Nonuniqueness in the energy spectra of anharmonic oscillators using the coupled-cluster method

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The coupled-cluster method (CCM) of quantum many-body theory has been widely and very successfully applied to a broad spectrum of condensed-matter systems. At a given level of approximation in a hierarchy of truncations which are necessary to implement the method in practice, the many-body Schrödinger equation is decomposed into a finite set of coupled nonlinear equations for the various amplitudes that otherwise exactly describe the correlated clusters or subsystems within the interacting many-body medium. The properties of the multiple solutions to these equations and their implications for the method itself are the primary concern here. We perform a detailed investigation for the simple but illustrative one-body problem of a quartic anharmonic oscillator, which provides a very stringent test of the convergence properties of any method rooted in perturbation theory. The problem is treated as a model field theory in 0+1 dimensions in order to illuminate general properties of the CCM. The various supercoherent states generated by the CCM at other than the lowest levels of truncation are unnormalizable but yield finite and well-defined estimates for quantities of physical interest. Their possible use as multiphoton generalizations of the two-photon squeezed coherent states is pointed out.

I. INTRODUCTION

The coupled-cluster method (CCM) has become firmly established as a rather powerful and accurate technique in quantum many-body theory, with a wide applicability across the spectrum of physical many-body systems. One of the main reasons for its success is that by parametrizing the exact interacting many-body ground-state wave function as an exponential operator $\exp(\hat{S})$, acting on some suitable noninteracting or model state,¹ the resultant perturbation or cluster expansion contains only linked terms. Coester² and Kümmel³ demonstrated further that the linked cluster correlation operator $\hat{S}$ can be used as the generator of a similarity transformation for the exact ground-state Schrödinger equation. In this way they originated the so-called $\exp(S)$ method of quantum many-body theory or, as it is generally referred to more recently, the CCM. A rather general and pedagogical discussion of the method may be found in Ref. 4.

The range of numerically very accurate applications has been very wide. It includes both finite and infinite systems in nuclear physics,⁵⁻⁷ atomic and molecular systems of interest in quantum chemistry,⁸⁻¹³ and the homogeneous electron liquid or one-component Coulomb plasma.¹⁴⁻¹⁷ After this successful array of applications to systems in the broad area of condensed-matter physics, the method has also been applied to such systems of interest in quantum relativistic field theory as the ϕ^4 model.¹⁸

In order to be able to continue to extend the range of applicability of the CCM, particularly in the area of relativistic field theories, the method itself and its various modes of implementation have lately come under close

scrutiny. It is largely with this aim in mind, rather than to study the specific model problems themselves, that the CCM has been applied to various one-body anharmonic oscillators.¹⁹⁻²³ Such one-body problems are simple enough for CCM calculations to be carried out to a very high order, and certainly to much higher orders than could ever be realized in practice for many-body systems of physical interest. Nevertheless anharmonic oscillators are systems which are both interesting in their own right and which present a serious challenge to any approximation scheme which is ultimately rooted in perturbation theory. Thus it is well known that a straightforward application of Rayleigh-Schrödinger perturbation theory leads to a ground-state energy expansion which diverges for *all* values of the coupling constant in the case of a quartic anharmonicity, for example.^{24,25}

In an earlier paper²² we first gave a rather detailed analysis of the simple (Hartree or Gaussian) variational approximation to the ground state of a very wide class of anharmonic oscillators. We further showed how this optimized Hartree wave function could be systematically improved upon. This was achieved by treating it as a zeroth-order or model wave function, and by applying to it a version of both the ground-state and, via the Emrich ansatz,²⁶ the excited-state CCM formalism. We stress again that these CCM calculations were carried out in such a way that makes it possible to enquire about the applicability of the method to related field-theoretical systems. The intention was not to use that version of the CCM which would achieve the most accurate results possible for these systems. We note in passing that the practical implementation of what is perhaps the most direct version of the CCM when applied to such one-body prob-

lems is exactly equivalent to diagonalization of the Hamiltonian in a truncated one-body basis of states. Such a procedure is known to be very accurate in general. On the other hand, the version of the CCM used in Ref. 22 was more concerned with later applications to quantum-field theory, and the resulting problems were used as simple models of actual many-body systems, for which the convergence properties of the standard truncation scheme could be studied. It was nevertheless demonstrated to be capable of giving extremely accurate results for both the ground-state and excitation energies of the various anharmonic oscillators studied.

The question of the possible nonuniqueness of the CCM ground-state wave function was briefly addressed in our earlier paper,²² and in some more detail in Ref. 23. One knows that the CCM parametrization of the wave function is exact if no approximations are made, and hence its associated energy eigenvalue would also be given exactly. Nevertheless a possible source of ambiguity arises because the normalizability of the exact wave function is nowhere explicitly imposed within the CCM methodology. Furthermore, the truncated approximate wave functions which arise in practical implementations of the method are manifestly unnormalizable. We stress that since the standard CCM calculation of the energy does not involve the norm of the wave function, the corresponding approximations to the energy remain perfectly well behaved and finite. We point out in passing that there also exists an extended version of the CCM²⁷⁻²⁹ which permits the evaluation of expectation values of *arbitrary* operators without reference to the norm of the wave function.

Even for such model problems as the various one-body anharmonic oscillators, the ground-state CCM equations cannot be solved exactly. Some approximation hierarchy is needed to truncate what is otherwise an infinite set of coupled multinomial equations for the various correlation coefficients in the expansion of the linked cluster operator $\hat{S}$. It is not surprising that the standard truncation scheme produces multiple solutions at each level of approximation. The number of possible such solutions grows without bound as the truncation index that marks the order of the approximation is increased. For the specific case of the quartic anharmonic oscillator this ambiguity in the ground-state CCM solution was first addressed by Kaulfuss and Altenbokum.²¹ They adopted the viewpoint of suppressing the extra solutions by performing a thermodynamic stability analysis. In order to do this they used a temperature-dependent extension of the CCM, and chose among the multiplicity of solutions at each level of approximation by performing a stability analysis which selected those levels which are stable against thermal fluctuations.

It was shown elsewhere²² how a very simple ansatz for initializing the numerical method of solution of the normal (zero-temperature) truncated CCM equations could reproduce, in all cases, these thermodynamically stable solutions. This solution was referred to as the "standard" solution. A single numerical example of a "non-standard" solution was also briefly discussed. In spite of the fact that this nonstandard solution represented a very

different wave function from the corresponding standard one, the surprising result was demonstrated that the respective energy eigenvalues were extremely close both to each other and to the exact result for this case. In view of this observation that the nonstandard solutions could also produce rather accurate approximations to the ground-state energy, we chose to examine them more closely in their own right,²³ rather than to continue to suppress them. We conjectured that as the truncation index of our chosen approximation scheme becomes very large, we tend towards an infinite set of different solutions for the ground-state wave function, all of which give asymptotically the exact energy eigenvalue when calculated via our standard CCM procedure, but only one of which is the usual physical (i.e., normalizable) state.

It is the primary purpose of the present paper to continue with the analysis of the multiple (nonstandard) solutions. To this end, we first present a brief summary of both the ground-state and excited-state CCM formalisms, together with the starting Hartree approximation, in Sec. II. We discuss in detail in Sec. III the method of solution for the ground-state CCM equations and we define various algorithms for generating nonstandard solutions. A number of such solutions are presented in Sec. IV and the resulting values for the ground-state energy are compared and contrasted with both the standard result and the exact value. By making use of the Emrich prescription²⁶ for excited states within the CCM, the excitation spectra generated from each of the ground-state solutions as input are also presented. Finally, these results are discussed in Sec. V both in terms of their consequences for the CCM itself and in a wider context of possible applicability elsewhere.

