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Energies and bounds from perturbative approximations to the Bloch-Horowitz effective Hamiltonian

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Bloch-Horowitz perturbation theory is applied to the calculation of approximate energies and model-space eigenvectors, for the solvable large-matrix Hamiltonian H used by Pittel, Vincent, and Vergados. Two types of upper and lower bounds to the energies are discussed: moment-theory bounds, obtained by applying moment theory to the terms of perturbation theory, and norm bounds, derived from the expectation $\bar{E}$ and variance σ^2 of H with respect to an eigenvector approximated by nth order perturbation theory ($n \leq 6$). It is shown that lower bounds cannot be constructed unless some fourth-order quantity is known. The upper bounds are generally stricter than the lower bounds. All of the bounds apply even when back-door intruder states cause perturbation theory to diverge; but they lose their rigor and become "quasibounds" when there are physical intruders. The moment-theory and norm lower quasibounds always require estimation of a parameter. For the solvable Hamiltonians, it is shown that this can be done quite reliably, and that the resulting quasibounds are tight enough to have some practical utility. The energy-independent effective interaction V is constructed and its errors are displayed and discussed. Finally, a certain [1/2] pseudo-Padé approximant is empirically shown to give energies with a mean absolute error of less than 0.3 MeV in all cases.

[NUCLEAR STRUCTURE Effective interactions, ^{18}O. Perturbation theory for energies and bounds to them; used large solvable matrices, included intruder states. Padé approximants.]

I. INTRODUCTION

The calculation of nuclear spectra from a given many-body Hamiltonian H is a familiar problem in theoretical nuclear physics. Often it is hoped that comparison of the results with experiment will permit conclusions regarding the physical validity of the basic Hamiltonian. Calculations that simply diagonalize the bare H within a space spanned by a large number of shell-model basis states are found to be inadequate for this purpose. For this reason, it is usual, instead, to include only a small number of configurations (which span a space called the "model space"), and compensate approximately for this truncation by replacing the bare H by what is called an "effective Hamiltonian." This maneuver has some hope of succeeding, because it is in principle possible to define an exact effective Hamiltonian which, acting on the model space, will exactly reproduce a few eigenstates of the original H. Given the effective Hamiltonian, one can also construct a two-body effective *interaction*, whose matrix elements can be used for calculations involving more than two valence nucleons. Effective transition operators are also often introduced. In practice, all these effective quantities can, of course, be calculated only approximately; an exact calculation would be as impossible as an exact diagonalization of H. One of our major purposes, then, is to investigate the errors that arise from these inevitable approximations.

In this article we examine perturbation theory (PT) as a method of approximating effective Hamiltonians and interactions, describe techniques for estimating the accuracy of our calculations, and test these methods by comparing their results with exact results for some solvable many-body Hamiltonians. More specifically, we use the Bloch-Horowitz[1] method to obtain effective Hamiltonians whose solutions represent the predominantly two-particle $J=0^+$, $T=1$ states in ^{18}O [composed mainly of $(d_{5/2})^2$, $(s_{1/2})^2$, and $(d_{3/2})^2$ configurations], the ground state of ^{16}O, and the single-particle states in ^{17}O. In addition, we construct the corresponding $J=0^+$, $T=1$ two-body effective-interaction matrix elements for the s-d shell. The present work is closely related to the earlier work by Pittel, Vincent, and Vergados,[2] henceforth referred to as PVV. PVV used the same Hamiltonians as we do, but investigated the energy-independent (Brandow) effective Hamiltonian rather than using the Bloch-Horowitz energy-dependent Hamiltonian, and did not attempt any theoretical error analysis.

Except for solvable models, PT can in practice be carried out only up to third and possibly fourth order. Therefore, tests of the accuracy of PT have no practical significance beyond fourth order. The PT series will diverge when there exist in-

truder states (i.e., collective states, lying mainly outside the model space, which are depressed enough to enter the energy region of those states that lie mainly inside the model space). However, even if the PT series ultimately diverges, it has been found (at least in some cases[2,3]) that low orders of PT can give results of useful accuracy. The investigation of this possibility is one of the objects of our study.

Since the pioneering works of Schucan and Weidenmüller,[4,5] the analytic properties of the effective Hamiltonian have been much discussed[6-11] because of their implications for the convergence properties of the perturbation series. Like Refs. 2 and 3, the present paper focuses attention on the estimation of the errors incurred by truncating the PT series, rather than on the question of mathematical convergence. However, unlike Refs. 2, 3, and 10, the present work departs from the Schucan-Weidenmüller approach in no longer using analytic properties of the effective Hamiltonian to estimate the errors of low-order PT. Instead, we use methods of estimation that are familiar in the numerical analysis of the algebraic eigenvalue problem.[12-16] These simple ideas depend on the notion of the vector-space norm, and allow us to restrict the coupling parameter to the real axis. Our approach avoids a persistent difficulty of the analyticity approach: that the strengths of singularities are harder to estimate than their locations. Related approaches have long been used in quantum chemistry and atomic physics.[15,17]

As already mentioned, our work differs from that of PVV in that we use the energy-dependent (Bloch-Horowitz) type of effective Hamiltonian rather than the energy-independent (Brandow) type. One advantage of this is that perturbation theory for the Bloch-Horowitz method is much easier to analyze, because it is based on a simple geometric series. It is also plausible that the Bloch-Horowitz perturbation theory may give better approximations, because it is not affected by the gap-cut singularities[11] that are often prominent in the Brandow method. Thus, part of the interest of the present work arises from the possibility of comparing the results of the Bloch-Horowitz and the Brandow methods.

Perturbation theory is by no means the only possible method for calculating effective Hamiltonians. Indeed, several other methods are known to converge in some cases for which PT diverges, and some of these[18-20] seem to be successful even in quite low orders. Of course, every one of these methods is still capable of benefitting from an error analysis. In this regard, it is worth remarking that some of our methods for estimating bounds are equally applicable to nonperturbative calculations. Although we are using PT largely as a technique for generating approximate results to which we can apply our error estimates, we actually find that PT is encouragingly accurate in the cases we consider. We can also point to other, more qualitative, advantages of PT. First, PT is a particularly systematic and well-known procedure, with a well-studied diagrammatic interpretation.[21-24] Second, the unperturbed Hamiltonian need not be an independent-particle Hamiltonian; this opens up the possibility of using a sophisticated nonperturbative method to construct a zero-order solution, and then using PT to refine this solution.

In Sec. II we establish necessary notations and formulate the energy-dependent effective Hamiltonian and the effective interaction. In Sec. III we describe techniques for calculating upper and lower bounds to the energies of simple states. The numerical results of calculations that use the solvable test Hamiltonians are given in Sec. IV, together with a discussion of the PT approximations and the error bounds, and a comparison of the present results with those of PVV. Finally, in Sec. V we summarize our conclusions.

II. FORMAL THEORY

A. Energy-dependent effective Hamiltonian

Let H be the full Hamiltonian of a system of nucleons. We denote by $\{\phi_j, j=1,2,\dots\}$ a complete set of orthonormal basis states of the system. With respect to this basis, H can be written as H_0+V, i.e., as the sum of a zero-order Hamiltonian H_0, which is diagonal on the ϕ_j basis, and a perturbation term V. We denote by ϵ_j the eigenvalues of H_0:

$$H_0\phi_j=\epsilon_j\phi_j \quad (j=1,2,\dots), \tag{2.1}$$

and we assume that $\epsilon_1\leq\epsilon_2\leq\epsilon_3\leq\dots$.

The perturbation expansion of any effective operator is a power series in a parameter z, introduced as follows:

$$H(z)=H_0+zV. \tag{2.2}$$

The parameter z essentially modifies the strength of V. The value $z=1$ is called the physical value of z, as $H(1)$ is the actual Hamiltonian of the system. By $\{\psi_j\}$ and $\{E_j\}$ we denote the set of the eigenvectors and eigenvalues of H:

$$H\psi_j=E_j\psi_j \quad (j=1,2,\dots). \tag{2.3}$$

To define formally an effective Hamiltonian we introduce some additional concepts and notations. The model space is a space spanned by a subset of the states $\{\phi_j\}$. This subspace, of a finite (and small) dimension M, is chosen on physical

grounds and usually is spanned by the M energetically lowest configurations. The projection operator P onto the model space is defined as

$$P=\sum_{m\le M}|\phi_m\rangle\langle\phi_m|. \tag{2.4}$$

We also define, by

$$Q=1-P, \tag{2.5a}$$

a projection operator onto the space spanned by the rest of the configurations. We call this space the excluded space or Q space. The projection operators have the following properties:

$$P^2=P,\quad Q^2=Q,\quad PQ=QP=0. \tag{2.5b}$$

In a realistic problem the excluded space has an infinite number of configurations. However, in our solvable test problems, this space has finite dimension.

Let χ_j denote the projection of ψ_j onto the model space; that is

$$\chi_j=P\psi_j. \tag{2.6}$$

Of particular interest is the set of M states ψ_m that have large components in the model space. We call these states the "represented" states, and regard χ_m as the representation of ψ_m.

Using the projection operators P and Q, we partition[1,17,25] the Hamiltonian as follows:

$$H=H_{PP}+H_{PQ}+H_{QP}+H_{QQ}, \tag{2.7}$$

where the notation $A_{PQ}\equiv PAQ$ is used. The H_{QQ} part of the Hamiltonian consists of an unperturbed piece and a perturbation, i.e.,

$$H_{QQ}=H_{0QQ}+z\,V_{QQ}. \tag{2.8}$$

Equations (2.3), (2.6), and (2.7) lead to the relation

$$\mathcal{H}(E_m,z)\chi_m=E_m\chi_m, \tag{2.9}$$

where

$$\mathcal{H}(\omega,z)=H_{PP}+z^2V_{PQ}\frac{1}{\omega-H_{QQ}}V_{QP}. \tag{2.10}$$

This is the Bloch-Horowitz[1] expression for the energy-dependent effective Hamiltonian. A subset of the solutions E_j of Eq. (2.9) are the eigenvalues E_m of H corresponding to the represented eigenstates ψ_m, and the corresponding eigenvectors χ_m are the projections of the ψ_m onto the model space. In this work, the dependence on z will be suppressed most of the time, being shown only when needed for a specific discussion.

