Anharmonic oscillator as a test of the coupled-cluster method

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Recent applications of the coupled-cluster method to the $(\phi^4)_2$ quantum field theory showed the necessity of a detailed analysis of its convergence behavior. The anharmonic oscillator has always served as a good test case for different approximation schemes. We treat the model both in the maximum-overlap condition and in the Hartree approximation. The ground-state energy is reproduced very well for all values of the coupling strength and already for a low-order truncation scheme. The expansion in correlation amplitudes can be carried out in extremely high order and shows a divergent tendency of the amplitudes. Introducing temperature dependence allows us to select the stable ground state out of a variety of solutions of the hierarchy of equations.

I. INTRODUCTION

The one-dimensional anharmonic oscillator has been studied intensively in the past by various authors utilizing several powerful methods. Bender and Wu[1] derived many high-order terms in the perturbation expansion of the ground-state energy obtaining the unsurprising result that the series diverges for all values of the coupling strength. Recently, a numerically and conceptually simple approach was proposed by Chern, Hsue, and Kümmel.[2,3] Using the familiar coupled-cluster method[4,5] they proposed to make use of the Hartree approximation refined by a four-particle correlation approximation [SUB(4)]. For all values of the coupling strength the ground-state energy is reproduced within an accuracy of less than 1%. For a long time it seemed to be obvious that it would be easy to extend these manipulations to quantum field theories. Intensive numerical evaluations were carried out in the $(\phi^4)_2$ model by different authors.[6,7] It became apparent that convergence in this model is worse that in the case of simple anharmonic oscillators. This motivated the investigation of the convergence of a SUB(n) approximation, which, although simple, had not been carried out up to now.

We finish the analytical calculations with a large system of nonlinear equations which in general do not show a unique solution. To select out the correct ground-state solution we require stability against thermal fluctuations. These ideas are easily extendable to quantum field theories.

II. APPROXIMATION SCHEMES, THE MODEL, AND THE COUPLED-CLUSTER EQUATIONS

The model Hamiltonian is described by

$$H=\tfrac{1}{2}\hat{p}^2+\tfrac{1}{2}\hat{x}^2+\frac{\lambda}{4}\hat{x}^4 . \tag{2.1}$$

Introducing creation and annihilation operators in the customary way yields the familiar representation of H,

$$H=a^\dagger a+\tfrac{1}{2}+\frac{\lambda}{16}(a+a^\dagger)^4 . \tag{2.2}$$

It is convenient to perform a Bogoliubov transformation first and take it in its normal-ordered form with respect to new quasiparticle operators $b^\dagger, b$.

The Bogoliubov transformation is defined by

$$a=\frac{b-tb^\dagger}{(1-t^2)^{1/2}} . \tag{2.3}$$

The resulting Hamiltonian, suitable for further calculations, looks like

$$H=E_0(\sigma)+\epsilon(\sigma)b^\dagger b+\alpha(\sigma)(b^2+b^{\dagger 2}) +\gamma(\sigma):(b+b^\dagger)^4: , \tag{2.4}$$

where

$$\sigma=\frac{1-t}{1+t} , \tag{2.5a}$$

$$E_0(\sigma)=\frac{1+\sigma^2}{4\sigma}+\frac{3\lambda}{16}\sigma^2 , \tag{2.5b}$$

$$\epsilon(\sigma)=\frac{1+\sigma^2}{2\sigma}+\frac{3\lambda}{4}\sigma^2 , \tag{2.5c}$$

$$\alpha(\sigma)=\frac{\sigma^2-1}{4\sigma}+\frac{3\lambda}{8}\sigma^2 , \tag{2.5d}$$

$$\gamma(\sigma)=\frac{\lambda}{16}\sigma^2 . \tag{2.5e}$$

Neglecting the interaction term proportional to $\gamma(\sigma)$ and fixing σ by $\alpha(\sigma)=0$ yields the ground-state energy $E_0(\sigma)$. This approach is referred to as the Hartree approximation. In the case of strong coupling the energy is

$$E_0(\sigma)\underset{\lambda\to\infty}{\sim}\tfrac{3}{8}(\tfrac{3}{2}\lambda)^{1/3} \tag{2.6}$$

which reproduces the exact energy within 2%. Chern, Hsue, and Kümmel[2] used the Hamiltonian (2.4) in the Hartree approximation and improved their results both with the coupled-cluster method (CCM) as well as via matrix diagonalization.

The CCM assumes the ground state to be a generalized coherent state

$$|\psi\rangle=e^{\hat{S}}|0\rangle \tag{2.7}$$

with $b\,|\,0\rangle=0$ for bosons. The operator $\hat{S}$ can be expanded in powers of $b^\dagger$:

$$\hat{S}=\sum_n \hat{S}_n \,, \tag{2.8a}$$

$$\hat{S}_n=\frac{1}{\sqrt{n!}}S_n(b^\dagger)^n \,. \tag{2.8b}$$

The coefficients S_n are called correlation amplitudes. Solving the Schrödinger equation is exactly equivalent to evaluating all S_n amplitudes.