II. FORMALISM

Although brief mention will be made in Sec. IV of more general anharmonic oscillators, we shall be mainly concerned with the one-dimensional quartic anharmonic oscillator described by the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda x^4, \quad \lambda > 0. \quad (1)$$

In order to keep the formalism as compact as possible, the discussion and results in the remainder of this section apply to the Hamiltonian of Eq. (1). The necessary extensions to more general anharmonicities are, for the most part, quite straightforward, and may be found elsewhere.²² In terms of the usual destruction operator a , defined as

$$a \equiv 2^{-1/2}(x + ip), \quad (2)$$

Eq. (1) may be written in the equivalent form

$$H = \frac{1}{2} + a^\dagger a + \frac{1}{4}\lambda(a + a^\dagger)^4. \quad (3)$$

The operator a and its Hermitian adjoint $a^\dagger$ obey the usual commutation relation,

$$[a, a^\dagger] = 1, \quad (4)$$

and have a (normalized) vacuum state, denoted as $|0\rangle$, defined in the usual way as

$$a|0\rangle=0. \quad (5)$$

It would be most straightforward to implement the CCM immediately by using the state $|0\rangle$ as the zeroth-order (uncorrelated) starting approximation to the exact ground state, and the creation operator $a^\dagger$ as the basic building block for the correlation operator $\hat{S}$, which is used to construct the exact ground state as described below. It is, however, very useful to perform first a change of basis via the Bogoliubov transformation,

$$\begin{aligned} b &\equiv (1-t^2)^{-1/2}(a-ta^\dagger), \\ b^\dagger &\equiv (1-t^2)^{-1/2}(a^\dagger-ta). \end{aligned} \quad (6)$$

For ease of later discussion, the parameter t in Eq. (6) is constrained from the outset to be real. It is trivial to show that for the transformation to be unitary we require $-1 < t < 1$, and that in this case the transformation is canonical,

$$[b, b^\dagger] = 1. \quad (7)$$

If we denote the new (normalized) vacuum state of the transformed operators as $|\phi\rangle$,

$$b|\phi\rangle=0, \quad (8)$$

it is not difficult to show that the relationship between the two normalized vacuum states can be given in terms of the original creation operator as

$$|\phi\rangle = (1-t^2)^{1/4} \exp(\tfrac{1}{2}ta^{\dagger 2})|0\rangle. \quad (9)$$

Furthermore, just as it is trivial to show that the coordinate representation $\langle x|0\rangle$ of the bare original vacuum is a Gaussian, $\langle x|\phi\rangle$ is a squeezed Gaussian state in the language made familiar by recent applications in quantum optics.³⁰ It is from this squeezed coherent vacuum state $|\phi\rangle$, with some appropriately chosen value for the parameter t , that we shall build up our CCM description of the quartic anharmonic oscillator. The extra freedom permitted by the single parameter t is by no means fundamental to our discussion. Its introduction does, however, very appreciably accelerate the convergence of the resulting CCM truncation scheme discussed below.

It is convenient to rewrite the Hamiltonian of Eq. (3) in terms of the new operators b and $b^\dagger$. If we denote the normal ordering with respect to b and $b^\dagger$ of some arbitrary operator $\theta = \theta(b, b^\dagger)$ as $:\theta:$, as usual, we readily obtain the particularly useful form

$$\begin{aligned} H = E_0(\omega) &+ \left[\frac{1+\omega^2}{2\omega} \right] b^\dagger b + \left[\frac{1-\omega^2}{4\omega} \right] (b^2 + b^{\dagger 2}) \\ &+ \left[\frac{3\lambda}{2\omega^2} \right] :(b + b^\dagger)^2: + \left[\frac{\lambda}{4\omega^2} \right] :(b + b^\dagger)^4: \end{aligned} \quad (10)$$

in terms of the new parameter $\omega = \omega(t)$ defined as

$$\omega \equiv (1-t)/(1+t). \quad (11)$$

The constant term $E_0(\omega)$ in Eq. (10) is given by

$$E_0(\omega) = \frac{(1+\omega^2)}{4\omega} + \frac{3\lambda}{4\omega^2}, \quad (12)$$

and, from Eq. (10), it is simply the expectation value $\langle \phi|H|\phi\rangle$ of the Hamiltonian in the squeezed vacuum state $|\phi\rangle$. The Hartree or Gaussian approximation to the ground-state energy is then obtained by minimizing this expectation value with respect to the parameter t or, equivalently, ω . Equation (12) then readily yields the equation

$$\omega^3 - \omega - 6\lambda = 0, \quad (13)$$

which determines ω variationally in this Hartree approximation. Although there would appear to be three solutions to Eq. (13), the extra restriction $|t| < 1$ or, equivalently, that ω be real and positive, may readily be shown to yield a unique solution $\bar{\omega}$ for the parameter ω for a given coupling constant $\lambda > 0$. We recall that this restriction on the parameter t was necessary for the Bogoliubov transformation to be unitary and, equivalently, for the state $|\phi\rangle$ of Eq. (9) to be normalizable. With this Hartree solution $\omega \rightarrow \bar{\omega}$, the Hamiltonian of Eq. (10) takes the simple form

$$H = \frac{(3\bar{\omega}^2 + 1)}{8\bar{\omega}} + \bar{\omega} b^\dagger b + \frac{(\bar{\omega}^2 - 1)}{24\bar{\omega}} :(b + b^\dagger)^4:. \quad (14)$$

The effectiveness of the Hartree approximation for applications to anharmonic oscillators and related field-theoretic problems has been discussed by a number of authors.^{20-22,31,32} For the present purposes it is simply a starting point for our full CCM description of these systems.

Our next step is to apply the CCM to the Hamiltonian of Eq. (1), now written in the equivalent form of Eq. (14). To this end we start from the Hartree vacuum state $|\phi\rangle$ of Eq. (9) with the parameter t taking the corresponding value $\bar{t}$,

$$\bar{t} = (1 - \bar{\omega}) / (1 + \bar{\omega}), \quad (15)$$

and with $\bar{\omega}$ the real positive solution of Eq. (13). Just as the vacua $|0\rangle$ and $|\phi\rangle$ represent (generalized) coherent-state approximations to the exact ground state $|\psi\rangle$ of H ,

$$H|\psi\rangle = E|\psi\rangle, \quad (16)$$

the standard CCM *exact* representation of $|\psi\rangle$ takes the supercoherent form

$$|\psi\rangle = \exp(\hat{S})|\phi\rangle, \quad (17)$$

where the operator $\hat{S}$ is written in terms of the transformed canonical creation operator $b^\dagger$ as

$$\hat{S} = \sum_{n=1}^{\infty} S_n (b^\dagger)^n. \quad (18)$$

The exact ground-state wave function $|\psi\rangle$ is thus exactly determined by the set of c -number parameters $\{S_n, n=1, 2, \dots\}$. We note in particular that although the state $|\phi\rangle$ of Eq. (9) is normalized (in the physical case $|t| < 1$), the state $|\psi\rangle$ of Eq. (17) is *not* normalized, but obeys instead only the intermediate normalization relation $\langle \phi|\psi\rangle = \langle \phi|\phi\rangle = 1$. In particular, there is no explicit guarantee that the CCM state $|\psi\rangle$ of Eqs. (17) and (18) is normalizable. Finally, we stress again that the CCM parametrization can be performed for *any* choice of param-

eter t or, equivalently, ω . The simple Hartree variational choice $t \rightarrow \bar{t}$ is dictated purely by practical considerations of speed of convergence. It seems intuitively clear that such a "best" possible choice of $|\phi\rangle$ in the usual Rayleigh-Ritz sense is likely to make the size of the correlation amplitudes $\{S_n\}$ smaller, and hence the convergence of the resulting approximation scheme discussed below more rapid.

The ground-state Schrödinger equation (16) is now decomposed in the normal CCM way by first premultiplying with the operator $\exp(-\hat{S})$, and then projecting in turn onto the states $\langle\phi|$ and $\langle\phi|b^n$, with $n=1,2,\dots$. This procedure produces, respectively, an expression for the ground-state energy,

$$E = \langle\phi|He^{\hat{S}}|\phi\rangle \quad (19)$$

and an infinite coupled set of equations for the correlation coefficients $\{S_n\}$,

$$\langle\phi|b^n(e^{-\hat{S}}He^{\hat{S}})|\phi\rangle = 0, \quad n=1,2,\dots \quad (20)$$

Insertion of Eq. (14) into Eqs. (19) and (20) produces, respectively, the explicit result

$$E = \frac{(3\bar{\omega}^2 + 1)}{8\bar{\omega}} + \frac{(\bar{\omega}^2 - 1)}{2\bar{\omega}}(S_2^2 + 2S_4) \quad (21)$$

for the ground-state energy and the coupled set of equations

$$\begin{aligned} &\delta_{n,4} + (n+1)(n+2)(n+3)(n+4)S_{n+4} + 4n(n+1)(n+2)S_{n+2} + 6n[n-1+4\bar{\omega}^2/(\bar{\omega}^2-1)]S_n + 4(n-2)S_{n-2} \\ &+ \sum_{j,k} jk \{ [2(j-1)(j-2) + 3(j-1)(k-1) + 2(k-1)(k-2)]\delta_{j+k,n+4} + 6n\delta_{j+k,n+2} + 6\delta_{j+k,n} \} S_j S_k \\ &+ 2 \sum_{j,k,l} jkl [(n+1)\delta_{j+k+l,n+4} + 2\delta_{j+k+l,n+2}] S_j S_k S_l + \sum_{j,k,l,m} jklm \delta_{j+k+l+m,n+4} S_j S_k S_l S_m = 0 \quad (22) \end{aligned}$$

for the correlation coefficients $\{S_n\}$, where the index n runs over all positive integers as do the summations over the indices j, k, l , and m (and where $S_{-1} \equiv 0 \equiv S_0$ by definition).