Since $\mathcal{H}$ depends on the energy, solution of Eqs. (2.9) and (2.10) requires an iteration process for each eigenvalue. Equation (2.9) can be regarded as a combination of the equations

$$\mathcal{H}(\omega)\chi=E(\omega)\chi \tag{2.11}$$

and

$$\omega=E(\omega). \tag{2.12}$$

We use the phrase "self-consistent solution" to mean that these equations are satisfied simultaneously. We denote a typical solution of Eq. (2.11) as a function of ω by $E(\omega)$; we denote a typical self-consistent solution by E (without the argument ω). We remark that for ω different from all eigenvalues, w_q, of H_{QQ}, each eigenvalue $E(\omega)$ of $\mathcal{H}(\omega)$ is a decreasing function[17] of ω. The function $E(\omega)$ has poles at the eigenvalues of H_{QQ}. In Fig. 1, we show the behavior of the eigenvalues $E(\omega)$ as a function of ω. The eigenvalues of H are the points of intersection of the curves $E=\omega$ and $E=E(\omega)$. In Ref. 26 it is shown that the slope of the curve $E_m(\omega)$ at $\omega=E_m$ is a measure of the Q-space overlap of the eigenvectors ψ_m, i.e.,

$$dE_m(\omega)/d\omega=-\langle\psi_m|Q|\psi_m\rangle/\langle\psi_m|P|\psi_m\rangle. \tag{2.13}$$

Therefore, only the solutions for which $dE_k(\omega)/d\omega\big|_{\omega=E_k}$ is small correspond to the energies of represented states.

By using Eq. (2.8) one can expand the effective Hamiltonian as a power series in z:

$$\mathcal{H}(\omega,z)=H_{0PP}+\sum_{l=0}^{\infty}z^{l+1}h_{l+1}, \tag{2.14}$$

where

$$h_{l+1}=PV(Q(\omega-H_{0QQ})^{-1}QV)^lP. \tag{2.15}$$

The nth order approximation to $\mathcal{H}(\omega,z)$ is

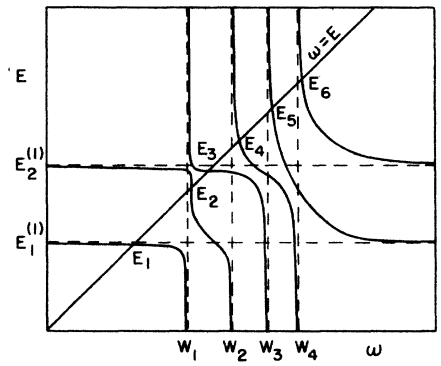

FIG. 1. Schematic graph of the eigenvalues $E_m(\omega)$ of $\mathcal{H}(\omega)$, for model and excluded spaces of dimensions two and four, respectively. The curves $E_m(\omega)$ $(m=1,2)$ intersect the line $\omega=E$ at points $E_1,\ldots,E_6$ corresponding to the eigenvalues of H. The represented states are E_1 and E_3; E_2 is an intruder state, while E_4, E_5, E_6 are excluded states of higher energies. The poles are at the eigenvalues of H_{QQ}, $w_1,\ldots,w_4$.

$$\mathcal{H}^{(n)}(\omega,z)=H_{0PP}+\sum_{l=0}^{n-1} z^{l+1}h_{l+1}. \tag{2.16}$$

The approximate eigenvalues of the effective Hamiltonian are found by self-consistently solving Eqs. (2.11) and (2.12) with $\mathcal{H}$ replaced by its nth order approximation $\mathcal{H}^{(n)}$. The resulting approximate eigenvalues and eigenvectors are denoted, respectively, by $E^{(n)}$ and $\chi^{(n)}$.

The Q-space part of ψ_m can be expressed in terms of its P-space part as follows:

$$Q\psi_m=Q(E_m-H_{QQ})^{-1}QV\chi_n. \tag{2.17}$$

We also write the nth order approximation to the wave function ψ_m as follows:

$$\psi_m^{(n)}=\Omega^{(n-1)}\chi_m^{(n)}, \tag{2.18}$$

where $\Omega^{(n)}$ is the nth order approximation to the wave operator Ω:

$$\Omega^{(n)}=\sum_{l=0}^{n}\left[zQ(E_m-H_{0QQ})^{-1}QV\right]^l P. \tag{2.19}$$

For later analysis of the bounds it is convenient to rewrite the effective Hamiltonian (2.10) as

$$\mathcal{H}(\omega,z)=H_{PP}-z^2\mathfrak{D}(\omega,z), \tag{2.20}$$

where

$$\mathfrak{D}(\omega,z)=-V_{PQ}[\omega-H_{QQ}(z)]^{-1}V_{QP}. \tag{2.21}$$

The operator just introduced is of particular interest in that it contains the effects of virtual excitations out of the model space. We call $\mathfrak{D}(\omega,z)$ the dispersion term of $\mathcal{H}$. In our discussions we use a notation in which, for a Hermitian operator A, $\min(A)$ is the lowest eigenvalue of A and $\max(A)$ is the largest one. We also use the concept of a positive operator, which is an operator A such that $\langle\xi|A|\xi\rangle>0$ for all vectors ξ. To find a convenient power expansion for $\mathfrak{D}(\omega,z)$, we first remark that it is always possible to ensure that

$$\min(H_{0QQ})-\omega>0. \tag{2.22}$$

If, for a given H_{0QQ}, the inequality above is not satisfied, then a constant s can be added to $\min(H_{0QQ})$ such that $\min(H_{0QQ})+s-\omega>0$. On the other hand, the same constant s can be subtracted from V_{QQ} so that H_{QQ}, and consequently H, remain unchanged. Henceforth, we always assume that Eq. (2.22) holds.

Equation (2.21) can be written in the form

$$\mathfrak{D}(\omega,z)=V_{PQ}G^{1/2}(\omega)[1-zK(\omega)]^{-1}G^{1/2}(\omega)V_{QP}, \tag{2.23}$$

where

$$G(\omega)\equiv(H_{0QQ}-\omega)^{-1} \tag{2.24}$$

is a positive Hermitian operator so that $G^{1/2}(\omega)$ exists [the eigenvalues of $G^{1/2}(\omega)$ are the positive square roots of the corresponding eigenvalues of $G(\omega)$]. We have also defined the operator

$$K(\omega)=-G^{1/2}(\omega)V_{QQ}G^{1/2}(\omega), \tag{2.25}$$

which is Hermitian, so that its eigenvalues $k_j(\omega)$ are real. To simplify subsequent expressions we will omit the explicit dependence of G, K, and k_j on ω, but it is important to keep this dependence in mind. The dispersion term has an expansion in powers of z of the form

$$\mathfrak{D}(\omega,z)=-\sum_{n=0}^{\infty} z^n h_n, \tag{2.26}$$

where

$$h_n=-V_{PQ}G^{1/2}K^nG^{1/2}V_{QP}. \tag{2.27}$$

We introduce "moments" μ_n, related to the expectation values of h_n by

$$\mu_n=-\langle\xi|h_n|\xi\rangle. \tag{2.28}$$

These are used in the discussion of bounds [Eq. (3.6)].

B. Effective interaction

The two-body effective interaction υ is a quantity of special interest in nuclear structure, because it can be used to perform calculations for systems of several valence nucleons that are distributed among the same set of orbitals for which υ was calculated. Therefore, one part of our investigation is to examine the accuracy with which we can estimate the matrix elements of υ by using PT.

Having determined the approximate eigenvalues E_m and eigenvectors χ_m of the energy-dependent effective Hamiltonian, we can construct an energy-independent operator $\tilde{\mathcal{H}}$ with model-space matrix elements $\langle\phi_m|\tilde{\mathcal{H}}|\phi_m\rangle$, such that its eigenvalues and eigenvectors are the E_m and $\chi_m(m\leq M)$. (This effective Hamiltonian $\tilde{\mathcal{H}}$ is denoted by $\mathcal{H}$ in PVV.)

In order to construct the effective-interaction matrix, we need to subtract (from the diagonal matrix elements of $\tilde{\mathcal{H}}$) the energy of the core and the single-particle energies. As discussed in PVV, the effective-interaction matrix elements are given by the relation:

$$\langle\phi_m|\upsilon|\phi_{m'}\rangle=\langle\phi_m|\mathcal{H}|\phi_{m'}\rangle-\delta_{mm'}[E_c-E_{c+1}(j_1)-E_{c+1}(j_2)], \tag{2.29}$$

where $E_{c+1}(j_1)$ and $E_{c+1}(j_2)$ are the correlated energies of the predominantly single-particle states of angular momenta j_1 and j_2 of the particles in the state ϕ_m. E_c is the ground-state energy of

the closed core containing c nucleons. The single-particle energies and the core energy can be calculated approximately by PT.

C. Intruder states

An "intruder state" is a state that lies mainly in the Q space, at a perturbed energy below the energy of some represented states. The unperturbed energy of an intruder state is higher than the unperturbed energies of the model states, but when the perturbation zV is turned on, a collective effect depresses it below some of the represented states. Intruder states that appear for $z=1$ are called "physical intruders"; intruder states appearing for $z=-1$ are called "backdoor intruders."[2] One of the solutions shown in Fig. 1 corresponds to an intruder state. As was mentioned previously, the slope of $E_m(\omega)$, at $\omega = E_m$ (the self-consistent energy), is a measure of the Q-space overlap of this state.[26] A large slope indicates that the state consists mostly of configurations of the Q space. Because this slope for an intruder state is extremely steep, the intruder solution is not likely to be found, unless the grid of the values of ω on which the curves $E(\omega)$ are constructed is very fine. Since we are interested in the represented states, not in the intruder, this is a convenient feature. If, by accident, an intruder state solution is found, its nature will be revealed by inspection of the slope $dE_i/d\omega$.

