b | O | \exp(\Sigma_3^6 S_n) \Phi_b \rangle}{\langle \exp(\Sigma_3^6 S_n) \Phi_b | \exp(\Sigma_3^6 S_n) \Phi_b \rangle} \qquad (3.2)$$

have been used. The truncation is defined by the prescription that at most three independent integrations are taken into account. This then includes all terms with $S_3 S_4$, $S_3^3 S_4$, and $S_4 S_5$. In [1–4] only the first term had been used. To arrive at a fair comparison, in the present paper also the second term has been added in the S_4 approximation, although it has only a small effect.

IV. NUMERICS

Far away from the critical region this coupled set of up to five-dimensional equations could be solved by iteration. The starting parameters t and ϵ_k were obtained from the Gauss approximation. Then in separate cy-

cles first the equations for S_3 and S_4 were solved iteratively with S_5 and S_6 set equal to zero. Afterwards the equations for S_5 and S_6 were solved by iteration, using t, ϵ_k, S_3, and S_4 from the first cycles. This was repeated until convergence within at least 1% was achieved. The number of iterations needed typically was quite small.

This procedure was not possible nearer to the critical region. Here the equation for S_6 naturally made some problems. The S_n's now being quite large, the cancellations between large terms, mentioned above, in combination with the high dimensionality lead to slow convergence. Thus, it was necessary to approach the critical region by changing the coupling strength in very small steps, using the results from the last step as input. First, the (1,2,3,4) particle equations were solved as in Ref. 2. Then a single iteration of the five- and six-particle equations was done, the results inserted into the one- to four-particle equations, which were solved as before. This was repeated until convergence was achieved to an accuracy of better than 1%. Thus in each step only one (very time consuming) iteration of the five- and six-body equations was needed. At the very end the latter equations were solved separately with a few iterations to make sure that indeed a solution was obtained. In all cases it turned out that these last iterations generated very little change. The maximum number of iterations needed was 65.

The number of mesh points for the (Gauss-Legendre) integrations mostly was 21 per dimension. Near the critical region also 23 points were used for comparison. There was less than 1% difference between both. At some values for λ the calculations were checked even with 25 points, leading to the same results. Thus very likely the mesh is dense enough. The maximum momentum included was around 250 (with $m = 1$), varying somewhat with the number of mesh points.

Exploiting the Feynman-Hellmann method, Eq. (3.1), for the field expectation value $\langle\Phi\rangle$ turned out to be quite a difficult task. The energy was calculated for several small values of the coupling γ around $\gamma = 0$ and the derivative at $\gamma = 0$ was obtained by interpolation. In approaching the critical region this method did break down quite early, because the numerical "dirt" becomes comparable to a tolerably small γ. There are two related reasons for this behavior: The energy changes more rapidly with γ. Also, it becomes impossible to obtain a numerical accuracy of better than 10^{-3} as required for small γ.

V. RESULTS AND CONCLUSIONS

The results are given in Figs. 1–4. Note that all plots end at $\lambda = 18$, since, for larger coupling strength S_4 and S_6, approximations rapidly become indistinguishable. The energy in Fig. 1 shows excellent convergence. This is not surprising. The (standard) CCM is known to be at its best for this quantity, because the energy is computed via a formally exact expression and not as an expectation value. Wave functions do less well. Thus, as to be expected, the field expectation values shown in Fig. 2 do not come out quite as good. Both the Feynman-

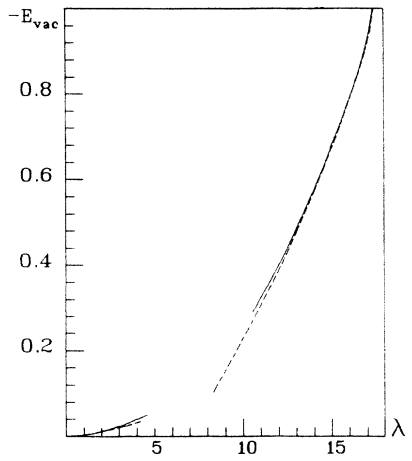

FIG. 1. Vacuum energy as function of coupling strength λ. Solid line: S_6 approximation; dashed line: S_4 approximation.