It is clear from Eq. (22) that there is a solution in which all of the coefficients S_n with n odd are zero, although it is certainly not clear that this is the only possibility for the odd-indexed coefficients. However, from Eqs. (17) and (18), this solution clearly leads to a wave function $|\psi\rangle$ which is a parity eigenstate, as expected from the symmetric form of the Hamiltonian of Eq. (1). Although solutions which do not conserve parity may also, in principle, exist both for the exact (infinite) set of multinomial equations given by Eq. (22) and for their approximate truncated counterparts discussed below, we shall for present purposes constrain ourselves to approximations which conserve parity. Henceforth we shall therefore confine ourselves to considering solutions of Eq. (22) and its finite truncations in which all S_n with n odd are zero, and hence where the indices j, k, l, m , and n run over the even positive integers. We note that Eq. (22) is a special case of the more general Hamiltonian treated in Ref. 22 and it was first presented by Kaulfuss and Altenbokum.²¹

Once we have parametrized the ground-state wave function in the above CCM fashion, we can also generate the excited states $|\psi'\rangle$ and their corresponding eigenvalues E' ,

$$H|\psi'\rangle = E'|\psi'\rangle, \quad (23)$$

by making use of the Emrich parametrization²⁶

$$|\psi'\rangle = \hat{S}'|\psi\rangle = \hat{S}'e^{\hat{S}}|\phi\rangle, \quad (24)$$

where the operator $\hat{S}$ is the same ground-state correlation operator as appears in Eqs. (17) and (18), and the new excitation correlation operator $\hat{S}'$ has a similar decomposition,

$$\hat{S}' = \sum_{n=1}^{\infty} S'_n (b^\dagger)^n. \quad (25)$$

A simple combination of the ground- and excited-state Schrödinger equations, (16) and (23), respectively, readily yields the equation

$$[H, \hat{S}']|\psi\rangle = (E' - E)\hat{S}'|\psi\rangle, \quad (26)$$

from which the excitation energy may be directly obtained. The set of coefficients $\{S'_n, n=1,2,\dots\}$ is obtained similarly as its ground-state counterpart by projecting Eq. (26) onto the states $\langle\phi|b^n \exp(-\hat{S})$ to obtain the equations

$$(n!)^{-1} \langle\phi|b^n (e^{-\hat{S}}[H, \hat{S}']e^{\hat{S}})|\phi\rangle = (E' - E)S'_n, \quad n=1,2,\dots \quad (27)$$

One assumes that the ground-state coefficients $\{S_n\}$ are (fixed) input to Eq. (27) from the previously obtained solution to Eq. (22). The set of equations (27) then serves as a set of linear eigenvalue equations to determine both the excited-state coefficients $\{S'_n\}$ belonging to each excited state, and their corresponding excitation energies. The manifest similarity of the nested-commutator expansions for the two terms in parentheses in the matrix elements of Eqs. (20) and (27) then leads to an explicit set of coupled equations for the coefficients $\{S'_n\}$, and their corresponding excitation energies, which may rather simply be generated from their ground-state counterparts in Eq. (22). This general symmetry between the ground-state and excited-state CCM equations was first commented upon by Emrich²⁶ and in the present context it has been discussed more fully in Ref. 22.

Emrich himself has explicitly demonstrated²⁶ that the excited-state cluster operator $\hat{S}'$ is also a fully linked operator, just as in the case of its ground-state counterpart $\hat{S}$. Its diagrammatic expansion thus contains no

disconnected pieces. We also point out that from the explicit form of the matrix element in Eq. (27), involving the similarity transformation of the commutator of the Hamiltonian with $\hat{S}'$, it is clear that only linked terms are again generated by this excited-state formalism. Thus, if Eq. (27) is developed diagrammatically, the formal expansion contains no unlinked terms, in exactly the same way as is also true for the ground state by Eq. (20). Just as this linked-cluster property for the ground state was formulated deliberately within the ground-state CCM in order to give a size-extensive estimate for the ground-state energy eigenvalue E (i.e., one that scales properly with particle number N as $N \rightarrow \infty$), the Emrich formalism hence also gives a size-extensive estimate for the excitation energies. This feature is again of vital importance for applications to real many-body or field-theoretic systems.

We now consider the ground-state CCM equations (22) in more detail. An exact solution of this infinite set of coupled multinomial equations for the coefficients $\{S_i\}$ will produce the exact ground-state wave function $|\psi\rangle$ in its CCM parametrization of Eqs. (17) and (18), and its corresponding energy eigenvalue from Eq. (21). This solution for the set $\{S_i\}$ may then be inserted into the infinite linear eigenvalue problem of Eq. (27) to generate the exact set of excitation energies and corresponding excited-state wave functions. In order to implement this procedure in practice, it is clear that some approximation scheme is required. The standard ground-state CCM approximation technique is referred to as the $SUB(n)$ scheme, where n is the truncation index that labels the order of the approximation. It takes the simple form of truncating the otherwise infinite set of equations by imposing the condition that all of the coefficients S_i are set to zero for $i > n$, and with the remaining lowest n equations solved consistently. The corresponding excited-state scheme is denoted by $SUB(m, n)$, and similarly imposes the approximation that all of the coefficients S'_i with $i > m$ are set to zero, and the remaining lowest m linear eigenvalue equations are solved exactly, with the ground-state input coefficients $\{S_i\}$ taken from $SUB(n)$ approximation.

In the remainder of this paper we shall consider the solutions to the ground- and excited-state CCM equations for the quartic anharmonic oscillator in the $SUB(m, n)$ truncation scheme. There are, of course, also other approximation schemes that one could consider. The $SUB(m, n)$ scheme has the two advantages of simplicity and having been extensively tested and successfully used for a variety of many-body problems. Furthermore, where other more complicated schemes have been considered in the present context,²¹ they have not been demonstrated to have any particular advantages.

III. METHOD OF SOLUTION

The untruncated set of equations (22) will clearly produce the exact ground-state wave function and energy eigenvalue to the Hamiltonian of Eq. (14). However it is by no means apparent that this will be the unique solution to

these equations, since we have at no point explicitly imposed that our CCM-parametrized wave function be normalizable, and we know that this requirement is certainly necessary for bound-state solutions to the Schrödinger equation to be unique. Thus we are assured that there exists a unique normalizable ground-state wave function, and Eq. (22) will produce the unique CCM correlation coefficients associated with it via Eqs. (17) and (18). In addition we may postulate the existence of a (possibly infinite) number of unnormalizable solutions to Eq. (22), all belonging to the same exact ground-state energy eigenvalue. We emphasize that this lack of normalizability is of no direct concern when calculating the ground-state energy since the norm of the state $|\psi\rangle$ is not involved in the calculation of the energy. As we have seen, it is calculated instead via Eq. (19) or, equivalently and explicitly, via Eq. (21).