Physical and back-door intruders cause divergence of the perturbation expansion of $\mathcal{H}$. This is a consequence of the following theorem, whose proof we relegate to Appendix A.

Define $\overline{H}_{QQ} \equiv H_{0QQ} - V_{QQ}$. Then if relation (2.22) holds:

(*a*) *The condition*

$$\min(H_{QQ}) < \omega \ [\text{or } \min(\overline{H}_{QQ}) < \omega] \tag{2.30}$$

implies that at least one eigenvalue of $K(\omega)$ *is greater than* 1 (*or less than* -1) *and in either case, the series* $1+zK+z^2K^2+\cdots$ *contained in Eq.* (2.23) *diverges at* $z=1$.

(*b*) *The conditions*

$$\min(H_{QQ}) > \omega \ \text{ and } \ \min(\overline{H}_{QQ}) > \omega \tag{2.31}$$

together imply that the series converges at $z=1$.

The above theorem is physically significant when ω is equal to the energy of a represented state. This theorem also helps us to give a precise definition of an intruder state in the energy-dependent effective-Hamiltonian case. Intruders appear when the energy of a represented state is above $\min(H_{QQ})$ or $\min(\overline{H}_{QQ})$; in the first case we have a physical intruder an in the second case we have a back-door intruder. Let $\hat{k}(\omega) = \max[K(\omega)]$ and $\hat{k} = \min[K(\omega)]$; then, according to the theorem, physical intruders imply that $\hat{k} > 1$ and back-door intruders imply that $\hat{k} < -1$. Finally, although the present work *is* concerned with the effects of intruders, questions of *convergence* are only a minor concern.

Having completed the formal description of effective Hamiltonians and interactions, in Sec. III we now go on to discuss the errors of approximate calculations of the energies.

III. CONSTRUCTION OF BOUNDS

A. General

In this section we describe several methods for upper and lower bounds to the exact represented eigenvalues of H. The methods to be described are divided into two categories: (a) Those that seek to use the numerical values of the terms of the perturbation expansion of $\mathcal{H}$ as input, to give moment-theory (MT) results characterized as "MT bounds." (b) Those that make essential use of the norm of the error vector $(H - E^{\text{approx}})\psi^{\text{approx}}$, will be referred to as "norm bounds." These have the advantage that they can be applied also to non-perturbative calculations of ψ^{approx} and E^{approx}

The idea of constructing bounds directly from the terms of PT has great appeal, so we devote considerable attention to the MT bounds. In atomic physics, where the perturbation V can be chosen to be non-negative, PT bounds have had some success. Unfortunately, in nuclear physics it is very difficult to ensure that V is non-negative, because the two-nucleon interaction has negative as well as positive parts. For arbitrary V it is actually impossible *in principle* to construct a lower bound on an energy, from knowledge of the terms of PT for $\mathcal{H}$ through fourth order only. This is proved in Appendix B, by constructing a counterexample to any supposed lower bound. An immediate consequence is that the terms of PT must be supplemented by other information, which can take various forms. We suppose first that the additional information takes the form of one or more bounds on K. Bounds on the energy can then be derived from the theory of moments. It will be seen that the lower bounds provided by this theory depend on $\hat{k} = \max(K)$. Unfortunately, obstacles are encountered in applying the theory for $\hat{k} > 1$, i.e., if there is a physical intruder. However, back-door intruders cause no difficulty.

The norm bounds can be applied even in the presence of intruders. The most rigorous norm bounds, called the σ bounds, provide a calculable interval inside which an eigenvalue is known to lie. More practical bounds are also discussed, in particular what we call the σ^2/ϵ bound, which

requires an energy denominator to be estimated nonrigorously.

B. MT bounds

It is convenient first to derive bounds for the expectation value of $\mathcal{H}$ with respect to an arbitrary model state ξ. Bounds on the eigenvalues $E_m(\omega)$ of $\mathcal{H}$ are then obtained by choosing ξ to be an eigenvector of $\mathcal{H}(\omega)$ or an adequate approximation to one, as will be discussed later. Finally, bounds on the self-consistent solution of $\omega = E_m(\omega)$ can be found.

We introduce the notation $g(z)$ for the expectation of $\mathfrak{D}(\omega, z)$:

$$g(z) \equiv \langle \xi \,|\mathfrak{D}(\omega,z)\,|\,\xi\rangle = \langle \xi \,|\, V_{PQ}G^{1/2}(1-zK)^{-1}G^{1/2}V_{QP} \,|\, \xi\rangle = \sum_j \frac{|\langle \xi \,|\, V_{PQ}G^{1/2}|k_j\rangle|^2}{1-zk_j} \,. \tag{3.1}$$

We have left implicit the dependence of G, K, and k_j on ω, for the time being.

Consider the function

$$h(k) = \sum_j |\langle \xi \,|\, V_{PQ}G^{1/2}\,|k_j\rangle|^2\,\delta(k-k_j)\,, \tag{3.2}$$

which is non-negative. We call this function the spectral distribution function[27] of $G^{1/2}V_{QR}\xi$. In terms of this distribution function, the expectation of the dispersion term can be expressed as

$$g(z) = \int_{-\infty}^{a} \frac{h(k)}{1-zk}\,dk\,, \tag{3.3}$$

where a is any upper bound to $\hat{k}$, i.e.

$$\hat{k} \le a\,. \tag{3.4}$$

As long as Eq. (3.4) is satisfied, any value of a can be used, because $h(k) = 0$ for $k > \hat{k}$. We now expand $g(z)$ in powers of z, with the result

$$g(z) = \sum_{l=0}^{\infty} \mu_l z^l\,, \tag{3.5}$$

where the coefficients

$$\mu_l \equiv \int_{-\infty}^{a} k^l h(k)\,dk \tag{3.6}$$

are the moments of the distribution $h(k)$. They are trivially related to the terms of PT though Eq. (2.28). The problem of moments[13,14] is to find bounds to $g(z)$ using only a finite number of these moments; its relation to our problem is now clear. Calculation of μ_0, μ_1, μ_2 is of the same order of difficulty as carrying the perturbation expansion for $\mathcal{H}$ to the fourth order. Because (as we have mentioned) higher orders are probably not practically feasible, we will try to calculate bounds assuming we have at our disposition only the three lowest moments.

The theory of moments is a well-established part of mathematics, and several well-known approaches are capable of being applied to our problem. The Tschebycheff inequalities[28] use the moments to provide upper and lower bounds to the integrated distribution function $\int_{-\infty}^{k} h(k')dk'$. Bounds on $g(z)$ can then be calculated, provided that we know a lower bound to δ, where $\delta \equiv |1-k_N|$ is the separation of the zero of the denominator at $k_s \equiv z^{-1} = 1$ from k_N, the eigenvalue of K nearest to 1. If $\hat{k} < 1$ (i.e., in the absence of intruders), we have $k_N = \hat{k}$, so that only $\hat{k}$ is required. We see that $\hat{k}$ is needed in this approach, as in other moment-theory treatments, even in the absence of intruders. If $\hat{k} > 1$, so that one or more physical intruders exist, μ_0, μ_1, μ_2, and $\hat{k}$ no longer suffice for the construction of a lower bound on the expectation of $\mathcal{H}$. Clearly, physical intruders introduce severe difficulties for the MT bounds.

Hamburger's[29] bounds on $g(z)$ require knowledge of the radius of convergence R of the series (3.5) and a finite number of moments. We have

$$R = 1/\max(|\check{k}|, |\hat{k}|)\,, \tag{3.7}$$

so that both physical and back-door intruders affect the Hamburger bounds. We have chosen not to apply the Hamburger bounds, because back-door intruders are important for our test case.[2,11] and probably also for more realistic cases. We note also that $R \to \infty$ the Hamburger bounds reduce to the Stieltjes bounds that we consider below.

Other treatments[30] give what are called "best possible bounds." A bound is a best possible bound if and only if a distribution function $h_1(k)$ exists such that: (a) $h_1(k)$ reproduces the assumed properties of $h(k)$ (e.g., μ_0, μ_1, μ_2, and $\hat{k}$), and (b) the bound is attained (or approached arbitrarily closely) by the function $g_1(z)$ obtained by substituting $h_1(k)$ in Eq. (3.3).

The theory of Stieltjes series yields best possible bounds in a natural way. First, Eq. (3.3) can be subjected to the transformation

$$k = k(x) = (\hat{k}-1)x + \hat{k}\,, \tag{3.8}$$

with the result that

$$g(z) = \int_0^{\infty} \frac{h[k(x)]}{u+zx}\,dx\,, \quad u = \frac{1-z\hat{k}}{1-\hat{k}}\,. \tag{3.9}$$

In obtaining Eq. (3.9), we have assumed $\hat{k} < 1$ (no physical intruder). For $\hat{k} > 1$ the transformation (3.8) does not lead to useful results. We therefore postpone the investigation of bounds in the more difficult case $\hat{k} > 1$ to a later work. Because we are interested only in the physical value, $z = 1$, for which $u = 1$, we can write

$$g(1)=f(1)\,, \tag{3.10}$$

where the new function f is defined by

$$f(t)=\int_0^\infty \frac{h[k(x)]\,dx}{1+tx}\,. \tag{3.11}$$

Because $h[k(x)]$ is non-negative, the expansion of this function in powers of t is by definition a Stieltjes series

$$f(t)=\sum_{r=0}^{\infty} m_r(-t)^r\,, \tag{3.12}$$

with coefficients given by

$$m_r=\int_0^\infty x^r h[k(x)]\,dx$$

$$=\int_{-\infty}^{a}\left(-\frac{k-\hat{k}}{1-\hat{k}}\right)^r \frac{h(k)}{1-\hat{k}}\,dk\,. \tag{3.13}$$

The relation between the original moments μ_r and the new moments m_r is easily derived from the second half of Eq. (3.13). The result is

$$m_r=\frac{1}{(1-\hat{k})^{r+1}}\sum_{l=0}^{r}(-1)^l\binom{r}{l}\hat{k}^{r-l}\,\mu_l\,. \tag{3.14}$$

The moments μ_r are necessarily positive for r even, while the m_r are positive for all r. Note that knowledge of μ_0, μ_1, and μ_2 permits calculation of m_0, m_1, and m_2.