Equations for these amplitudes can be obtained by projecting onto states $\langle n\,|\,e^{-\hat{S}}$:

$$\langle 0\,|\,e^{-\hat{S}}He^{\hat{S}}\,|\,0\rangle=E \,, \tag{2.9a}$$

$$\langle n\,|\,e^{-\hat{S}}He^{\hat{S}}\,|\,0\rangle=0 \,. \tag{2.9b}$$

The first equation defines the exact ground-state energy whereas (2.9b) determines the coefficients S_n. It is a well-known trick to proceed to expand $e^{-S}He^{S}$ in a sum of multiple commutators. This takes into account the important linked cluster theorem.[8] A lengthy but straightforward calculation yields an infinite hierarchy of equations for the S_n:

$$\begin{aligned}0=&\sqrt{2}\alpha\delta_{n,2}+\sqrt{24}\gamma\delta_{n,4}+[\epsilon+6\gamma(n-1)]nS_n+[(n+1)(n+2)]^{1/2}(\alpha+4\gamma n)S_{n+2}+4\gamma(n-2)[(n-1)n]^{1/2}S_{n-2}\\&+\gamma[(n+1)(n+2)(n+3)(n+4)]^{1/2}S_{n+4}+\sum_{K+L=n+2}\sqrt{n!}\frac{KL}{\sqrt{K!L!}}[\alpha+12\gamma(L-1)]S_KS_L\\&+6\gamma\sqrt{n!}\sum_{K+L=n}\frac{KL}{\sqrt{K!L!}}S_KS_L\\&+\gamma\sqrt{n!}\sum_{K+L=n+4}\frac{KL(L-1)(4n-K+5)}{\sqrt{K!L!}}S_KS_L+4\gamma\sqrt{n!}\sum_{K+L+M=n+2}\frac{KLM}{\sqrt{K!L!M!}}S_KS_LS_M\\&+6\gamma\sqrt{n!}\sum_{K+L+M=n+4}\frac{KLM(M-1)}{\sqrt{K!L!M!}}S_KS_LS_M+\gamma\sqrt{n!}\sum_{K+L+M+P=n+4}\frac{KLMP}{\sqrt{K!L!M!P!}}S_KS_LS_MS_P \,.\end{aligned} \tag{2.10}$$

We used a more general Hamiltonian (2.4) with α arbitrary. Within the set (2.10) the equation for S_n depends on S_{n+1} up to S_{n+4}. To receive an approximate solution of the first n_0 equations, one has to make assumptions on $S_{n>n_0}$. The S_n truncation scheme assigns zero values to all higher amplitudes than S_{n_0}.

The coefficient σ in (2.5a) is up to now a free parameter which has to be fixed by a suitable condition. Here we discuss two manifest ways.

(1) σ is a solution of $\alpha(\sigma)=0$ and amplitudes S_2, S_4, $S_6,\ldots,S_n$ have to be calculated from (2.10). It should be noted that all odd-indexed S_n amplitudes vanish by the requirement of a well-defined parity of the ground state [Hartree approximation and SUB(n)].

(2) Here S_2 should vanish and σ is a solution of (2.10) for $n=2$. Only amplitudes $S_4,S_6,\ldots$ appear (maximum overlap condition).[9]

We analyze both possibilities numerically but in general problems appear because the nonlinear equations (2.10) do not show a unique solution. To exclude unphysical solutions we perform a stability analysis with respect to thermal fluctuations. Therefore, in the next section, we introduce a temperature-dependent coupled-cluster formulation.

III. TEMPERATURE DEPENDENCE AND STABILITY ANALYSIS

The truncated hierarchy (2.10) of nonlinear coupled equations will have more than one solution in general. Intuitively, one would expect the solution corresponding to lowest energy to be the physical one. Unfortunately, an explicit calculation disproves this assumption. There are solutions with large S amplitudes promoting the energy (2.9a) significantly below the well-known exact values. Therefore, it is desirable to have a reliable criterion not depending on the energy which selects the correct solution out of a variety of possible ones. Our proposal for such a criterion is based on the property of thermodynamical stability.

Insert the anharmonic oscillator in a heat bath. Unstable states, although lower in energy than the exact energy, can now decay in stable solutions because the energy of the anharmonic oscillator itself is no longer conserved. The oscillator gets heated up and finally approaches a stable state. To describe such a process the temperature-dependent coupled-cluster formalism[10] is set up. That formalism for fermions was applied to the model of Lipkin, Meshkov, and Glick by one of the authors.[11] Here we propose a direct transfer of the technique originally developed for fermions to the boson case. The Schrödinger equation for zero temperature is replaced by the Bloch equation for the statistical operator ρ,

$$\left[H+\frac{d}{d\beta}\right]\rho=0 \,, \tag{3.1}$$

where we make use of the ansatz for ρ:

$$\rho=e^{\tilde{S}}\left[\sum_{m,n=0}^{\infty}|\,m\rangle e^{-\beta(m+n)\epsilon/2}\times[\delta_{mn}+C_{mn}(\beta)]\frac{1}{\sqrt{m!n!}}\langle n\,|\right]e^{\tilde{S}^\dagger} \tag{3.2}$$

and

$$\tilde{S}_n(\beta)=S_0(\beta)+\hat{S}(\beta)=S_0(\beta)+\sum_{n=1}^{\infty}\hat{S}_n(\beta)\ . \tag{3.3}$$