Furthermore, this situation carries over into the truncated version of the problem obtained in $SUB(n)$ approximation. Indeed it is not difficult to show that for *all* finite values $n > 2$ of the truncation index, and for $n=2$ if $|S_2| > \frac{1}{2}$, the truncated CCM wave function of the form of Eqs. (17) and (18) is not normalizable. Once again, this is of no concern in calculating the corresponding $SUB(n)$ approximation to the ground-state energy. Clearly we are by no means guaranteed *a priori* that any $SUB(n)$ approximation to either the exact normalizable wave function or any of its possible corresponding unnormalizable counterparts should give an accurate calculation of the energy eigenvalue. In particular, the convergence properties of the $SUB(n)$ scheme are far from being obvious. Indeed it was one of the purposes of our earlier paper²² to investigate the accuracy and convergence of the method. We showed that one particular solution, which was demonstrated for the quartic anharmonic oscillator to be identical to the thermodynamically stable solution of Kaulfuss and Altenbokum,²¹ and to approximate the physical (normalizable) solution, achieved extremely high accuracy for the energy eigenvalue at quite low values of the truncation index n . We shall demonstrate here that many of the other solutions that we find are also capable of giving results very close to the exact ones. It is clear that the coupled multinomial equations (22) are capable, in principle, of producing multiple solutions. Thus, if the n th equation in the hierarchy is considered as a polynomial in the variable S_n , one sees that the order of the equation is 3 for $n=2$, 2 for $n=4$, and 1 for $n \geq 6$. If we restrict ourselves to the solutions where each of the coefficients S_n is real, in keeping with what is expected of a normal bound-state solution, it is not possible to enumerate the number of different possible solutions to Eq. (22) at a given $SUB(N)$ level of approximation. However the total number of solutions certainly increases rapidly as a function of the truncation index N .

Faced with a multiplicity of solutions to the CCM equations (22) in a given $SUB(N)$ truncation, one reaction is to adopt some criterion to suppress all but a single solution. Kaulfuss and Altenbokum²¹ adopted this viewpoint, and went so far as to extend the CCM formalism described here for pure states to a temperature-dependent description for mixed states. In this way they

could perform a thermodynamic stability analysis on the various solutions and so select the unique solution which was stable against thermal fluctuations. We showed in an earlier paper²² that a very straightforward numerical procedure for finding a specific solution of the $SUB(N)$ -truncated CCM equations (22) leads to the same thermodynamically stable solution in all cases where comparison can be made. We describe this procedure more fully below.

An alternative and perhaps more straightforward approach to reducing the number of multiple solutions would be to extend the static CCM formalism considered here to its time-dependent counterpart. One may then perform the usual dynamical stability analysis by considering small perturbations away from each stationary solution. By linearizing the equation of motion around a stationary point we readily find the general feature of linear response theory that the excitation energies of the system may also be calculated as the eigenvalues of the resulting dynamical matrix. If the stationary state obtained from the ground-state calculation is dynamically stable, the associated dynamical matrix constructed from it will only have real eigenvalues. We do not consider this approach further here, but further details may be found in Refs. 27 and 29 in the wider context of the extended version of the CCM.

We view the truncated Eq. (22) as simply a set of N nonlinear algebraic equations in N real unknowns, where with no loss of generality for bound states we consider only real solutions for the coefficients $\{S_i\}$. A very efficient and robust method of solution for such problems is the hybrid Powell method,³³ which we henceforth refer to as method 1. As input this method requires some initial set of starting values. It then generates successive approximations by use of first derivatives (via the Jacobian) in its search for a solution. It is clear that different sets of initial starting values can lead to different solutions. Perhaps the simplest and most obvious choice of starting values is to set all $S_i = 0$. Indeed this choice produces, in all cases, the thermodynamically stable solution produced in Ref. 21 by the temperature-dependent CCM extension for the quartic anharmonic oscillator.

An alternative method of solution stems from viewing the n th equation in the CCM hierarchy (22) as a polynomial equation in the particular variable S_n itself, and with the remainder of the set of coefficients $\{S_k\}$ assumed known and fixed. In this way, each of the $SUB(N)$ -truncated polynomial equations can be solved sequentially, starting from the lowest ($n = 2$) equation.

Once some suitable set of initial values has been chosen this procedure may be iterated until convergence is achieved (assuming that the process *does* converge). We shall refer to this technique for solving the CCM equations (22) in $SUB(N)$ truncation as method 2. In addition to the previous ambiguity that can arise from the choice of initial values, we now have the extra ambiguity that arises from the possibility of multiple solutions to the nonlinear equations for the cases $n \leq 4$.

Just as in the previous case of method 1, we find that a very simple prescription to resolve these ambiguities leads to method 2 reproducing all of the thermodynamically

stable solutions of Ref. 21. Specifically, the algorithm that achieves this is to set all $S_i = 0$ for our starting values and, furthermore, to choose the real root of smallest absolute value whenever one of the polynomial equations produces multiple *real* solutions.

In practice, our preferred method of solution is actually a combination of methods 1 and 2. Thus we first perform one iteration of method 2 (initialized as above with all of the fixed coefficients S_i set to zero). The resultant set of approximate coefficients $\{S_i\}$ is made unique by choosing in each case the real root of smallest absolute value, and after this single iteration of method 2 this set is used as input to method 1, which is then iterated to convergence in the usual way. We have found that this procedure can, in practice, lead to a considerable acceleration of the convergence, as compared to using method 1 with the $\{S_i = 0\}$ initialization.

It is clear that one may also choose other roots that arise from the single iteration of method 2, and we have found that such alternative input choices for use in method 1 provide a rather effective technique for generating nonstandard solutions. At each iteration of method 2 there are in principle three possible solutions for the cubic equation for S_2 and two possible solutions for the quadratic equation in S_4 from the cases $n = 2$ and 4, respectively, of Eq. (22). The equations with $n > 4$ are all linear in the corresponding variable S_n . Thus we have 6 possible solutions (but not necessarily all real) for the set of coefficients $\{S_n\}$ from each iteration of method 2 in the case where only the solutions with $S_k \equiv 0$ for k odd are considered, as done here. In order to distinguish between those particular cases of the various possible solutions that we have found useful as initial values, we first introduce a new parameter R . In the two cases ($n = 2$ and 4) of Eq. (22) where each method 2 iteration may in principle lead to multiple real roots, we first number these real roots of each equation according to size, with the smallest root being labeled the first, etc. The parameter R is then a positive integer which determines the number of the real root in each of the truncated CCM equations (22), considered as a polynomial equation in the coefficient S_n for given index n , wherever such a choice may arise, namely, only for $n \leq 4$. If the index R is larger than the number of real roots obtained from a particular equation, we simply pick the largest. For example if the $n = 4$ equation produces the two real roots -2.1 and 0.5 for S_4 , and the parameter R is set to 2 or 3, the root 0.5 would be specified.

While a specification of the parameter R completely removes any ambiguity about the choice of roots, we still need to deal with the choice of initial values. We have already discussed the possibility of initializing each of the coefficients $\{S_i\}$ to zero, as in the case of the standard solution. Another possibility is to use as initial values the output from a different solution or a different $SUB(n)$ approximation. We have made use of both such choices and in order to specify completely a particular method of solution, we introduce the following notation. Each solution is denoted in the first place by $S_R^n : I$ where n now denotes the truncation index of the $SUB(n)$ approxima-

tion, R denotes the parameter which indicates the choice of roots in our initial method 2 iteration, and the index I denotes how the parameters $\{S_i\}$ are initialized. (We assume in this notation that the Hamiltonian is held fixed and specified separately.) We shall use the special notation $R \rightarrow S$ to denote the choice of roots in the "standard" case, namely, where any ambiguity after the initial method 2 iteration is resolved by choosing that root for each coefficient S_i which is smallest in absolute value (and not in actual size, as would correspond to the case $R=1$). Thus one way of denoting the standard solution in $SUB(n)$ approximation is $S_5^n:0$, where the index $I=0$ indicates a starting value of zero for each of the coefficients $\{S_n\}$.

We note that the above notation is not unique, since there exist in principle many other routes to obtaining a given solution. For example, the usual way of obtaining a $SUB(n)$ solution is to use as the starting values the output of a $SUB(n-1)$ calculation, since this is a speedy practical route to convergence. Thus, the standard $SUB(6)$ solution may be found via the $S_5^6:0$ procedure, but it may also be obtained using the output of the $SUB(4)$ calculation denoted by $S_5^4:0$ as initial values. We would denote this latter procedure to obtain the standard $SUB(6)$ solution as $S_5^6:S_5^4:0$. Similarly, the standard $SUB(8)$ solution may be generated via the procedure denoted as $S_5^8:S_5^6:S_5^4:0$ or, more compactly, as $S_5^8::S_5^4:0$, where the double colon notation denotes that we have simply incremented the n index from $n=4$ one step at a time (through the corresponding even values) with no change in the corresponding index R in each case.