Best possible bounds to the function f defined by Eq. (3.11) can be derived either from the theory of Pade approximants[31] or from the theory of Gaussian quadrature.[32] For given input the results are necessarily the same, since both methods give best possible bounds. We quote the Padé results, which are more convenient in form. The $[N/L]$ Padé approximant to $f(t)$, denoted by $f_{[N/L]}(t)$, is the ratio of two polynomials $P_N(t)$ and $Q_L(t)$, of orders N and L, respectively, whose coefficients are chosen so that $P_N(t)/Q_L(t)$ agrees with $f(t)$ through order t^{N+L}. For uniqueness, the convention $Q_L(0)=1$ is used. Subject to these restrictions on $P_N(t)$ and $Q_N(t)$ we have

$$f_{[N/L]}(t)=P_N(t)/Q_L(t)\,. \tag{3.15}$$

For $t\geq 0$ and $N\geq 1$ the Pade bounds are

$$f_{[N-1/N]}(t)\leq f(t)\leq f_{[N/N]}(t)\,. \tag{3.16}$$

The highest Padé approximants that can be calculated from m_0, m_1, and m_2 are

$$f_{[0/1]}(1)=m_0^2/(m_0+m_1) \tag{3.17a}$$

and

$$f_{[1/1]}(1)=(m_0m_1-m_1^2-m_0m_2)/(m_1+m_2)\,. \tag{3.17b}$$

In terms of the original moments μ_r, these are

$$g_{[0/1]}(1)=\mu_0^2/(\mu_0-\mu_1) \tag{3.18a}$$

and

$$g_{[1/1]}(1)=\frac{\mu_0(\mu_2-\mu_1)-\mu_1^2+\mu_0(\mu_1+\mu_0)\hat{k}-\mu_0^2\hat{k}^2}{(1-\hat{k})[\mu_2-\mu_1+\hat{k}(\mu_0-\mu_1)]}\,, \tag{3.18b}$$

where we have applied Eq. (3.10).

Equations (3.16) and (3.18) finally provide bounds to $g(1)=\langle\xi\,|\mathfrak{D}(\omega,1)\,|\,\xi\rangle$, from which bounds to $\langle\xi\,|\mathfrak{K}(\omega)\,|\,\xi\rangle$ can easily be calculated by means of Eq. (2.20) (with $z=1$). To obtain strict bounds on a represented eigenvalue of H, it is necessary to have upper and lower bounds $E^{MU}(\omega)$ and $E^{ML}(\omega)$, respectively, to the appropriate eigenvalue $E(\omega)$ of $\mathfrak{K}(\omega)$. Solving the self-consistency equations

$$E^{MU}(E^{MU})=E^{MU}\,,\quad E^{ML}(E^{ML})=E^{ML} \tag{3.19}$$

then yields upper (lower) bounds E^{MU} (E^{ML}), as can be seen from Fig. 2. In this figure, we show in detail a piece of the graph of $E(\omega)$ in the vicinity of the intersection with the straight line $\omega=E(\omega)$. From the curves representing the bounds we deduce that the bounds given by $E^{MU}(E^{(n)})$ and $E^{ML}(E^{(n)})$ will, if $E^{(n)}(\omega)$ lies between $E^{MU}(\omega)$ and $E^{ML}(\omega)$, be looser than the self-consistent values E^{ML} and E^{MU}. Thus we see that the bounds will be tightened if they are obtained self-consistently. Unfortunately, $E^{MU}(\omega)$ and $E^{ML}(\omega)$ cannot be calculated exactly because we cannot simply take $\xi=\chi$

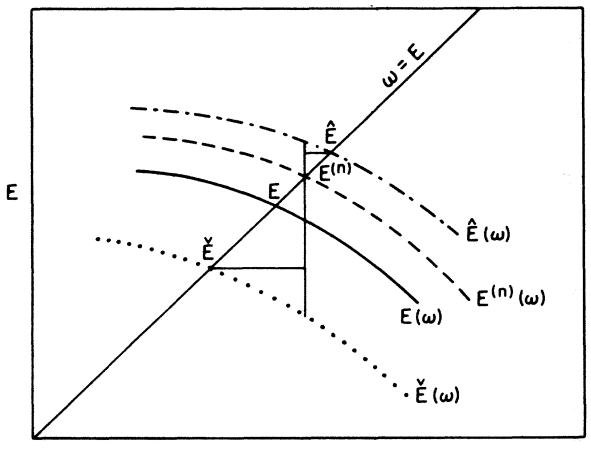

FIG. 2. Schematic graph of several approximations to an exact eigenvalue $E(\omega)$ of $\mathfrak{K}(\omega)$. PT of nth order gives $E^{(n)}(\omega)$; $\hat{E}(\omega)$ is an upper bound to $E(\omega)$; $\check{E}(\omega)$ is a lower bound to $E(\omega)$. If $\check{E}(\omega)<E^{(n)}(\omega)<\hat{E}(\omega)$, as assumed here here, the self-consistent upper- and lower-bound solutions $\hat{E}$ and $\check{E}$ are closer to the exact E than the non-self-consistent results $\hat{E}(\omega=E^{(n)})$ and $\check{E}(\omega=E^{(n)})$. See Eq. (3.22) of the text.

in Eq. (3.1), since the exact χ is not known. Instead, we have to use the approximations

$$E^{ML}(\omega) \approx \langle \chi^{(n)}(\omega) | \mathcal{H}(\omega) | \chi^{(n)}(\omega) \rangle_{[1/1]} , \quad (3.20a)$$

$$E^{MU}(\omega) \approx \langle \chi^{(n)}(\omega) | \mathcal{H}(\omega) | \chi^{(n)}(\omega) \rangle_{[0/1]} , \quad (3.20b)$$

where $\chi^{(n)}$ is the appropriate eigenvector of $\mathcal{H}^{(n)}$, the nth order PT approximation to $\mathcal{H}(\omega)$, and the subscripts [1/1] and [0/1] refer to the bounds obtained from Eq. (3.18). We can show that for the cases we have tested, the errors of the approximations (3.20) are in fact negligible compared with the errors that result from replacing $\mathcal{H}(\omega)$ by $\mathcal{H}^{(n)}(\omega)$ in Eq. (3.20). For the overlap between exact and approximate model wave functions we always find that $c = \langle \chi | \chi^{(n)} \rangle [\langle \chi | \chi \rangle \langle \chi^{(n)} | \chi^{(n)} \rangle]^{-1/2} \geq 0.995$. An overestimate of the error in Eq. (3.20) is then easily shown to be

$$(1 - c^2) \| \mathcal{H} - E \| . \quad (3.21)$$

This overestimate is approximately 0.13 MeV for the highest and lowest represented states, if their separation is about 13 MeV, as in our test problems. We found that the actual values of this error were less than 0.005 MeV, however, and so we neglected them as small compared with the main errors.

Instead of calculating the bounds using the self-consistent Eqs. (3.19) with the functions $E^{MU}(\omega)$ and $E^{ML}(\omega)$ given by Eq. (3.20), one can make the simplifying assumptions that their ω dependence is so smooth near $\omega = E^{(n)}$ that the curves $E^{ML}(\omega)$ and $E^{MU}(\omega)$ can be taken as linear and that both have slope $\alpha \approx dE^{(n)}/d\omega \big|_{\omega = E^{(n)}}$. Then we can derive improved approximate expressions for the self-consistent upper bound E^{MU} and the self-consistent lower bound E^{ML} in terms of already known quantities. The resulting expressions are:

$$E^{MU} = E^{MU}(E^{(n)}) + \alpha(1 - \alpha)^{-1}[E^{MU}(E^{(n)}) - E^{(n)}] \quad (3.22a)$$

and

$$E^{ML} = E^{ML}(E^{(n)}) + \alpha(1 - \alpha)^{-1}[E^{ML}(E^{(n)}) - E^{(n)}] . \quad (3.22b)$$

For small α, the absolute error involved in neglecting the corrections in Eqs. (3.22a) and (3.22b) is roughly $|\alpha| \cdot |\omega - E^{(n)}|$, as can be seen from Fig. 2. For the cases we test, α is less than 0.36 but $E^{ML}(E^{(n)}) - E^{(n)}$ can be 3.9, so that the error of replacing ω by $E^{(n)}$ is as much as 1 MeV.

If the terms proportional to α, in Eqs. (3.22), are neglected, we obtain the following bounds from Eqs. (3.19) and (3.20):

$$E^{ML} \approx E^{ML}(E^{(n)}) = \langle \chi^{(n)}(E^{(n)}) | \mathcal{H}(E^{(n)}) | \chi^{(n)}(E^{(n)}) \rangle_{[1/1]} \quad (3.23a)$$

and

$$E^{MU} \approx E^{MU}(E^{(n)}) = \langle \chi^{(n)}(E^{(n)}) | \mathcal{H}(E^{(n)}) | \chi^{(n)}(E^{(n)}) \rangle_{[0/1]} . \quad (3.23b)$$

These bounds and the adjusted bounds using Eqs. (3.22), are evaluated and discussed in Sec. IV. The lower bounds depend on $\hat{k}$, while the upper bounds depend purely on the terms of PT. The bounds remain valid when $\hat{k}$ is replaced by any upper bound a, such that

$$\hat{k} \leq a < 1 . \quad (3.24)$$

Unfortunately, it is quite difficult to obtain estimates of $\hat{k}$ that satisfy Eq. (3.24). We have tried applying the method of Gershgorin disks[16] to estimate $\hat{k}$ from the matrix elements[33] of K. The results are discouragingly pessimistic; for the first excited state in the DEG (discussed in Sec. IV A) case the Gershgorin method gives

$$\hat{k} \leq 1.997 , \quad (3.25)$$

while the actual value is $\hat{k} = 0.743$. Thus, we are obliged, in practice, to rely on informal estimates of $\hat{k}$.