The $\beta=\infty$ ground state, i.e., $T=0$, is completely specified by amplitudes S_n^g whereas the density matrix $\langle m\,|\,\rho\,|\,n\rangle$ needs additional amplitudes C_{mn} to avoid overcompleteness. $S_0(\beta)$ is a c-number function which ensures correct normalization of the partition function. It turns out that the Bloch equation is completely equivalent to an infinite hierarchy of equations

$$\left\langle k\left|e^{-s\left[H+\frac{d}{d\beta}\right]}\rho\right|l\right\rangle=0\ . \tag{3.4}$$

Here we are interested in the special case $l=0$, $k>0$, which yields the $S_n(\beta)$ equations

$$\frac{dS_k(\beta)}{d\beta}=-\langle k\,|\,e^{-\hat{S}(\beta)}He^{\hat{S}(\beta)}\,|\,0\rangle \tag{3.5}$$

with boundary conditions $S_k(\infty)=S_k^g$. Each solution of the $\beta=\infty$ hierarchy (3.10) can now be extrapolated to finite temperature. (3.5) is not explicitly dependent on β: therefore the solutions are translationally invariant on the β axis and we can push a solution from finite β to arbitrarily large β.

Assume the $\beta=\infty$ equations to have two solutions S_n^{I} and S_n^{II}. S_n^{II} may be unphysical but lower in energy than S_n^{I}. Equation (3.5) has solitonlike solutions connecting S_n^{I} and S_n^{II}. These "amplitude solitons" can easily be obtained by a numerical solution of (3.5). They may be centered around $\beta\neq 0$ but by translational invariance they can be pushed to arbitrary values of β.

Now, β-independent c numbers S_n^{I} and S_n^{II} are certainly special solutions of (3.3). Assume β to be very large and $S_n^i(\beta)=S_n^i$ for $\beta>\beta_0$. At β_0 there may be an infinitesimal deviation $\delta S_n^i=S_n^i(\beta_0)-S_n^i$. It is now possible to analyze the behavior of this δS_n^i by an ansatz

$$\delta S_n^i(\beta)=\delta S_n^i(\beta_0)e^{i\nu(\beta-\beta_0)}\ , \tag{3.6}$$

where ν are stability frequencies and the unstable solution S_n^{II} will have frequencies with positive imaginary parts. Therefore, infinitesimal deviations δS_n^i will grow exponentially. Stable states have real stability frequencies and can be identified by this criterion.

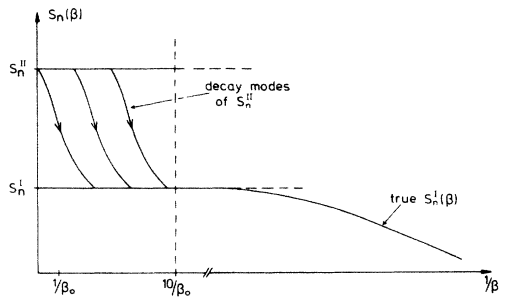

FIG. 1 The expected typical behavior of finite-temperature amplitudes is sketched for illustration. S_n^{I} is a smooth function of $1/\beta$, whereas S_n^{II} decays via amplitude solitons into S_n^{I}. Shifting the decay process to arbitrary small temperature allows us to ignore the unknown temperature dependence of the true S_n^{I} and replace it by its value at $T=0$.

Why did we push β_0 to very large values? Besides these "decay modes" of S_n^{II} into S_n^{I} there are further solutions which describe the "true" amplitudes $S_n(\beta)$ at finite β. Certainly, at arbitrarily large β we can ignore the β dependence of these solutions since they should be slowly varying functions of β whereas the amplitude solitons appear almost as step functions, at least on the T axis very close to $T=0$. Therefore, at infinitesimal temperature, the deviations of these true $S_n(\beta)$ from S_n can still be ignored and we can replace them by their $T=0$ values. (See Fig. 1.)

IV. NUMERICAL INVESTIGATIONS

The numerical evaluation of the coupled-cluster equations (2.10) is by no means involved and could even be done with a conventional microcomputer for the case that the number of amplitudes has not been chosen too large. First of all, we mention that there is no remarkable difference between results gained by the Hartree approximation or by the maximum overlap condition. To compare the calculations of the energy with the exact one, we use an ordinary matrix diagonalization of the Hamiltonian which shows convergence already for a 30×30 matrix.