We conclude this section with a few more examples. One class of nonstandard solutions that we have studied is generated via the procedure denoted by $S_1^n:0$. Thus in this case we first initialize all coefficients S_i to zero and then perform an initial method 2 iteration from which the smallest (in size, not in absolute magnitude) root in each case is chosen. This set of parameters $\{S_i\}$ is then used as initial-value data for method 1. A broader class of nonstandard solutions has also been obtained by using a specific case of the previous nonstandard solution as the initial values. Specifically, we have investigated the solutions obtained first by the procedure denoted as $S_2^4:S_1^4:0$, where in the $SUB(4)$ approximation the final ($R=2$) solution is obtained by using the above $S_1^4:0$ solution as initial values to our by now familiar practical method. Similarly we may generate a family of such solutions at different $SUB(n)$ levels of truncation via the procedures denoted by $S_2^6:S_2^4:S_1^4:0$, etc., and where the solutions with higher truncation index n in this series are compactly denoted as $S_2^n::S_2^4:S_1^4:0$.

It is clear that the above notation for distinguishing the nonstandard solutions is by no means the most general. However, it is not the intention of the present paper to give an exhaustive list of all possible solutions. Rather, we wish to demonstrate that the alternative solutions to the CCM equations, which are usually either not discussed at all, or are discarded, can be of interest in their own right. In this spirit, the limited notation introduced above for the nonstandard solutions is quite adequate.

IV. RESULTS

In this section we present results for various solutions to the CCM equations (22) for the quartic anharmonic oscillator, as well as a brief discussion of more general anharmonicities. In Table I we define shorthand notations for the several nonstandard solutions which we consider since the full notation is somewhat cumbersome.

In the following discussion we will frequently refer to a particular solution ranging over various $SUB(n)$ truncations and different values of the perturbation parameter(s). In fact, this is quite a reasonable approach to take for the standard solution, at least for the quartic anharmonic oscillator of Eq. (1), since small changes in the perturbation parameter λ and incremental changes in the truncation index n produce quite gradual changes in the solution $\{S_i\}$ and in the resultant ground-state energy. This is not, however, always the case for the nonstandard solutions, and for these it is perhaps best to interpret a particular solution as meaning a particular prescription for obtaining this solution.

A few words should be said concerning the nonstandard solution denoted $N_R(n)$ in Table I. This solution, first discussed in Ref. 22, was obtained there by a somewhat *ad hoc* procedure, and it has not proven possible to give a *general* prescription for obtaining it in terms of the somewhat limited notation defined in the previous section. Nevertheless, for certain values of the truncation index n and perturbation parameter λ a well-defined procedure can be given. For example, for $\lambda=0.1$ and $n=18$, it can be generated via $S_2^{18}::S_1^{22}::S_1^{12}:0$. In general, however, it is generated by starting at some known example of it (for example, the original solution discussed in Ref. 23, which is for $\lambda=0.1$ and $n=18$), and then either slowly varying λ or incrementally changing n to the desired value. This procedure will generate a slowly varying solution for $18 \leq n \leq 24$ and for $\lambda \leq 2$. Outside these ranges either no solution can be found or it degenerates to some other solution.

In Table II we display results for the ground-state energy of the quartic anharmonic oscillator with $\lambda=10$ for various solutions to the CCM equations (22) and over a range of the truncation index n . The standard solution shows the typical behavior found in Ref. 22, namely, very rapid initial convergence followed by a slow oscillatory approach to the correct energy. In contrast, the solutions $N_1(n)$ and $N_2(n,8)$ show behavior typical of many nonstandard solutions, namely, while not producing energies

TABLE I. Definitions of various solutions of the CCM equations for the anharmonic oscillator with the notation described in the text.

Shorthand	Full notation	Remarks
S	$S_5^n:0$	standard solution
$N_1(n)$	$S_1^n:0$	
$N_2(n,m)$	$S_1^n::S_1^m:0$	$n \geq m$
$N_3(n,m)$	$S_2^n::S_1^m:0$	$n \geq m$
$N_R(n)$		nonstandard solution from Ref. 22

TABLE II. Various nonstandard solutions along with the standard results for the quartic anharmonic oscillator with $\lambda=10$. The exact ground-state energy value is 1.504 97.

n	Standard	$N_1(n)$	$N_2(n, 8)$	$N_3(n, 8)$
2	1.531 25			
4	1.508 03	1.508 03		
6	1.504 83	1.504 83		
8	1.504 65	1.290 52	1.290 52	1.290 52
10	1.504 82	1.420 26	1.420 26	1.420 26
12	1.504 94	a	1.495 25	1.495 25
14	1.505 00	1.258 87	1.467 75	1.514 34
16	1.505 02	1.384 32	1.384 32	1.514 01
18	1.505 02	a	1.473 56	1.510 31
20	1.504 99	1.262 49	1.427 15	1.507 57
22	1.504 94	1.367 16	1.367 16	1.506 07

^aNo solution can be found.

which are grossly inaccurate, they show no clear signs of convergence as the truncation index n is increased, to the extent that talking about a particular solution ranging over various truncation index values is really quite dubious and as discussed above, one should really consider the definitions given for these solutions simply as prescriptions for finding them for any given set of parameters n and λ . The remaining nonstandard solution $N_3(n, 8)$ is, however, clearly different. While being identical to $N_2(n, 8)$ for $n \leq 12$, for $n \geq 12$ it produces a well-behaved and convergent ground-state energy. By $n=22$, in fact, we find a percentage error for the ground-state energy of 0.07%, which, while larger in magnitude than the -0.002% error for the standard solution, is still quite small.

This solution is looked at more closely in Tables III and IV, where it is displayed along with the standard solution and with the solution $N_R(n)$ for $18 \leq n \leq 24$ and for $\lambda=0.1$ and 2, respectively. There are two points to note from these tables. The first is that one can obtain quite similar (and accurate) energies with very dissimilar solutions for the parameters $\{S_i\}$. There are a number of reasons for this behavior. Firstly, one can see from Eq. (21) that the CCM ground-state energy only depends explicitly on S_2 and S_4 . Thus, for example, for $\lambda=0.1$ and $n=18$, S_{18} can differ by six or seven orders of magnitude between the standard and nonstandard solutions, and yet the energies produced by these solutions are very nearly the same. Secondly, one can see from Eq. (21) that the energy actually only depends on S_4 and S_2^2 , i.e., the sign of S_2 is irrelevant. The effect of this can be seen in the $SUB(18)$ results for $\lambda=0.1$, where the S_2 value for $N_R(18)$ is nearly equal to $-S_2$ for the standard solution, and so the energies are very close. The final cause for this ability to obtain similar energies with dissimilar $\{S_i\}$ solutions is that the energy is not terribly sensitive to changes in S_2 and S_4 , since a large part of the ground-state energy will generally come from the S_i -independent piece of Eq. (21), which is just the Hartree approximation to the energy. Since this approximation is quite accurate here, any solution to the CCM equation whose S_2 and S_4 values do not

TABLE III. Various solutions for the CCM equations for the quartic anharmonic oscillator with $\lambda=0.1$ for four values of the truncation index N . The last two rows are the corresponding ground-state energy values and percentage errors, respectively, with the exact value being 0.559 15.