In passing, we mention the existence of some simpler bounds, which are not the best possible bounds, however. Leinaas and Kuo[26] show that in odd orders Brillouin-Wigner PT gives upper bounds to the ground-state energy:

$$E_1 \leq E_1^{(2n+1)} . \quad (3.26)$$

Next we note that for the Stieltjes series, Eq. (3.12), it can be shown that

$$(-1)^{n+1}[f(1) - f^{(n)}(1)] = \int_0^\infty \frac{h[k(x)]x^{n+1}}{1+x}\, dx \leq m_{n+1} , \quad (3.27)$$

where

$$f^{(n)}(t) = \sum_{l=0}^{n} m_l (-t)^l . \quad (3.28)$$

The right-hand side of Eq. (3.27) provides upper (lower) bounds of $f(1)$ for n even (odd), from which lower (upper) bounds on the energy can be constructed.

C. Norm bounds

It is well known that a variational calculation (i.e., expectation value) for the ground-state energy of a system gives an upper bound to its energy. However, an expectation value of H with respect to an approximate excited-state eigenvector is *not* guaranteed to be an upper bound to the corresponding energy. Nevertheless, if M

approximate eigenvectors $\{\psi_m^{\text{approx}}, m=1,\ldots,M\}$ are known, they can be used to define an M-dimensional subspace. Let p be the projection operator on this subspace. Suppose H_{pp} is now diagonalized[34] to get orthonormal eigenvectors ξ_m (lying in the subspace) and corresponding eigenvalues $\bar{E}_m, m=1,\ldots M$. Then the $\bar{E}_m$ are strict upper bounds[35] to the corresponding[36] eigenvalues E_m:

$$\bar{E}_m \geq E_m . \tag{3.29}$$

The construction of lower bounds is a more complicated case. For any approximate eigenvector, say ξ_m, let λ be a corresponding approximate eigenvalue. The variance of H about λ,

$$\sigma_m{}^2 \equiv \langle \xi_m | (H-\lambda)^2 | \xi_m \rangle , \tag{3.30}$$

takes on its minimum value for

$$\lambda = \langle \xi_m | H | \xi_m \rangle = \bar{E}_m . \tag{3.31}$$

If H has no eigenvalues in the interval $|\lambda - E_m| \leq \sigma_m$, it will follow, in contradiction to Eq. (3.30), that $\langle \xi_m | (H-\lambda)^2 | \xi_m \rangle$ will be *larger* than $\sigma_m{}^2$, because the mean square deviation is larger than the minimum deviation. It follows[37] that H must have at least one eigenvalue, say E_m, that satisfies

$$\bar{E}_m - \sigma_m \leq E_m \leq \bar{E}_m + \sigma_m . \tag{3.32}$$

Only the first inequality is of much consequence, since Eq. (3.29) already gives a good upper bound to E_m. Note that if $\sigma_m = 0$, Eq. (3.32) becomes

$$E_m = \bar{E}_m , \tag{3.33}$$

and Eq. (3.30) implies that ξ_m must be an exact eigenvector, because $\sigma_m{}^2$ is a norm. To apply the theory outlined above, we in practice use the nth order PT eigenvectors $\psi_m^{(n)}$ given by Eq. (2.18) for the approximate eigenvectors ψ_m^{approx}. Because the vectors ψ_m^{approx} are not exactly orthogonal, we have to exercise appropriate care[34] in constructing the projection operators p.

Of all lower bounds that we discuss, the bound $\bar{E}_m - \sigma_m$ is the least dependent on assumptions. It is ironic to notice that even this bound is incomplete in quite an important respect, which can be illustrated by imagining an attempt to calculate the ground-state energy from an approximate wave function. The σ_m bound will tell us that at least one state lies between $\bar{E}_m$ and $\bar{E}_m - \sigma_m$; but of course it has nothing to say on the question of whether the *ground state* is one of those states! This seems to be a fundamental difficulty, which cannot be rigorously solved without constructing bounds on *all* eigenvalues (a most unwelcome requirement in many-body theory). In practice one must rely on a combination of past experience and experimental results for assurance that the ground state has been correctly identified.

We now introduce a lower bound that makes use of σ_m, but is more dependent on assumptions than the σ_m bound. Its advantage is that it is usually a closer estimate than the σ_m bound. We use the previously mentioned orthonormal approximate eigenvectors ξ_m, which span the space on which p is the projection. By introducing the complementary projection

$$q = 1 - p , \tag{3.34}$$

we can partition H, by analogy with Eq. (2.7), and so introduce an operator $h(\omega)$, defined by

$$h(\omega) \equiv H_{pp} - d(\omega) , \tag{3.35}$$

in terms of the operator

$$d(\omega) \equiv H_{pq}(H_{qq} - \omega)^{-1} H_{qp} . \tag{3.36}$$

Carrying through the analogy, the represented eigenvalues ψ_m and eigenvectors E_m of H satisfy

$$h(E_m)\psi_m = E_m \psi_m . \tag{3.37}$$

It is easy to see that, if the quantity

$$\epsilon(\omega) \equiv \min(H_{qq}) - \omega \tag{3.38}$$

is positive for ω in the region of interest, the following operator inequality holds:

$$d(\omega) < H_{pq} H_{qp} / \epsilon(\omega) . \tag{3.39}$$

Because $\epsilon(\omega)$ has only one zero, the equation

$$[H_{pp} - H_{pq} H_{qp} / \epsilon(E_m^{NL})] \psi_m^{NL} = E_m^{NL} \psi_m^{NL} \tag{3.40}$$

can be shown to have *exactly* M solutions E_m^{NL} $[m \leq M,\ E_m^{NL} \leq \min(H_{qq})]$. A well-known theorem[38] states that the effect of adding any positive Hermitian operator to a Hermitian operator is to increase each of its eigenvalues. From Eqs. (3.35), (3.36), (3.37), and (3.39) this theorem can be used to show that each solution E_m^{NL} of Eq. (3.40) is a lower bound to the corresponding eigenvalue E_m of H so that

$$E_m^{NL} \leq E_m . \tag{3.41}$$

Use of the bound given by (3.41) involves estimation of the energy denominator

$$\epsilon \equiv \epsilon(E_m^{NL}) = \min(H_{qq}) - E_m^{NL} . \tag{3.42}$$

If the vectors $\{\psi_m^{\text{approx}}\ (m \leq M)\}$ are all close approximations to the corresponding exact eigenvectors, the space on which q projects will be almost an invariant subspace of H. Consequently, $\min(H_{qq})$ can be approximated by E_{i_0}, the lowest *excluded* eigenvalue of H. If $E_{i_0} < E_M^{NL}$, the method fails because ϵ is no longer positive. Therefore, the method is adversely affected by the presence of intruder states. If it is assumed that the lowest intruder-state energy is above the M'th repre-

sented-state energy, then $E_{M'}$ can be used as a lower bound on E_{i_0}, so that

$$\epsilon \simeq E_{M'} - E_m^{NL} , \tag{3.43}$$

where the dependence of ϵ on m is left implict. If intruder states are absent, one can take $E_{M'} = E_M$.

In practice we take the self-consistency aspects of Eq. (3.40) into account only approximately. First, we replace E_m^{NL} in Eq. (3.43) by a fixed estimate

$$E_m^{NL} \simeq \bar{E}_m . \tag{3.44}$$

Second, we approximate the appropriate eigenvalue of the full operator in Eq. (3.40) by the expectation

$$\langle \xi_m | [H_{pp} - H_{pq} H_{qp} / \epsilon] | \xi_m \rangle = \bar{E}_m - \sigma_m^2/\epsilon , \tag{3.45}$$

where σ_m is given by Eq. (3.30). The errors of these approximations are small, of the same order as the error of Eq. (3.20). The end result is the approximate bound

$$\bar{E}_m - \sigma_m^2/\epsilon \leq E_m, \tag{3.46}$$

which closely resembles well-known results given by Wilkinson[39] and Temple.[40] We call Eq. (3.46) the σ^2/ϵ bound; this bound and the σ bound [Eq. (3.32)] will be applied to get the lower bounds in Sec. IV. Upper bounds are available from Eq. (3.29).

IV. NUMERICAL RESULTS

A. Solvable test Hamiltonians

The model space chosen for 0^+ states of ^{18}O consists of the three 0^+ configurations of two particles distributed in the s-d shell outside the ^{16}O core. We call these states 2p-0h states, where p (h) denotes a particle (hole) relative to the ^{16}O closed core. For our solvable test Hamiltonians, the excluded space consists of 168 3p-1h and 4p-2h 0^+ configurations, altogether. Holes are restricted to the $1p_{1/2}$ shell; particles are restricted to the $2s$-$1d$ and $2p$-$1f$ shells. Configurations with holes in the $1p_{3/2}$ shell are important in producing collective effects, but we omit them to keep the problem computationally feasible.

Two sets of single-particle energies were used. The first choice, denoted STD, arbitrarily uses experimental single-particle energies with respect to the ^{16}O core. Namely, we use $\epsilon(1p_{1/2}) = -10.67$, $\epsilon(1d_{5/2}) = -4.15$, $\epsilon(2s_{1/2}) = -3.28$, and $\epsilon(1d_{5/2}) = +0.96$ (henceforth, all energies are given in MeV units). The p and f shells are taken to be degenerate at the unrealistically low energy of 8.83 MeV. The second choice, denoted DEG, differs from the STD case only in the choice of the single-particle energies in the s-d shell. Here we use a $(2j+1)$-weighted average energy of -2.3017 MeV, degenerate in the three s-d orbitals. For the matrix elements of V, the two-body matrix elements of Kuo and Lee[41] were used. PVV[2] give an extensive discussion of the above choice of the configuration space, the single-particle energies, and the two-body matrix elements, so it will not be repeated here.

In the STD case, a physical intruder state arises, as well as several back-door intruders, but there are no intruders in the DEG case. This permits study of the influence of the intruders.

In the next two subsections, we will discuss calculations of the energies of the 0^+ represented states and the 0^+ matrix elements of the effective interaction. The PT results are compared with exact calculations. Results with Padé approximants to the perturbation series and error bounds to the energies are also given and discussed.