The results for the ground-state energy are presented in Tables I and II. First of all, it becomes obvious that the exact energy is reproduced very well by our method. Already a S_6 truncation yields an accuracy of less than 0.01% for all values of the coupled strength. This is a remarkable result for the simplicity of the approach. Some remarks have to be made on the dependence of the energy on the truncation scheme.

For small values of the coupling strength ($\lambda\leq 2.0$) the energy converges rapidly for all values of the maximum number of S_n amplitudes taken into account ($n_{\max}\leq 50$). Increasing the coupling strength, significant fluctuations around the exact values show up, depending slightly on the applied truncation scheme. For $\lambda=10.0$ the fluctuation amplitudes are only 0.007% but they become as large as 0.03% for $\lambda=100.0$. In this range the deviations from exact values achieve their maximum whereas for a very large coupling strength they decrease again. This behavior is widely independent of the approximation schemes used, the Hartree procedure and the maximum overlap condition.

Tables III and IV show the values of the correlation amplitudes if a total number of 30 S_n amplitudes is considered. These tables give insight into the fluctuations of the ground-state energy. For small values of the coupling strength ($\lambda\approx 0.1$) the sequence of amplitudes seems to tend towards zero. A detailed analysis, taking almost 70 amplitudes into account, disproves this assumption. This behavior becomes apparent if we observe the relation between two adjacent amplitudes $|S_{n+2}/S_n|$. There is always a critical index n_{crit} for which this quantity is less than 1 but also a region $n\geq n_{\mathrm{crit}}$ where the relation becomes larger than 1. To become concrete now, we find in the case of the maximum overlap calculation that $n_{\mathrm{crit}}=20$ for $\lambda=1.0$ and 10.0, $n_{\mathrm{crit}}=18$ for $\lambda=1000.0$ In the case of the Hartree calculation these critical values be-

TABLE I. Ground-state energy as a function of the coupling strength and the maximum number of S_n amplitudes taken into account (maximum-overlap condition).

n_{max}	$\lambda=0.1$	$\lambda=0.5$	$\lambda=1.0$	$\lambda=5.0$	$\lambda=10.0$	$\lambda=100.0$	$\lambda=1000.0$
4	0.517 366	0.571 008	0.621 114	0.847 630	1.010 917	2.007 326	4.234 215
6	0.517 365	0.570 947	0.620 917	0.846 530	1.009 152	2.002 046	4.230 998
8	0.517 365	0.570 951	0.620 919	0.846 476	1.009 031	2.001 514	4.229 671
10	0.517 365	0.570 951	0.620 925	0.846 520	1.009 100	2.001 703	4.230 090
12	0.517 365	0.570 951	0.620 927	0.846 547	1.009 154	2.001 900	4.230 564
14	0.517 365	0.570 951	0.620 927	0.846 558	1.009 179	2.002 020	4.230 872
16	0.517 365	0.570 951	0.620 927	0.846 561	1.009 187	2.002 081	4.231 041
18	0.517 365	0.570 951	0.620 927	0.846 559	1.009 186	2.002 103	4.231 117
20	0.517 365	0.570 951	0.620 927	0.846 556	1.009 179	2.002 086	4.231 097
22	0.517 365	0.570 951	0.620 927	0.846 551	1.009 166	2.001 960	4.231 243
24	0.517 365	0.570 951	0.620 927	0.846 546	1.009 142	2.001 729	4.231 221
26	0.517 365	0.570 951	0.620 927	0.846 539	1.009 115	2.001 575	4.231 210
28	0.517 365	0.570 951	0.620 927	0.846 535	1.009 101	2.001 525	4.231 182
30	0.517 365	0.570 951	0.620 927	0.846 535	1.009 102	2.001 551	4.231 152
Exact	0.517 365	0.570 951	0.620 927	0.846 554	1.009 170	2.001 996	4.230 821

come smaller, that is, $n_{crit}=16$ for $\lambda=1.0$, $n_{crit}=14$ for $\lambda=10.0$, decreasing to its minimum values $n_{crit}=10$ for values of the coupling strength larger than 10^3.

It should be noted that S_n amplitudes become independent of the coupling strength for large values of λ because of an asymptotic form of the Hamiltonian

$$H=(\tfrac{3}{2}\lambda)^{1/3}[\tfrac{3}{8}+b^{\dagger}b+\tfrac{1}{24}:(b+b^{\dagger})^4:] \ . \tag{4.1}$$

Summarizing now, it is not recommendable to consider the convergence of S_n amplitudes as a function of n. Very high S_n will always become arbitrarily large. Nevertheless, the low S_n amplitudes like S_2 and S_4 are nearly uninfluenced by this divergence. Our numerical study exhibits small fluctuations of S_2 and S_4 as a function of the truncation scheme. It would be interesting to prove or disprove analytically that they tend towards an asymptotic value.