i	S	$SUB(18)$ $N_R(18)$	$N_3(18, 8)$	S	$SUB(20)$ $N_R(20)$	$N_3(20, 8)$	S	$SUB(22)$ $N_R(22)$	$N_3(22, 8)$	S	$SUB(24)$ $N_R(24)$	$N_3(24, 8)$
2	1.60×10^{-3}	-1.75×10^{-3}	-4.02×10^{-2}	1.60×10^{-3}	5.20×10^{-4}	-4.26×10^{-2}	1.60×10^{-3}	1.18×10^{-3}	-3.06×10^{-2}	1.60×10^{-3}	1.35×10^{-3}	-1.62×10^{-2}
4	-2.89×10^{-3}	-2.45×10^{-3}	-5.92×10^{-2}	-2.89×10^{-3}	-2.37×10^{-3}	-3.14×10^{-2}	-2.89×10^{-3}	-2.95×10^{-3}	-1.14×10^{-2}	-2.89×10^{-3}	-2.84×10^{-3}	-3.47×10^{-3}
6	7.41×10^{-5}	1.42×10^{-3}	3.09×10^{-2}	7.41×10^{-5}	4.05×10^{-4}	2.56×10^{-2}	7.41×10^{-5}	2.74×10^{-4}	1.60×10^{-2}	7.41×10^{-5}	1.72×10^{-4}	7.95×10^{-3}
8	-2.65×10^{-6}	-4.64×10^{-4}	2.29×10^{-3}	-2.65×10^{-6}	-2.04×10^{-4}	-8.40×10^{-4}	-2.65×10^{-6}	-4.47×10^{-5}	-2.33×10^{-3}	-2.65×10^{-6}	-3.91×10^{-5}	-1.96×10^{-3}
10	1.09×10^{-7}	-3.96×10^{-5}	-2.66×10^{-3}	1.09×10^{-7}	1.26×10^{-5}	-2.04×10^{-3}	1.09×10^{-7}	-1.25×10^{-5}	-1.12×10^{-3}	1.09×10^{-7}	-2.00×10^{-6}	-4.16×10^{-4}
12	-4.90×10^{-9}	4.12×10^{-5}	3.54×10^{-4}	-4.86×10^{-9}	1.15×10^{-5}	2.72×10^{-4}	-4.85×10^{-9}	5.88×10^{-6}	2.85×10^{-4}	-4.85×10^{-9}	3.09×10^{-6}	1.99×10^{-4}
14	2.32×10^{-10}	-6.12×10^{-6}	-1.99×10^{-4}	2.29×10^{-10}	-2.91×10^{-6}	-4.00×10^{-5}	2.26×10^{-10}	-6.13×10^{-7}	6.44×10^{-8}	2.25×10^{-10}	-5.36×10^{-7}	-1.17×10^{-5}
16	-1.08×10^{-11}	-2.15×10^{-7}	8.84×10^{-5}	-1.12×10^{-11}	1.40×10^{-7}	4.81×10^{-5}	-1.10×10^{-11}	-8.01×10^{-8}	9.66×10^{-6}	-1.08×10^{-11}	-3.65×10^{-9}	-1.23×10^{-6}
18	3.58×10^{-13}	1.19×10^{-7}	-8.08×10^{-6}	5.22×10^{-13}	4.45×10^{-8}	-9.08×10^{-6}	5.57×10^{-13}	2.75×10^{-8}	-5.99×10^{-6}	5.47×10^{-13}	1.35×10^{-8}	-1.39×10^{-6}
20				-1.67×10^{-14}	-6.97×10^{-9}	-9.88×10^{-7}	-2.57×10^{-14}	-2.75×10^{-9}	7.10×10^{-7}	-2.81×10^{-14}	-1.94×10^{-9}	3.39×10^{-7}
22							7.88×10^{-16}	7.50×10^{-11}	2.75×10^{-7}	1.28×10^{-15}	8.76×10^{-11}	6.92×10^{-8}
24									-3.76×10^{-17}		3.79×10^{-12}	-2.66×10^{-8}
	0.559 15	0.559 32	0.536 83	0.559 15	0.559 35	0.548 04	0.559 15	0.559 12	0.555 89	0.559 15	0.559 16	0.558 96
	-5.5×10^{-7}	0.032	-3.99	-5.7×10^{-7}	0.037	-1.99	-5.4×10^{-7}	-0.005	-0.582	-5.1×10^{-7}	0.003	-0.033

TABLE V. Various energies calculated via the ground- and excited-state CCM equations for the quartic anharmonic oscillator over a range of the perturbation parameter λ calculated in the *SUB*(22) and *SUB*(22,22) approximations, with percentage errors displayed beneath the energy values. The solutions shown are the standard method (marked *S*), N_R (22), and N_3 (22,8).

λ	Solution	E_0	E_1	E_2	E_3	E_4
0.1	Exact	0.559 15	1.769 50	3.138 62	4.628 88	6.220 30
	<i>S</i>	0.559 15	1.769 50	3.138 62	4.628 88	6.220 26
		-5.4×10^{-7}	2.7×10^{-6}	6.7×10^{-6}	-1.5×10^{-4}	-5.6×10^{-4}
	N_R	0.559 12	1.767 10	3.130 39	4.710 94	6.443 90
		-0.005	-0.14	-0.26	1.77	3.59
	N_3	0.555 89	1.813 57	3.152 81	4.982 46	7.143 43
		-0.58	2.49	0.45	7.64	14.84
1.0	Exact	0.803 77	2.737 89	5.179 29	7.942 40	10.963 6
	<i>S</i>	0.803 77	2.737 76	5.176 65	7.942 92	11.061 12
		-2.4×10^{-4}	-0.005	-0.005	0.007	0.89
	N_R	0.804 09	2.736 35	5.155 29	7.893 01	11.143 0
		0.04	-0.05	-0.46	-0.62	1.64
	N_3	0.804 09	2.736 35	5.155 29	7.893 01	11.143 0
		0.04	-0.05	-0.41	-0.62	1.64
2.0	Exact	0.951 57	3.292 87	6.303 88	9.727 32	13.481 3
	<i>S</i>	0.951 56	3.292 33	6.293 95	9.740 54	13.967 0
		-0.001	-0.02	-0.16	0.14	3.60
	N_R	0.951 88	3.284 56	6.256 04	9.687 07	13.800 3
		0.03	-0.25	-0.76	-0.41	2.37
	N_3	0.951 96	3.289 41	6.325 11	10.552 28	14.361 9
		0.04	-0.10	0.34	8.48	6.53
10	Exact	1.504 97	5.321 61	10.347 1	16.090 1	22.408 8
	<i>S</i>	1.504 94	5.317 57	10.260 76	16.230 6	23.787 8 ^a
		-0.002	-0.08	-0.83	0.87	6.15
	N_3	1.506 07	5.322 95	10.398 4	16.394 3	22.733 5
		0.07	0.02	0.50	1.89	1.45
100	Exact	3.131 38	11.187 2	21.906 9	34.182 5	47.707 2
	<i>S</i>	3.131 25	11.169 7	21.526 8	34.791 3	44.983 0 ^a
		-0.004	-0.16	-1.73	1.78	-5.71
	N_3	3.134 05	11.196 1	22.015 4	34.243 0	47.591 5
		0.08	0.08	0.49	0.18	-0.24
1000	Exact	6.694 22	23.972 2	47.017 3	73.419 1	102.51 6
	<i>S</i>	6.693 89	23.928 4	46.091 3	74.923 7	94.993 ^a
		-0.005	-0.18	-1.97	2.05	-7.34
	N_3	6.700 09	23.994 2	47.245 7	73.261 9	101.89 2
		0.09	0.09	0.49	-0.21	-0.61

^aEnergy has an imaginary component (not shown).

method, this might be a source of concern. Our point here, however, is that these nonstandard solutions give rise to excitation spectra which do contain accurate approximations to the actual energy levels.

We have also done some work on more complicated anharmonic oscillators. In general, if one is working with a system which does not naturally allow one to set all of the odd-indexed parameters S_i to zero, then the limited scheme we have used to produce nonstandard solutions is not very successful, in the sense that, while nonstandard solutions are found, they do not behave well, as do the solutions $N_3(n, 8)$ and $N_R(n)$ for the quartic anharmonic oscillator, but instead behave somewhat chaotically, as do the solutions $N_1(n)$ and $N_2(n, 8)$ for this system. Another oscillator for which we have found well-behaved nonstandard solutions is the positive-definite double-well Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}(x^2 - \frac{1}{2}Z^2)^2. \quad (28)$$

As discussed in Ref. 22, if one builds upon a Hartree wave function centered around $x=0$, then one again finds that all the odd-indexed parameters S_i can be naturally set equal to zero. For $Z^2 \leq 2$, corresponding to very shallow wells, one finds that both the centered Hartree approximation and the CCM built upon it produce reasonable approximations to the ground state, and for the latter, excitation energies. It is for this case that we can also find well-behaved nonstandard solutions. For example, for $Z^2 = \frac{1}{2}$, we find percentage errors for the ground state energy of -6.5 , -1.4 , and 0.45 for truncation indices of 10, 12, and 14, respectively, from the $N_3(n, 10)$ solution. The standard solution produces an error of 0.004% for the corresponding *SUB*(14) standard solution.

V. DISCUSSION

One of the main aims of the present work has been to continue and extend the earlier work^{22,23} involving the application of the CCM to anharmonic oscillators. Our overall motivation has been that since the CCM has proved to be such a powerful and highly successful tool when applied to a wide variety of many-body systems, it seems timely and worthwhile to subject the method itself to closer scrutiny. In this light we have been particularly interested in an examination of the convergence properties of the method within the standard $SUB(n)$ and $SUB(m,n)$ truncation schemes for the ground-state energy and excitation energies, respectively. These schemes have been widely applied to various condensed matter systems, and it is of considerable interest to enquire about their range of validity, their convergence properties, their possible future extension, and whether there are any indications that they might need to be modified or abandoned altogether in certain circumstances.