B. Energies

The exact energies E_m and the (normalized) model-space projections χ_m of the corresponding represented states ψ_m are given in Table I for the STD and the DEG cases. Considerable mixing of model-space configurations is seen, although ψ_m lies mainly in the model space.

The PT calculations of the energies were carried out through sixth order. In effective-interaction calculations that do not arbitrarily limit intermediate-state degrees of freedom, the num-

TABLE I. Exact eigenvalues E_m and amplitudes $\langle \phi_{m'} | \chi_m \rangle$ for model-space projections of represented eigenvectors ψ_m, with norms $\langle \chi_m | \chi_m \rangle$.

		STD			DEG		
$\phi_{m'}$	E_m	−57.689	−54.775	−44.806	−55.695	−52.603	−49.095
$(d_{3/2})^2$		0.212	−0.059	−0.815	0.491	−0.230	0.720
$(s_{1/2})^2$		0.354	0.831	0.039	0.361	0.835	0.013
$(d_{5/2})^2$		0.808	−0.373	0.179	0.668	−0.305	−0.507
$\langle \chi_m \vert \chi_m \rangle$		0.823	0.833	0.679	0.819	0.843	0.776

TABLE II. Terms of PT for expectation $g=\langle\chi^{(4)}|\mathfrak{D}(E_m^{(4)},z)|\chi^{(4)}\rangle=g_0+zg_1+z^2g_2+\cdots$.

	STD			DEG		
E_m	−57.689	−54.775	−44.806	−55.695	−55.603	−49.095
$\hat{k}$	0.611	0.687	1.229	0.653	0.743	0.881
$\check{k}$	−0.669	−0.779	−1.836	−0.587	−0.669	−0.796
g_0	−3.683	−3.307	−4.101	−3.377	−3.137	−3.896
g_1	−0.120	−0.076	+0.129	−0.303	−0.122	+0.096
g_2	−0.304	−0.235	−0.717	−0.262	−0.195	−0.400
$\mathcal{K}$ [a]	0.318	0.289	0.385	0.353	0.285	0.295
$\langle\chi_m^{(4)}\|\chi_m^{(4)}\rangle$	0.839	0.841	0.743	0.843	0.853	0.801
α [b]	−0.192	−0.189	−0.346	−0.186	−0.172	−0.248

[a] Defined by Eq. (4.2).
[b] Defined by $\alpha=(1-\langle\chi_m^{(4)}|\chi_m^{(4)}\rangle)/\langle\chi_m^{(4)}|\chi_m^{(4)}\rangle$.

ber of intermediate states increases rapidly with the order of PT. This fact has so far prevented the application of PT beyond the third order,[21] except for averaged matrix elements.[42] In the present calculation, we have made a concession to practicality by keeping the number of intermediate states fixed, and so we are able to carry the calculation to higher orders (at least 20). This helps us to observe the dependence of the errors and bounds on the order of PT. Table II shows the terms through sixth order in PT for $g(1)$, defined by Eq. (3.9), for the STD and DEG cases, taking $\xi=\chi^{(4)}$, $\omega=E^{(4)}$, and $z=1$. Even in those cases where the series is known to converge (because the values of $\hat{k}$ and $\check{k}$ are both numerically less than unity), the (fourth-order term g_2 is often larger than the (third-order) term g_1. On the other hand, the (third- and fourth-order) terms g_1, g_2 are always much smaller than the second-order term g_0. This behavior contrasts with that of the Rayleigh-Schrödinger (RS) perturbation series,[2,11] where the third-order term is often larger than second order (but nevertheless produces an improvement). The quantity $g(1)$ represented by this series is not directly meaningful, so we do not quote its value.

Each energy $E^{(n)}$ was calculated by constructing and diagonalizing $\mathfrak{IC}^{(n)}(\omega)$ and then solving Eqs. (2.11) and (2.12) self-consistently by the Regula Falsi method.[43] Because we preferred to eliminate contamination of the errors studied by spurious errors from lack of self-consistency, we iterated until self-consistency was achieved to four decimal places. Four iterations usually sufficed.

In Table III we display the errors of PT for the energies in the STD case and the DEG case. From column 3, we see that the energies obtained from PT are higher than the corresponding exact values, with only one exception: in the STD case, the energy of the third state for sixth-order PT is lower than the exact value. We believe that this exception is associated with the interaction of this state with the intruder, whose influence becomes stronger as the order of PT increases. However, we are not aware of any general proof that PT energies are upper bounds, except in the case of odd orders when physical intruders are absent. Our observation that odd orders of PT form upper bounds, even when $\hat{k}>1$, can be interpreted as evidence that the intruders have limited influence, in these low orders.

In the STD case, the errors of second-order PT range from 0.343 to 0.574, while the errors of third-order PT range from 0.263 to 0.755. Thus, the quality of agreement is about the same in second and third orders; and the DEG case is similar in this respect. In both cases, fourth order brings a considerable improvement: the error becomes less than 0.18 MeV for all three represented states. This is a good enough level of accuracy to be very useful, if it could be attained in realistic calculations. In both DEG and STD cases, the error for the two lowest energies continues to decrease as the order n increases, although odd n produces less improvement than even n. For the third energy, these same remarks apply to the DEG case, but in the STD case higher orders behave unpredictably. This feature of the STD case is probably due to the intruder state.

In column 2 of Table III, we tabulate the radian measure of θ, the (positive) angle between the exact and approximate model-space projections of the represented states, defined by

$$\cos\theta=|\langle\chi_m|\chi_m^{(n)}\rangle|/(\langle\chi_m|\chi_m\rangle\langle\chi_m^{(n)}|\chi_m^{(n)}\rangle)^{1/2}. \tag{4.1}$$

This way of representing the overlap between states is especially convenient when a small num-

TABLE III. Errors of Bloch-Horowitz perturbation theory for energies. All results in a given row n use wave operators Ω through order $n-1$.

	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
				Upper bounds			Lower bounds				
	n	θ	$E^{(n)}-E$	$\bar{E}-E$	$E^{MU}-E$	$E-(\bar{E}-\sigma)$	$E-(\bar{E}-\sigma^2/\epsilon)$	$E-E^{ML}$	σ	$\hat{k}_{\text{vir}}$	ϵ_{vir}
	I_Q	$n-1$	$n-1$	$2n-2$	$n-1$	$2n-1$	$2n-1$	$n-1$	$2n-1$	...	...
						(a) STD case					
$E=-57.689$, $\hat{k}=0.613$, $\check{k}=-0.669$	1	0.022	4.227	4.227	a	5.512	35.903	a	9.739	a	22.44
	2	0.075	0.480	0.377	a	2.290	2.184	a	2.667	a	18.87
	3	0.020	0.384	0.087	0.372	1.105	0.422	a	1.193	a	16.36
	4	0.018	0.121	0.029		0.624	0.121	0.232	0.652	0.385	14.66
	5	0.006	0.094	0.010		0.220	0.068		0.223		4.97
	6	0.006	0.039	0.004		0.362	0.043		0.372		35
$E=-54.775$, $\hat{k}=0.687$, $\check{k}=-0.779$	1	0.045	3.677	3.677	a	4.966	27.933[b]	a	8.643	a	20.32
	2	0.103	0.343	0.259	a	1.947	1.494[b]	a	2.206	a	18.79
	3	0.034	0.263	0.047	0.255	0.852	0.243[b]	a	0.899	a	17.20
	4	0.033	0.059	0.014		0.452	0.062[b]	0.338	0.466	0.320	15.51
	5	0.013	0.051	0.005		0.179	0.006[b]		0.181		6.55
	6	0.013	0.014	0.002		0.269	0.024[b]		0.275		38
$E=-44.806$, $\hat{k}=1.1229$, $\check{k}=-1.836$	1	0.035	4.815	4.815[c]	a	3.748	26.208[b]	a	8.563	a	15.23
	2	0.026	0.574	0.689[c]	a	2.030	1.197[b]	a	2.719	a	10.73
	3	0.053	0.755	0.484[c]	0.648[d]	2.282	2.255[b]	a	2.765	a	15.80
	4	0.012	0.098	0.356[c]		2.090	1.741[b]	2.884[e]	2.446	0.402	16.81
	5	0.062	0.439	1.535[c]		3.920	8.544[b]		5.378		18.84
	6	0.026	−0.074	1.458[c]		3.918	8.839[b]		5.454		20
						(b) DEG case					
$E=-55.695$, $\hat{k}=0.653$, $\check{k}=-0.587$	1	0.048	4.108	4.018	a	5.350	8.984	a	9.457	a	21.77
	2	0.049	0.675	0.400	a	2.094	0.588	a	2.493	a	15.54
	3	0.023	0.406	0.107	0.363	1.039	0.091	a	1.145	a	12.25
	4	0.014	0.178	0.040		0.614	0.026	0.243	0.654	0.434	10.69
	5	0.008	0.114	0.016		0.385	0.009		0.401		10.05
	6	0.005	0.064	0.007		0.248	0.003		0.255		9.3
$E=-52.603$, $\hat{k}=0.743$, $\check{k}=-0.669$	1	0.034	3.527	3.527	a	5.091	13.659[f]	a	8.617	a	21.05
	2	0.071	0.357	0.242	a	1.774	0.913[f]	a	2.016	a	16.79
	3	0.037	0.243	0.045	0.235	0.758	0.130[f]	a	0.803	a	14.33
	4	0.026	0.073	0.013		0.380	0.030[f]	0.394	0.393	0.346	11.88
	5	0.016	0.048	0.005		0.212	0.008[f]		0.217		9.42
	6	0.012	0.020	0.002		0.131	0.003[f]		0.133		9
$E=-49.095$, $\hat{k}=0.881$, $\check{k}=-0.796$	1	0.072	4.339	4.339	a	4.560	13.987[g]	a	8.898	a	18.25
	2	0.011	0.369	0.452	a	2.105	1.405[g]	a	2.556	a	14.45
	3	0.029	0.453	0.115	0.452	1.156	0.320[g]	a	1.272	a	14.06
	4	0.016	0.115	0.044		0.682	0.104[g]	1.845[h]	0.727	0.410	12.01
	5	0.018	0.124	0.018		0.441	0.041[g]		0.458		11.65
	6	0.013	0.044	0.009		0.304	0.019[g]		0.313		11