There is one more comment on the convergence of the S_n amplitudes. Even if it would take place, the limit of the functions S_n has no physical meaning. It is easy to check that the norm of the $e^S|0\rangle$ state is given by

$$\langle 0|e^{S^{\dagger}}e^{S}|0\rangle=1+\sum_{\lambda_2\cdots\lambda_N=0}^{\infty}C_{\lambda_2\cdots\lambda_N}\prod_{j=1}^{N/2}S_{2j}^{\lambda_{2j}} \tag{4.2}$$

and

$$C_{\lambda_2\cdots\lambda_N}=\sum_{n,m=1}^{\infty}\frac{1}{n!m!}\sum_{\substack{\mu_1\cdots\mu_n\nu_1\cdots\nu_m=2\\ \sum\mu=\sum\nu}}^{N}{}'\frac{\left[\sum_1^n\mu_i\right]!}{\left[\prod_1^n\mu_i!\prod_1^m\nu_i!\right]^{1/2}} \tag{4.3}$$

TABLE II. Ground-state energy as a function of the coupling strength and the maximum number of S_n amplitudes taken into account (Hartree approximation).

n_{max}	$\lambda=0.1$	$\lambda=0.5$	$\lambda=1.0$	$\lambda=5.0$	$\lambda=10.0$	$\lambda=100.0$	$\lambda=1000.0$
4	0.517 366	0.517 004	0.621 096	0.847 482	1.010 661	2.006 477	4.241 207
6	0.517 365	0.570 947	0.620 915	0.846 498	1.009 089	2.001 795	4.230 380
8	0.517 365	0.570 950	0.620 920	0.846 477	1.009 032	2.001 509	4.229 652
10	0.517 365	0.570 951	0.620 926	0.846 525	1.009 112	2.001 751	4.230 210
12	0.517 365	0.570 951	0.620 927	0.846 551	1.009 161	2.001 941	4.230 672
14	0.517 365	0.570 951	0.620 927	0.846 559	1.009 182	2.002 040	4.230 925
16	0.517 365	0.570 951	0.620 927	0.846 560	1.009 186	2.002 077	4.231 033
18	0.517 365	0.570 951	0.620 927	0.846 558	1.009 182	2.002 077	4.231 044
20	0.517 365	0.570 951	0.620 927	0.846 554	1.009 174	2.002 041	4.230 957
22	0.517 365	0.570 951	0.620 927	0.846 551	1.009 163	2.001 934	4.230 629
24	0.517 365	0.570 951	0.620 927	0.846 547	1.009 145	2.001 764	4.230 153
26	0.517 365	0.570 951	0.620 927	0.846 543	1.009 128	2.001 649	4.229 869
28	0.517 365	0.570 951	0.620 927	0.846 541	1.009 120	2.001 621	4.229 811
30	0.517 365	0.570 951	0.620 927	0.846 541	1.009 123	2.001 659	4.229 914
Exact	0.571 365	0.570 951	0.620 927	0.846 554	1.009 170	2.001 996	4.230 821

TABLE III. Magnitude of correlation amplitudes for different values of the coupling strength and a fixed number of 30 amplitudes (maximum overlap condition).