It is manifestly clear that while the CCM provides a formally exact cluster decomposition of the N -body Schrödinger equation for both the ground and excited states, in each case there results an N -fold hierarchy of coupled equations, which are nonlinear in the ground-state amplitudes and linear in those for the excited states. Such systems cannot be exactly solved except for a few trivial applications, and some approximation scheme will essentially always be required in practice. The systematics of if and how such schemes converge to the otherwise exact results of the untruncated equations is therefore of considerable practical as well as theoretical interest. We have demonstrated previously²² that the broad class of anharmonic quantum oscillators is particularly well suited for the study of the convergence systematics for two main reasons. On the one hand, such one-body problems are well known to be extremely challenging for any calculational scheme ultimately rooted in perturbation theory. On the other hand, they are sufficiently simple to permit approximate solutions of the CCM equations to be obtained up to very high orders in the indices that characterize their level of truncation.

The ground-state CCM equations are intrinsically nonlinear in the cluster correlation amplitudes that completely characterize a given physical system. The basic underlying reasons for this nonlinearity lie at the heart of its successful applicability to many-body systems and are by now very well understood.⁴ Thus this nonlinearity is not only to be expected but also is positively desired for such applications. Nevertheless, such nonlinear coupled sets of equations as those in Eq. (22) will almost inevitably have multiple solutions at all levels of truncation, and perhaps also for the exact (untruncated) sets. One then has as a matter of principle to choose between the various solutions obtained from a given level of approximation.

This problem has received surprisingly little discussion in view of the very wide and successful use that the CCM enjoys. It was first addressed by Kaulfuss and Altenbokum²¹ in the context of applications to anharmonic oscillators. These authors adopted the viewpoint that at each order of approximation only one solution is physically meaningful. They used a temperature-dependent

extension of the zero-temperature ground-state CCM considered here to perform a thermodynamic stability analysis on the multiple solutions. In this way they were able to choose a single solution in an unambiguous fashion, and to discard the remainder.

Our own viewpoint has been quite different. In earlier work²² we took a more direct approach, as discussed in the previous section. By remaining with the usual zero-temperature (pure-state) version of CCM, we devised a straightforward and simple prescription for generating in all cases the thermodynamically stable solutions obtained by Kaulfuss and Altenbokum for the single-well quartic anharmonic oscillator. We further applied this prescription to the solution of the (truncated) CCM equations for a much broader class of anharmonic wells. In almost all cases we obtained approximate solutions which gave highly accurate estimates for the ground-state energy and which varied slowly both as a function of the coupling strengths and with the truncation index. Furthermore, these solutions also produced an accurate and stable excitation spectrum when used as input to the excited-state CCM formalism. The only observed weakness of the method was in the case of an anharmonic oscillator with a deep double well, where the standard CCM could not easily and accurately resolve the nearly degenerate energy-level doublets, due to its inability to incorporate any aspect of tunneling at the level of the zeroth-order or model wave function.

We also presented in Ref. 22 a single example of a solution to the ground-state (truncated) CCM equations, which differed from the standard one. The cluster amplitudes that characterized the two solutions were radically different from each other, even varying by many orders of magnitude for the higher-order amplitudes. Although it is perhaps not surprising at first glance that various solutions may differ widely, since the possibility must exist that the nonstandard solutions are simply spurious and unphysical, nevertheless this nonstandard set of cluster amplitudes also produced a very accurate estimate for the ground-state energy eigenvalue. The further work reported in this paper has shown that there exists in general a plethora of solutions to the ground-state CCM equations which differ widely from each other and yet many of which give very close and accurate estimates for the corresponding energy.

It is of interest to inquire into the possible mechanisms for producing such sets of multiple solutions. Mathematically, the situation seems clear. Thus, we have a complicated nonlinear set of coupled multinomial equations, the number of distinct solutions of which grows rapidly and without bound as the truncation index (and hence the number of equations) is increased. Since we restrict ourselves to real solutions $\{S_i\}$, it is not possible, however, to specify the number of such solutions in a given $SUB(n)$ approximation. From the physical viewpoint we are more used either to obtaining a unique solution to the underlying linear Schrödinger eigenvalue problem or to discarding any extra solutions as spurious and unphysical artifacts of the approximations used.

Nevertheless, other more subtle mechanisms arising from the detailed workings of the CCM may also exist to

provide the explanation for these multiple solutions. In the first place we recall that the basic CCM parametrization of Eq. (17) of the exact ground state $|\psi\rangle = \exp(\hat{S})|\phi\rangle$ is given in terms of a correlation operator $\hat{S}$ and a rather general model wave function $|\phi\rangle$. However, a hidden assumption behind the statement that this is an exact parametrization in terms of a correlation operator constructed as in Eq. (18) is that the overlap $\langle\phi|\psi\rangle$ should be nonzero. In principle, this so-called ground-state CCM formalism can produce as a solution *any* exact eigenfunction of the Hamiltonian whose overlap with the model state $|\phi\rangle$ is nonzero. The main reason why one usually expects the formalism to produce the actual ground-state wave function is simply that the starting wave function $|\phi\rangle$ is normally chosen to resemble our preconceived notions of the important attributes or symmetry properties of the exact ground state. On the other hand, one might anticipate the existence of nonstandard solutions to the truncated CCM equations which approximate *excited* states rather than the ground state.

As we have previously mentioned, a second possibility arises from the fact that the CCM does not explicitly impose the requirement that the wave functions $|\psi\rangle$ or their approximate truncated representations should be normalizable. Indeed, we have already observed that their $SUB(n)$ truncations are manifestly of infinite norm for all $n > 2$. Since it is well known that the imposition of normalizability for the bound states is necessary to obtain a unique discrete spectrum in the usual formulation of boundary conditions for the linear eigenvalue problem of the Schrödinger equation, the absence of its explicit imposition in the CCM raises the possibility of obtaining nonunique solutions. One might even imagine that in the exact implementation of the CCM or its n th-order $SUB(n)$ approximation as $n \rightarrow \infty$, the method could produce an infinite number of solutions whose CCM decompositions are very different, yet all of which produce the same *exact* energy eigenvalue when calculated as $E = \langle\phi|H|\psi\rangle$. In the same spirit, one might also then expect a finite number of distinct approximate solutions at a finite level of $SUB(n)$ truncation, each of which could approximate a different wave function in the $n \rightarrow \infty$ limit. We reiterate the important point that even though the $SUB(n)$ truncated wave functions have infinite norm, this does not enter into the calculation of the energy eigenvalue by the method of Eq. (19), as may be immediately seen from its explicit evaluation for the quartic anharmonic oscillator in Eq. (21).

In spite of the above discussion, it is still possible that the occurrence of multiple solutions is simply an artifact of the truncation scheme used to produce them. Thus it is still quite conceivable that the various solutions to the ground-state equations at a given $SUB(n)$ level of truncation all converge to the same normalizable solution in the $n \rightarrow \infty$ limit. Even in this case, the fact that widely different solutions obtained from the same truncated set of equations can yield such very close and accurate estimates of the energy would remain a remarkable feature of the method. It is, of course, also possible that more than one of the above causes and/or others act together. Finally, we remark that the question of the convergence of

the CCM solutions should also address the detailed behavior of the various solutions as the truncation index $n \rightarrow \infty$, particularly whether and in what senses this limit exists, and, if it does, in what sense is the limiting wave function equal to the exact state $|\psi\rangle$.

We turn now to the data presented in Sec. IV to see how far they support any of the above mechanisms. In the first place it is clear that all of the ground-state approximation solutions presented here give energies which are close to the corresponding exact ground-state energies, and most are *very* close. Even the nonstandard solutions $N_1(n)$ and $N_2(n,8)$ shown in Table II, which display the poorest convergence characteristics with increasing truncation index n , show errors of about 15% in the worst cases. Thus it is not possible to dismiss any of the solutions lightly as being spurious. Equally, it is clear that there is no indication at all for any of our solutions to be an approximation to any state other than the ground state.