[a] No MT bound exists.
[b] Quasibound, using $\epsilon = E_2^{(n)} - E_1^{(n)}$, appropriate to the $E=-57.689$ case.
[c] Quasibound, because an intruder state lies below this represented state.
[d] Quasibound, because $\hat{k} > 1$, although the value is independent of $\hat{k}$.
[e] Quasibound, using $\hat{k}$ from the corresponding DEG case.
[f] Rigorous bound, using $\epsilon = E_3^{(n)} - E_2^{(n)}$.
[g] Quasibound, using $\epsilon = E_3^{(n)} - E_2^{(n)}$, appropriate to the $E=-52.603$ case.
[h] Uses exact $\hat{k}$, corresponding STD case.

ber of decimal places is desirable in the presentation. For small θ, θ is approximately the norm of $\chi - \chi^{(n)}$, the error vector. Overlap $\cos\theta \geq 0.99$ corresponds to $\theta \leq 0.14$. Our results show that, for every order of PT, the overlap between the exact and the approximate model states is good, at worst 0.9947. The reason for such high overlaps may be connected with the fact that the energy range of the

represented states is quite large, so that the off-diagonal elements have rather small influence. However, the overlaps are very similar in the STD case (where the energy range is $E_3 - E_1 = 12.883$) and the DEG case (where the energy range is only $E_3 - E_1 = 6.600$), and the mixing among model-space basis states is quite strong (Table I). This suggests that χ is determined mainly by H_{PP} and is little affected by $\mathfrak{D}$ in Eq. (2.20). The procedure of ordinary[44] degenerate PT begins by diagonalizing H_{PP}; the θ values show that this may be appropriate for our cases.

C. Norm bounds; quasibounds

Before comparing the different bounds shown in Table III we must discuss what comparisons are most appropriate.

Table III is arranged so that all results in a given row are obtained with the use of a wave operator Ω approximated to the *same* order $n-1$. For orientation, the reader may like to think in terms of the nondegenerate case, $M=1$, where the wave operator is essentially just $\Omega^{(n)} = |\psi_1^{(n)}\rangle\langle\phi_1|$, but with $\psi_1^{(n)}$ normalized so that $\langle\psi_1^{(n)}|\phi_1\rangle = 1$. For example, the $n=3$ row contains $E^{(3)} - E$; $E^{(3)}$ is calculated from $\mathcal{H}^{(3)}(\omega)$, which uses $\Omega^{(2)}$ [because of Eq. (2.18)]. Therefore, the θ in this row is obtained from $\psi^{(3)}$, which also uses $\Omega^{(2)}$. Similarly, the calculation of all the bounds shown in this row involves at most $\Omega^{(2)}$. If the calculation of a wave operator $\Omega^{(n-1)}$ of given order $n-1$ is considered to be the limiting factor, this type of comparison is appropriate.

However, a different criterion of difficulty may be more relevant in practice: I_Q, the maximum number of Q-space intermediate-state sums that must be performed to construct a given term. Expressions for I_Q are therefore shown in the first row of Table III. As an example, $E^{(n)}$ and E^{ML} for $n=4$ involve the same value of I_Q as $\overline{E} - \sigma$ and $\overline{E} - \sigma^2/\epsilon$ for $n=2$, namely $I_Q = 3$. We shall often give weight to the I_Q criterion.

Column 4 of Table III shows the deviations from the exact energy of the variational upper bound $\overline{E}$; we see that the quantities $\overline{E}$ are indeed upper bounds, as the theory predicts. They are always closer to the exact values than are the $E^{(n)}$, and more so for higher orders (which is not unreasonable, since $I_Q = 2n-2$ for $\overline{E}$). The errors are very similar for $E^{(3)}$ and for $\overline{E}$ in second order, even for the third state in the STD case (in spite of the presence of intruder states).

The quantities $\overline{E}$ can be regarded as norm upper bounds to the energies, so discussion of other norm bounds is now appropriate. In column 9 of Table III, we display the values of σ_m, defined by Eq. (3.30). They decrease with increasing order of PT except for the third state in the STD case, where σ_m increases, probably because of mixing with the intruder state. For all other cases in second-order PT the lower bounds $\overline{E} - \sigma$ (column 6) are about 2 MeV below the exact value, but the difference decreases to about 1 and 0.5 MeV in the third and fourth orders. Except for solvable test cases, the quantity σ_m is not calculable for $n \geq 3$, and computing σ_m for $n=2$ is about as difficult as doing fourth-order PT. Nevertheless, we calculated norm bounds for higher orders to examine their behavior.

The other norm bounds, $\overline{E} - \sigma^2/\epsilon$, are usually better than the $\overline{E} - \sigma$ bound, as shown by comparing columns 6 and 7 of Table III. Exceptions occur both when the estimate of ϵ is small ($\lesssim \sigma$) and when ϵ is nonexistent (because an intruder state lies below the represented state). To simulate a possible practical procedure, we began by assuming only that no intruder exists in the DEG case, so that $\epsilon = E_3^{(4)} - E_1^{(4)}$ and $\epsilon = E_3^{(4)} - E_2^{(4)}$ were justifiable estimates for the E_1 and E_2 cases, respectively. This provided no estimate of ϵ for the E_3 case, so $\epsilon = E_3^{(4)} - E_2^{(4)}$ was arbitrarily tried. Although there is no proof that $\overline{E} - \sigma^2/\epsilon$ will generally give a lower bound, for this value of ϵ, we find that $E - (\overline{E} - \sigma^2/\epsilon)$ in fact turns out to be positive.

Except where noted, $\epsilon = E_{M'}^{(n)} - E_M^{(n)}$ is used in Table III. This choice corresponds to Eqs. (3.43) and (3.44).

To discuss other possible choices of ϵ, we introduce the idea of a *quasibound*. Given a formula that has been proved, under certain conditions, to give a rigorous inequality, a quasibound is any number obtained by substituting, for some input data, *ad hoc* values that may violate one or more conditions of the proof. A quasibound may or may not be a bound; its use as an estimate involves some element of risk. The concept can be useful only if there are simple empirically founded rules for choosing the *ad hoc* data. One method of formulating such rules is to use solvable test cases to compute virtual values of the *ad hoc* data, i.e., values such that they give the *exact* energy, when substituted into the formula for the bound.

In this spirit we have computed virtual values ϵ_{vir} of the parameter ϵ, which are tabulated in column 11 of Table III. The smallest value of ϵ_{vir} is 4.97; consequently, the quasibound $\overline{E} - \sigma^2/\epsilon$ will be a bound in all our test cases, provided that $0 < \epsilon < 4.97$. The small and systematic variation of ϵ_{vir} gives hope that a minimum value can be quite easily and safely inferred from experience. For comparison with the other lower bounds, we can mention that $\epsilon = 4$ would give $E - (\overline{E} - \sigma^2/\epsilon) = 0.267$ for the STD ground state in third order.

Quasibounds are of course not a new idea. For example, in variational calculations of the energies of three-nucleon bound states, lower bounds are estimated by techniques[45] very similar to those giving our quasibound, $\overline{E}-\sigma^2/\epsilon$.

D. PT bounds and quasibounds

The simplest MT upper bound, E^{MU}, given by Eq. (3.20), depends only on knowledge of μ_0 and μ_1, i.e., on information through third order in PT. No knowledge of $\hat{k}$ of $\check{k}$ is needed,[46] as is shown explicitly by Eq. (3.18). Column 5 of Table III lists the deviations of these MT upper bounds from the exact energies. Encouragingly, they are slightly tighter upper bounds than the $\overline{E}$ bounds for $n=2$, and are equally easy to calculate, requiring at most I_Q intermediate-state sums. Because of this success, we do not need to discuss higher-order MT upper bounds, which would correspond to odd $n \geq 5$.

The simplest MT lower bound, E^{ML}, depends on μ_0, μ_1, and μ_2, i.e., on information through fourth order in PT, and on $\hat{k}$ in addition. As the derivation of Eq. (3.18b) for $g_{[1/1]}(1)$ shows, only a quasibound results if $\hat{k}>1$. Of course the value of $\hat{k}$ is not known, in a realistic calculation, but must be estimated. To develop a strategy for this, we first calculate the exact values of $\hat{k}$, by numerically diagonalizing K. Table III shows, in column 8, values of $E-E^{ML}$ calculated with $n=4$ and the exact values of $\hat{k}$. These are best possible bounds, and any larger value of $\hat{k}$ would lead to looser bounds. These E^{ML} bounds tend to lie between the $\overline{E}-\sigma$ and $\overline{E}-\sigma^2/\epsilon$ bounds. For the third state in the STD case, the value of E^{ML} was calculated using $\hat{k}=0.881$, instead of the true value 1.229 (which would not be admissible). Therefore, this entry in the table is only a quasibound.

Virtual values $\hat{k}_{\rm vir}$ of $\hat{k}$ can also be computed[47] such that $E^{MU}(\hat{k}_{\rm vir},\mu_0,\mu_1,\mu_2)=E$. These appear in column 10. They are strikingly uniform, ranging from 0.320 to 0.434 for all the STD and DEG cases considered. It may, therefore, be easy to estimate $\hat{k}_{\rm vir}$, which might perhaps be related to the quantity[48]

$$\mathcal{K}=\frac{\mu_1}{\mu_0}+\left[\frac{\mu_2}{\mu_0}-\left(\frac{\mu_1}{\mu_0}\right)^2\right]^{1/2} \tag{4.2}$$

which was given in Table II. Apparently such a choice as

$$\hat{k} \leq 2\mathcal{K} \tag{4.3}$$

would provide quite safe quasibounds, in our cases. Fortunately, E^{ML} is a slowly varying function of $\hat{k}$, so that the exact value does not matter much, as long as it is not too near $\hat{k}=1$. Using Eq. (4.3) gives $E-E^{ML}=1.140$ (0.184) for the third state in the STD (DEG) case, and $E-E^{ML}>0$ always.