	$\lambda=0.1$	$\lambda=0.5$	$\lambda=1.0$	$\lambda=5.0$	$\lambda=10.0$	$\lambda=100.0$	$\lambda=1000.0$
S_4	$-5.807\,14\times10^{-3}$	$-1.572\,43\times10^{-2}$	$-2.062\,45\times10^{-2}$	$-2.934\,09\times10^{-2}$	$-3.167\,52\times10^{-2}$	$-3.531\,99\times20^{-2}$	$-3.558\,06\times10^{-2}$
S_6	$3.690\,18\times10^{-4}$	$2.425\,68\times10^{-3}$	$3.994\,40\times10^{-3}$	$7.655\,46\times10^{-3}$	$8.851\,07\times10^{-3}$	$1.082\,50\times10^{-2}$	$1.060\,14\times10^{-2}$
S_8	$-4.687\,33\times10^{-5}$	$-7.081\,37\times10^{-4}$	$-1.438\,53\times10^{-3}$	$-3.545\,58\times10^{-3}$	$-4.196\,31\times10^{-3}$	$-5.096\,80\times10^{-3}$	$-5.965\,35\times10^{-3}$
S_{10}	$8.940\,42\times10^{-6}$	$3.004\,71\times10^{-4}$	$7.471\,86\times10^{-4}$	$1.889\,67\times10^{-3}$	$1.864\,64\times10^{-3}$	$1.361\,03\times10^{-3}$	$5.314\,77\times10^{-3}$
S_{12}	$-2.265\,72\times10^{-6}$	$-1.658\,80\times10^{-4}$	$-4.983\,49\times10^{-4}$	$-6.997\,56\times10^{-4}$	$5.634\,85\times10^{-5}$	$1.852\,58\times10^{-3}$	$-5.941\,66\times10^{-3}$
S_{14}	$7.136\,48\times10^{-7}$	$1.119\,96\times10^{-4}$	$3.909\,25\times10^{-4}$	$3.107\,45\times10^{-4}$	$-3.761\,98\times10^{-4}$	$-1.687\,67\times10^{-3}$	$6.339\,31\times10^{-3}$
S_{16}	$-2.680\,02\times10^{-7}$	$-8.865\,73\times10^{-5}$	$-3.452\,42\times10^{-4}$	$-2.562\,29\times10^{-3}$	$-4.373\,53\times10^{-3}$	$-7.994\,00\times10^{-3}$	$-5.001\,69\times10^{-3}$
S_{18}	$1.166\,58\times10^{-7}$	$8.055\,48\times10^{-5}$	$3.782\,10\times10^{-4}$	$1.027\,60\times10^{-2}$	$1.903\,09\times10^{-2}$	$3.549\,83\times10^{-2}$	$1.057\,81\times10^{-3}$
S_{20}	$-5.767\,23\times10^{-8}$	$-8.543\,40\times10^{-5}$	$-6.009\,26\times10^{-4}$	$-2.576\,12\times10^{-2}$	$-4.788\,00\times10^{-2}$	$-9.099\,70\times10^{-2}$	$4.061\,73\times10^{-3}$
S_{22}	$3.189\,58\times10^{-8}$	$1.088\,28\times10^{-4}$	$1.197\,65\times10^{-3}$	$4.866\,29\times10^{-2}$	$9.340\,38\times10^{-2}$	$1.925\,02\times10^{-1}$	$-4.282\,53\times10^{-3}$
S_{24}	$-1.955\,16\times10^{-8}$	$-1.580\,21\times10^{-4}$	$-2.292\,21\times10^{-3}$	$-7.514\,01\times10^{-2}$	$-1.595\,57\times10^{-1}$	$-3.841\,20\times10^{-1}$	$-1.293\,85\times10^{-2}$
S_{26}	$1.324\,04\times10^{-8}$	$2.263\,16\times10^{-4}$	$3.661\,24\times10^{-3}$	$1.007\,88\times10^{-1}$	$2.590\,99\times10^{-1}$	$7.486\,25\times10^{-1}$	$6.330\,55\times10^{-2}$
S_{28}	$-9.561\,27\times10^{-9}$	$-2.692\,69\times10^{-4}$	$-4.434\,60\times10^{-3}$	$-1.230\,46\times10^{-1}$	$-3.969\,24\times10^{-1}$	$-1.304\,47$	$-1.441\,54\times10^{-1}$
S_{30}	$5.780\,89\times10^{-9}$	$2.028\,14\times10^{-4}$	$3.275\,82\times10^{-3}$	$1.194\,72\times10^{-1}$	$4.483\,62\times10^{-1}$	$1.548\,19$	$1.786\,13\times10^{-1}$

TABLE IV. Magnitude of correlation amplitudes for different values of the coupling strength and a fixed number of 30 amplitudes (Hartree approximation).