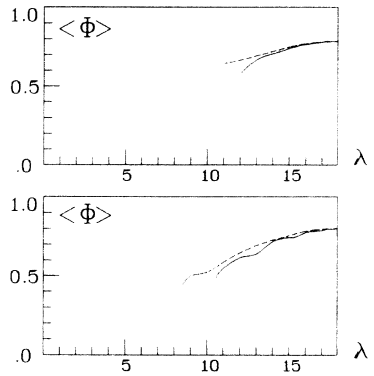

FIG. 2. Field expectation value as function of coupling strength λ. Solid and dashed lines, respectively: S_4, S_6 approximations. Top: Using the Feynman-Hellmann theorem. Bottom: Using series expansion of (3.2). For notations see Fig. 1.

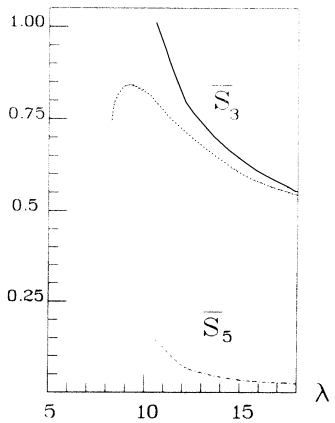

FIG. 3. Average over S_3 in S_6 approximation (solid line) and in S_4 approximation (dashed line). Average over S_5 (dash-dotted line).

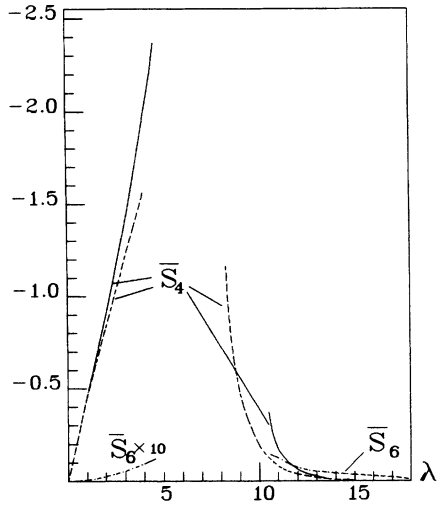

FIG. 4. Average over S_4 in S_6 approximation (solid line) and in S_4 approximation (dashed line). Average over S_6 (dash-dotted line), enlarged by a factor 10 in small λ region.

Hellmann theorem [Eq. (3.1)] as well as the expansion in powers of S_n based on (3.2) have been applied within the S_4 and the S_6 approximation. Because of the problems discussed before, the region where (3.1) could be applied successfully was somewhat smaller than the overall accessible region. In both cases the S_6 approximation leads to a more rapid decrease than does the S_4 approximation. The curves from the series expansion show more structure than the old plot of Ref. 2. This is due to the appearance of more terms carrying different signs. Comparison with the Feynman-Hellman results suggests that the neglected higher order terms will make the curves smoother. Except for this, the agreement between both methods as well as both approximations is quite reasonable, the differences being at most of the order of 20%. In Figs. 3 and 4 the averages over S_3 to S_6 are shown. Wherever the amplitudes S_n are large, and therefore important, the differences between S_4 and S_6 approximations for S_3 and S_4 are reasonably small. In the region around $\lambda = 11$, where the averaged S_4 is small, there is a larger but tolerable deviation between both approximations. The averaged S_5 and S_6 behave as expected, being small far away from the critical region and large near to it.

It seems that the critical region has been moved towards larger coupling strength and that it has been increased slightly. The latter fact is somewhat disappointing since one might have expected that this region becomes smaller instead. Possibly this feature is not genuine, but merely due to the limitations of the iterative computational methods applied to solve the equations for S_5 and S_6. This interpretation is supported by the observation that the symmetrical phase behaves better. Naturally, in this case numerical stability is somewhat better than in the symmetry-breaking phase.

Thus, again the CCM in its simplest ("normal") form successfully has passed a test. This may not seem surprising since an enormous number of terms has been taken into account. The surprise originates from the fact that many of the individual terms are quite large. Thus, there must be very effective cancellations between them. The success of the approximation schemes suggested by the CCM equations derives from this feature. It is not well understood why this is so. There are some plausibility arguments for it and no proofs.

ACKNOWLEDGMENTS

The author thanks Raymond Bishop and Martin Funke for discussions during the early stages of this work.

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