Whereas the two sequences of nonstandard solutions $N_1(n)$ and $N_2(n,8)$ seem to produce only fair estimates of the ground-state energy, the other two nonstandard solutions $N_3(n,8)$ and $N_R(n)$ which we have examined more closely clearly yield rather good comparable estimates. This close agreement is achieved in spite of the fact that their corresponding cluster coefficients $\{S_i\}$ are usually very different both from each other and from their counterparts for the comparable standard solution. A particularly striking example is observed in Table III where the coefficients S_{24} in the standard and $N_3(24,8)$ solutions in $SUB(24)$ approximation differ by nine orders of magnitude. It would also appear that the three solutions displayed in Table III are unlikely to converge to a common solution at the $SUB(\infty)$ limit. One is certainly tempted to assert that they represent approximations to different solutions with identical energy eigenvalues in this limit, and that it is therefore the lack of normalizability which has produced the nonuniqueness.

On the other hand, the data in table IV seem to indicate that both the $N_R(n)$ and $N_3(n,8)$ solutions are approaching the standard solution as n increases. In this case one is tempted to suggest that we see here an example of three solutions which will converge towards the common exact, and hence normalizable, ground state as $n \rightarrow \infty$. Their differences at finite truncations would thus be attributable to the approximation scheme itself, although *why* such multiple copies of the same solution should exist is far from clear.

All of the data presented support the notion that the multiple solutions to the ground-state CCM equations are neither spurious nor uninteresting. We regard their existence and properties as additional positive features that indicate the richness of the method rather than technical problems that need to be overcome. On one hand it is possible with a very simple and practical method of solution to find one particular solution for a very broad class of anharmonic oscillators which is everywhere well behaved and which we have termed our standard solution. That this seems also to be the thermodynamically stable solution is gratifying. It yields results of very high

precision even in relatively low orders of truncation. On the other hand, we also observe the possibility of a plethora of other solutions which provide alternative descriptions of the ground-state wave function, but which also yield accurate estimates for the energy eigenvalue when calculated via the CCM prescription of Eq. (19).

Rather than treating these additional solutions as curiosities, we feel that they deserve more serious consideration both for a thorough understanding of the method, and in particular its convergence properties, and for possible practical applications. For example, there are many situations of physical interest where one would regard a calculational technique which permits alternative descriptions of the system as being of real value. For many-body systems this typically arises for values of the interaction parameters or such external parameters as the density, where the system is close to undergoing a phase (or shape) transition. In such cases, two quite different wave functions are generally competing for dominance in terms of minimizing the energy. In principle, the flexibility of the CCM should suffice to allow for such distinct descriptions of the system within a given calculational framework based upon a *single* model wave function or zeroth-order description. Indeed, this ability of the CCM to deal with phase transitions has already been demonstrated. A rather general discussion has been given elsewhere by one of the present authors.³⁴ More specifically, in the case of infinite nuclear matter, for example, it has been shown³⁵ how the existence of such clustered phases at low densities as deuteron and other paired-nucleon condensates, or α -particle matter, are automatically described within the CCM based upon a single Slater determinant of noninteracting nucleons for the model state, in terms of "deexcited" states (i.e., states of negative excitation energy) that arise from the (so-called) excited-state version of CCM as described in Sec. II. For such simpler spin-algebraic models as the Lipkin model,³⁶ which is used to model the shape transition in atomic nuclei from spherical to deformed configurations, the ability of the CCM (at least in its extended version²⁷) to describe both branches of this transition with a single reference starting wave function has also been well documented.³⁷

It is perhaps worth pointing out that although the so-called ground-state and excited-state CCM formalisms described in Sec. II generally do produce, in their $SUB(n)$ truncations, approximations to the actual ground and excited states, this is by no means always the case, as we have already pointed out above with regard to the case where the model state $|\phi\rangle$ is for some reason an inappropriate choice for the actual ground state. One common such example is where the ground state of a given phase of the system has some broken symmetry properties which are preserved by $|\phi\rangle$. Furthermore it is quite possible in principle for the so-called ground state CCM to produce excited states either in addition to or instead of the actual ground state. One should note in this context that the only constraint placed by the ground-state formalism on any exact eigenstate $|\psi\rangle$ produced by it is that it has nonzero overlap with the model state $|\phi\rangle$. In fact, the intermediate normalization scheme actually specifies this overlap, $\langle\phi|\psi\rangle=1$. Conversely, the

excited-state CCM formalism of Emrich is designed to calculate those exact states with a zero overlap, $\langle\phi|\psi\rangle=0$.

In principle, the well-known Hubbard-Coester result^{1,2} that the cluster operator $\hat{S}$ of the ground-state CCM formalism is a linked operator extends readily to excited states also. For each such excited state the model wave function $|\phi\rangle$ may be taken as an excited model state (e.g., a Slater determinant formed from core and valence orbitals for a realistic many-fermion problem), and the creation and destruction operators may be redefined in terms of this new state. This particular approach has been shown to be applicable to certain excited states of relatively simple molecules of interest in quantum chemistry^{38,39} when used with a clearly defined reference function, and implemented to convergence at such a relatively low level of truncation as $SUB(2)$. As expected theoretically,³⁸ this has been shown to be possible in practice for a molecule like LiH³⁹ when an excited state has both a clearly defined principal model state as a single Slater determinant and is well approximated by the one- and two-body correlations constructed on top of this by the $SUB(2)$ approximation. The stability of this single model-state or "closed-shell" CCM scheme for excited states is rather closely tied to the size of the contribution of the principal determinant to the correlated wave function. Under the right conditions, convergence can occur even to states of quite high excitation energy.³⁹ Nevertheless, its general applicability to many-body or field-theoretic systems is hedged around by questions connected with the strong implicit assumption of adiabaticity in the development of the excited states as one formally "switches on" the interaction terms.

As we have seen above, the Emrich parametrization of Sec. II is not the only possible parametrization of the excited states. For such few-body problems as occur in quantum chemistry and nuclear physics, for example, various formulations of the open-shell or degenerate version of perturbation theory have also been suggested and applied.⁴⁰ Such open-shell schemes typically again utilize a full exponential operator acting on a multireference uncorrelated state constructed from a suitable subspace of Slater determinants of single-particle orbitals. Such open-shell CCM schemes in principle yield as many eigenstates and eigenvalues at any level of implementation as the dimensionality of the subspace. The theoretical basis of the method lies in the fact that the degenerate version of perturbation theory also leads to definite linked-cluster or exponential structures. They differ from their ground-state counterparts mainly by the appearance of the so-called folded diagrams.⁴¹ It is quite possible that the nonuniqueness discovered here in the closed-shell or single-reference ground-state CCM formalism will also be seen in the open-shell or multireference scheme. In the present paper we have focused attention for the excited states on the Emrich formulation, since the division of the single-particle orbitals into core, valence, and particle states which typifies the open-shell formulation is rather unnatural for most field-theoretic applications on which we wish to focus present attention.

A final reason for investigating the properties of the

CCM solutions in the $SUB(n)$ truncation scheme is their connection with the problem of supercoherent states in quantum optics and allied fields. Thus the CCM wave functions of Eqs. (17) and (18) when truncated at the $SUB(1)$ or $SUB(2)$ level (with $|S_2| < \frac{1}{2}$) are just the usual single-photon Glauber coherent states and the two-photon squeezed coherent states, respectively, in terms of a single photon mode created by the operator $b^\dagger$ with respect to a vacuum $|\phi\rangle$. For these two cases, the CCM truncated wave functions can also be represented as a unitary (displacement or squeezing), and hence norm-preserving, operator acting on the state $|\phi\rangle$. Conversely, for all $SUB(n)$ truncations with $n > 2$ [or for $SUB(2)$ with $|S_2| > \frac{1}{2}$] our CCM wave functions are clearly supercoherent generalizations of the previous states, but since they are not normalizable they cannot be defined in terms of a comparable unitary transformation with respect to the vacuum.

The impossibility of naively generalizing the squeezed ($n=2$) two-photon coherent state to *normalizable* multiphoton ($n > 2$) coherent states has been pointed out elsewhere,⁴² and much effort has gone into alternative attempts to construct them. Within the CCM we have dropped the requirement of normalizability, and yet we

still have a methodology in which the quantities of physical interest are well defined and finite. The seeming price that we have paid is the loss of uniqueness of the wave function. However, in view of our earlier discussion, at worst this problem seems capable of simple elimination. At best, the multiplicity of solutions may allow a useful and powerful extra flexibility.

In conclusion, it is clear that the method has features which impinge upon a number of areas of considerable theoretical and practical interest. We hope to return to some of them in future work.

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