	$\lambda=0.1$	$\lambda=0.5$	$\lambda=1.0$	$\lambda=5.0$	$\lambda=10.0$	$\lambda=100.0$	$\lambda=1000.0$
S_2	$3.835\,72\times10^{-4}$	$2.792\,19\times10^{-3}$	$4.758\,92\times10^{-3}$	$9.364\,58\times10^{-3}$	$1.077\,49\times10^{-2}$	$1.308\,35\times10^{-2}$	$1.366\,03\times10^{-2}$
S_4	$-5.807\,68\times10^{-3}$	$-1.574\,91\times10^{-2}$	$-2.069\,29\times10^{-2}$	$-2.957\,17\times10^{-2}$	$-3.196\,06\times10^{-2}$	$-3.570\,30\times10^{-2}$	$-3.600\,86\times10^{-2}$
S_6	$3.689\,50\times10^{-4}$	$2.427\,22\times10^{-3}$	$4.003\,84\times10^{-3}$	$7.702\,13\times10^{-3}$	$3.916\,71\times10^{-3}$	$1.096\,70\times10^{-2}$	$1.147\,87\times10^{-2}$
S_8	$-4.685\,39\times10^{-5}$	$-7.081\,87\times10^{-4}$	$-1.441\,27\times10^{-3}$	$-3.599\,70\times10^{-3}$	$-4.307\,49\times10^{-3}$	$-5.376\,48\times10^{-3}$	$-5.611\,33\times10^{-3}$
S_{10}	$8.934\,87\times10^{-6}$	$3.003\,73\times10^{-4}$	$7.485\,33\times10^{-4}$	$2.017\,00\times10^{-3}$	$2.108\,39\times10^{-3}$	$1.813\,00\times10^{-3}$	$1.663\,85\times10^{-3}$
S_{12}	$-2.263\,88\times10^{-6}$	$-1.657\,81\times10^{-4}$	$-5.001\,08\times10^{-4}$	$-8.944\,26\times10^{-4}$	$-2.727\,28\times10^{-4}$	$1.447\,32\times10^{-3}$	$1.950\,04\times10^{-3}$
S_{14}	$7.129\,40\times10^{-7}$	$1.119\,26\times10^{-4}$	$3.943\,86\times10^{-4}$	$4.444\,21\times10^{-4}$	$-1.688\,22\times10^{-4}$	$-1.605\,00\times10^{-3}$	$-1.955\,51\times10^{-3}$
S_{16}	$-2.676\,90\times10^{-7}$	$-8.861\,93\times10^{-5}$	$-3.499\,13\times10^{-4}$	$-2.397\,12\times10^{-3}$	$-4.208\,12\times10^{-3}$	$-7.915\,02\times10^{-3}$	$-8.980\,74\times10^{-3}$
S_{18}	$1.165\,02\times10^{-7}$	$8.048\,78\times10^{-5}$	$3.793\,37\times10^{-4}$	$9.585\,91\times10^{-3}$	$1.839\,64\times10^{-2}$	$3.622\,21\times10^{-2}$	$4.101\,22\times10^{-2}$
S_{20}	$-5.758\,65\times10^{-8}$	$-8.516\,37\times10^{-5}$	$-3.891\,38\times10^{-4}$	$-2.443\,73\times10^{-2}$	$-4.670\,17\times10^{-2}$	$-9.353\,41\times10^{-2}$	$-1.064\,25\times10^{-1}$
S_{22}	$3.184\,28\times10^{-8}$	$1.081\,48\times10^{-4}$	$1.165\,00\times10^{-3}$	$4.644\,51\times10^{-2}$	$9.043\,05\times10^{-2}$	$1.952\,23\times10^{-1}$	$2.265\,66\times10^{-1}$
S_{24}	$1.951\,56\times10^{-8}$	$-1.570\,07\times10^{-4}$	$-2.244\,76\times10^{-3}$	$-7.058\,48\times10^{-2}$	$-1.497\,61\times10^{-1}$	$-3.798\,65\times10^{-1}$	$-4.557\,67\times10^{-1}$
S_{26}	$1.321\,39\times10^{-8}$	$2.256\,81\times10^{-4}$	$3.627\,29\times10^{-3}$	$8.994\,36\times10^{-2}$	$2.318\,59\times10^{-1}$	$7.287\,90\times10^{-1}$	$9.031\,81\times10^{-1}$
S_{28}	$-9.542\,29\times10^{-9}$	$-2.700\,13\times10^{-4}$	$-4.447\,41\times10^{-3}$	$1.019\,00\times10^{-1}$	$-3.429\,72\times10^{-1}$	$-1.277\,35$	$-1.611\,50$
S_{30}	$5.771\,76\times10^{-9}$	$2.045\,73\times10^{-4}$	$3.323\,24\times10^{-3}$	$9.224\,18\times10^{-2}$	$3.864\,74\times10^{-1}$	$1.546\,65$	$1.959\,89$

TABLE V. The dependence of the amplitudes on the truncation scheme becomes obvious (here for a coupling strength $\lambda=100.0$).

	$n=4$	$n=8$	$n=12$	$n=16$	$n=20$	$n=24$	$n=28$
S_2	$1.439\,26\times10^{-2}$	$1.331\,80\times10^{-2}$	$1.302\,72\times10^{-2}$	$1.306\,19\times10^{-2}$	$1.313\,79\times10^{-2}$	$1.323\,79\times10^{-2}$	$1.315\,09\times10^{-2}$
S_4	$-3.119\,94\times10^{-2}$	$-3.585\,24\times10^{-2}$	$-3.543\,53\times10^{-2}$	$-3.530\,77\times10^{-2}$	$-3.534\,43\times10^{-2}$	$-3.560\,95\times10^{-2}$	$-3.574\,10\times10^{-2}$
S_6		$1.044\,88\times10^{-2}$	$1.074\,19\times10^{-2}$	$1.043\,96\times10^{-2}$	$1.025\,37\times10^{-2}$	$1.033\,64\times10^{-2}$	$1.081\,06\times10^{-2}$
S_8		$-3.766\,51\times10^{-3}$	$-5.919\,68\times10^{-3}$	$-5.783\,05\times10^{-3}$	$-5.268\,84\times10^{-3}$	$-4.446\,01\times10^{-3}$	$-4.917\,16\times10^{-3}$
S_{10}			$3.963\,50\times10^{-3}$	$4.805\,54\times10^{-3}$	$4.306\,92\times10^{-3}$	$2.041\,60\times10^{-3}$	$1.329\,26\times10^{-3}$
S_{12}			$-2.044\,47\times10^{-3}$	$-4.743\,81\times10^{-3}$	$-5.419\,69\times10^{-3}$	$-2.698\,16\times10^{-3}$	$9.481\,52\times10^{-4}$
S_{14}				$4.276\,17\times10^{-3}$	$7.996\,00\times10^{-3}$	$8.971\,21\times10^{-3}$	$1.570\,21\times10^{-3}$
S_{16}				$-2.550\,54\times10^{-3}$	$-1.078\,13\times10^{-2}$	$-2.349\,27\times10^{-2}$	$-1.529\,19\times10^{-2}$
S_{18}					$1.145\,87\times10^{-2}$	$-4.609\,73\times10^{-2}$	$4.742\,10\times10^{-2}$
S_{20}					$-7.620\,30\times10^{-3}$	$-7.123\,76\times10^{-2}$	$-1.039\,40\times10^{-1}$
S_{22}						$8.637\,89\times10^{-2}$	$1.915\,68\times10^{-1}$
S_{24}						$-7.004\,97\times10^{-2}$	$-3.229\,58\times10^{-1}$

and the summation $\sum'$ is restricted due to the subsidiary condition

$$\lambda_j=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{-ij\phi}\left[\sum_{\alpha=1}^{n}e^{i\phi\mu_\alpha}+\sum_{\beta=1}^{m}e^{i\phi\nu_\beta}\right]. \tag{4.4}$$

This does not define a normalizable state because the $C_{\lambda_2\cdots\lambda_N}$ all tend towards infinity. Only for $N=2$ is there a finite radius of convergence of the Taylor series. In all other cases the radius of convergence is zero. It may become even more apparent if one investigates the Fock-space representation of $e^S|0\rangle$ in the most simple case of $S=S_4$ only. The coefficients $C_n=\langle n|e^S|0\rangle$ seem to tend towards zero numerically for small n but it can be shown that

$$C_{4n}\rightarrow\left[\frac{2}{\pi}\right]^{1/4}\exp\left[-\tfrac{1}{4}\ln n+n\ln\left[\frac{8nS_4}{e\sqrt{6}}\right]\right],\quad n\rightarrow\infty \tag{4.5}$$

and this becomes arbitrarily large. Therefore $\sum_n|C_n|^2$ is not finite and $e^{S_4}|0\rangle$ does not belong to the Hilbert space of normalizable states. This may already show a significant complication if the CCM is applied to bosons. CCM states cannot be physical ones which are normalizable.

In Table V we compare S_n amplitudes for a fixed value of the coupling strength and different S_n-truncation schemes. It is obvious that inclusion of only one additional amplitude creates significant changes in the amplitude calculated before, but it is also interesting to see that nevertheless the energy is hardly influenced by this fluctuating property of the higher amplitudes.

The very large values of higher S_n demonstrate the breakdown of the S_n-truncation scheme. It is a bad approximation to assign zero values to S_{n+2} and S_{n+4}. Recently, one of the authors[12] proposed a different truncation scheme with the assignments

$$S_{n+2}=-\frac{4\gamma}{\epsilon}n\left[\frac{n+1}{n+2}\right]^{1/2}S_n\ , \tag{4.6a}$$

$$S_{n+4}=\frac{16\gamma^2}{\epsilon^2}n(n+2)\left[\frac{(n+1)(n+3)}{(n+2)(n+4)}\right]^{1/2}S_n\ . \tag{4.6b}$$

The proposal was based upon the observation that this truncation allows a renormalization of the $(\phi^4)_3$ quantum field theory compatible with the CCM. We checked this alternative for the anharmonic oscillator.

In the case of the Hartree approximation the change in energy is about $10^{-4}\%$ whereas the amplitudes vary at maximum 1%. These irrelevant effects of the different values for S_{n+2} and S_{n+4} are easy to understand. The enormous number of terms in the higher S_n equations is not affected by a minor change of a very few terms. Also, in this truncation scheme the high S_n are very large. It is probable that this will be the case in all truncation schemes. There may exist proper combinations C_n of amplitudes which decrease to zero fast enough so that the C_n truncations are physical. To find these combinations is extremely desirable in applying CCM to field theory suc-

cessfully. It should be noted that Eqs. (4.6) yield more significant changes in the energies when used together with the maximum overlap condition. This is again obvious because the vanishing of S_2 reduces the number of terms in the equation enormously and gives more importance to a change of a very few terms.

V. DISCUSSION AND OUTLOOK

Some important consequences have come out of our investigations. We have to draw the conclusion that the method works very well for calculations of the ground-state energy but the amplitudes themselves should be handled with care.

Our numerical analysis could not reveal whether there is real convergence or divergence of the energy. The most important observation is certainly that already low-order approximations like a S_6-truncation scheme give excellent results which cannot be improved by the inclusion of higher amplitudes. The simplicity of the maximum overlap condition together with the S_6 truncation makes this the most promising candidate for use in quantum field theory.

The fluctuations around the exact energy are small enough to call the method numerically convergent. Extensions to quantum field theory will probably show a comparable behavior; there are already a few hints supporting this statement.[7]

In comparison with the fermion case, the fluctuations seem to indicate some new phenomena if CCM is applied to bosons. Most experience with CCM has been made with Fermi systems where the method works extremely well. It is most successful in quantum chemistry, although, as noticed by Coester,[13] this has not been understood at all. The very sparse experience with bosons again shows up in the problem of how to formulate the correct truncation scheme. This will certainly be one of the major questions to be asked in the future. As long as there are no real convincing physical arguments for approximations, some doubts remain inherent in the method when applied to bosons.

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