E. Effective interaction $\mathcal{V}$ from the Bloch-Horowitz method (Ref. 49)

The energy-independent interaction $\mathcal{V}$ is obtained from Eq. (2.29). From the self-consistent eigenvalues and eigenvectors of the lowest three represented states, obtained for each order of PT, we constructed the effective Hamiltonian $\mathcal{H}$. The energy of the core and the single-particle energies were also calculated self-consistently for each order of PT. The errors in the energies for ^{16}O are displayed in Table IV, together with norm and MT upper and lower bounds, for STD and DEG, as for the ^{18}O case. Perturbation theory succeeds much better here than for ^{18}O. The exact effective interaction matrix elements are shown in Table V, together with the matrix elements of the difference

$$e_n \equiv \mathcal{V}-\mathcal{V}^{(n)} \tag{4.4}$$

between the exact and the approximate $\mathcal{V}$. In the last column an average absolute error, $\bar{e}_n$, was calculated for each order of PT as a guide to the

TABLE IV. Energies for ^{16}O (STD case) with error analysis.

	(1) n	(2) $E^{(n)}-E$	(3) $\overline{E}-E$	(4) $E^{MU}-E$	(5) $E-(\overline{E}-\sigma)$	(6) $E-(\overline{E}-\sigma^2/\epsilon)$	(7) $E-E^{ML}$	(8) σ	(9) $\hat{k}_{\rm vir}$	(10) $\epsilon_{\rm vir}$
$E=-44.770$	1	2.090	2.090	a	3.681	0.463[b]	a	5.770	a	15.93
$\hat{k}=0.297$	2	0.019	0.079	a	1.198	0.046[b]	a	1.276	a	20.6
$\check{k}=-0.536$	3	0.079	0.004	0.078	0.256	0.001[b]	a	0.260	a	17
$\mathcal{K}=0.166$	4	0.004	0.000		0.084	0.000[b]	0.010	0.084	0.228	c
	5	0.005	0.000		0.024	0.000[b]		0.024		c
	6	0.000	0.000		0.011	0.000[b]		0.011		c

[a] No MT bound exists.

[b] Quasibounds using $\epsilon=13.04$, the lowest zero-order excitation energy.

[c] Four-decimal accuracy is inadequate to compute $\epsilon_{\rm vir}$.

TABLE V. Errors e_n in energy-independent $\mathcal{U}$, calculated by Bloch-Horowitz (Ref. 49) perturbation theory of order n, with mean absolute errors $\bar{e}_n$. [1 $= (d_{5/2})^2$, $2 = (s_{1/2})^2$, $3 = (d_{3/2})^2$.]

		n \ (m,m')	(1,1)	(1,2)	(1,3)	(2,1)	(2,2)	(2,3)	(3,1)	(3,2)	(3,3)	Present $\bar{e}_n$	PVV[2] $\bar{e}_n$
STD	$\langle m\|e_n\|m'\rangle$	1	−0.492	−0.294	0.532	−0.202	−0.274	−0.093	0.246	−0.084	−0.145	0.262	0.262
		2	−0.135	−0.215	−0.202	−0.137	−0.165	−0.194	−0.040	−0.125	−0.263	0.164	0.213
		3	−0.028	−0.130	+0.683	−0.047	+0.029	−0.104	0.096	−0.058	−0.244	0.158	0.054
		4	0.005	−0.084	−0.140	−0.046	−0.060	0.003	0.000	−0.037	−0.068	0.049	0.198
		5	−0.117	−0.073	0.800	−0.019	+0.012	0.001	0.048	−0.017	−0.164	0.139	0.260
		6	0.061	−0.027	−0.270	−0.040	−0.029	0.122	−0.012	−0.015	0.026	0.067	0.514
	$\langle m\|\mathcal{U}\|m'\rangle$		−1.838	−0.989	−2.630	−0.897	−1.897	−0.661	−2.916	−0.652	−0.200		
DEG	$\langle m\|e_n\|m'\rangle$	1	−0.390	−0.263	0.351	−0.260	−0.282	−0.031	0.202	−0.117	−0.065	0.218	0.218
		2	−0.144	−0.220	−0.028	−0.196	−0.139	−0.079	−0.095	−0.154	−0.096	0.128	0.183
		3	+0.040	−0.118	+0.166	−0.113	+0.021	−0.009	0.036	−0.080	−0.077	0.073	0.056
		4	−0.058	−0.085	+0.054	−0.083	−0.045	0.009	−0.025	−0.052	−0.024	0.048	0.063
		5	+0.024	−0.054	0.087	−0.061	−0.014	0.024	−0.005	−0.032	−0.014	0.035	0.034
		6	−0.035	−0.040	0.046	−0.048	−0.021	0.026	−0.018	−0.022	+0.003	0.029	0.033
	$\langle m\|\mathcal{U}\|m'\rangle$		−1.736	−0.958	−2.811	−0.955	−1.889	−0.599	−2.960	−0.685	−0.120		

trend of agreement. In the DEG case the error decreases steadily by uniform factors, whereas in the STD case the decrease is less rapid for the first three orders and there are fluctuations rather than a monotonic decrease. For both STD and DEG cases, the average absolute error $\bar{e}_4$ for the matrix elements calculated through fourth order is less than 0.05 MeV. We note that the Bloch-Horowitz[49] errors are smaller than the Brandow[50] errors, for orders $n \geq 4$; however, Brandow PT gives better approximations in third order. The errors in the STD case are dominated by the (1,3), (2,3), and (3,3) matrix elements, as in the PVV calculation by Brandow PT. The behavior of the individual errors is not so obvious in the DEG case.

F. Energies from the Brandow method (Ref. 50)

PVV[2] calculated $\tilde{\mathcal{H}}$ for the STD and DEG cases, using the Brandow[22,50] version of PT. Since $\tilde{\mathcal{H}}^{(n)}$ is neither symmetric nor equal to $\tilde{\mathcal{H}}$, it is not *a priori* clear that it has real eigenvalues and eigenvectors. However, consideration of the Gershgorin disks[16] shows that if the antisymmetric part of $\mathcal{H}^{(n)}$ is sufficiently small compared with the spacing of the eigenvalues of the real part, the eigenvalues and eigenvectors are *exactly* real. This turns out to be true for both the STD and DEG cases, so we obtain real energies from the approximate $\tilde{\mathcal{H}}^{(n)}$. These are compared with the ex-

TABLE VI. Comparison of errors of eigenvalues (B-RS) computed from Brandow (Ref. 50) calculation (Ref. 2) of energy-independent $\tilde{\mathcal{H}}$, with present results (B-H) from Bloch-Horowitz (Ref. 49) PT for ^{18}O.

		DEG		STD	
	n	B-RS	B-H	B-RS	B-H
$E = -55.695$	1	4.108	4.108	4.227	4.227
	2	0.778	0.675	1.001	0.480
	3	0.263	0.406	0.186	0.384
	4	−0.272	0.178	−0.166	0.121
	5	−0.032	0.114	−0.354	0.094
	6	+0.116	0.064	1.044	0.039
$E = -52.603$	1	3.527	3.527	3.677	3.677
	2	0.497	0.357	0.664	0.343
	3	0.314	0.243	0.354	0.263
	4	−0.162	0.073	−0.416	0.059
	5	−0.066	0.048	−0.147	0.051
	6	0.061	0.020	0.191	0.014
$E = -49.095$	1	4.339	4.339	4.815	4.815
	2	−0.059	0.369	0.198	0.574
	3	0.417	0.453	0.757	0.755
	4	−0.036	0.115	−0.347	0.098
	5	−0.127	0.124	0.105	0.439
	6	−0.001	0.044	0.688	−0.074

act energies, and with the present results of Bloch-Horowitz PT, in Table VI. The results are hard to interpret. The Brandow results depend less sytematically on order n than the Bloch-Horowitz results.

G. Pseudo-Padé approximants

This subsection deals with empirical tests of an arbitrary method that aims to improve on PT. We write the energy E of a represented state as a power series in x, as follows:

$$E(x) = E^{(0)} + x\Delta E^{(1)} + x^2\Delta E^{(2)} + \cdots , \tag{4.5}$$

where

$$\Delta E^{(n)} \equiv E^{(n)} - E^{(n-1)} . \tag{4.6}$$

[Note that Eq. (4.5) is not the Rayleigh-Schrödinger perturbation series.] Then we calculate the Padé approximants to the series (4.5).

The Brillouin-Wigner perturbation expansion for the effective Hamiltonian is a geometric series, so the Padé approximants to the matrix $\tilde{\mathcal{H}}(\omega)$ [denoted $\mathcal{H}_{[N/L]}(\omega)$] would be a natural approximation. Kuo and others[26,20] have tested Padé approximants, and it has been found that approximate energies obtained from $\mathcal{H}_{[n+1/n]}(\omega)$ are better than those obtained from $\mathcal{H}^{(n)}(\omega)$. In contrast, our method is only empirically motivated, and so we call the Padé approximants in the series (4.5) "pseudo-Padé approximants" (PPA).

In Table VII, we display the results of the [1/2] and [2/1] PPA to the series for $E(x=1)$. The [0/1] PPA (not tabulated) gives poor approximations. Both the [1/2] and [2/1] PPA use information from PT through third order. The [2/1] approximants are negligibly better than the third-order PT results. However, the [1/2] PPA provides remarkably better approximations than the corresponding third-order PT.

We also applied the same technique to the individual matrix elements of the effective interaction v[Eq. (2.29)]. The [1/2] PPA in the DEG case gives an average error $\bar{e}^{\rm PPA}_{[1/2]} = 0.053$ compared with $\bar{e}_4 = 0.048$ from PT. In the STD case the [1/2] PAA error is $\bar{e}^{\rm PPA}_{[1/2]} = 0.095$ compared with $\bar{e}_4 = 0.158$. So this method does not give reliable improvement over PT.

It would be interesting to see whether the observed success of the pseudo-Padé approximants to the energies persists for other Hamiltonians.

TABLE VII. Differences $E - E_{[N/L]}$ of pseudo-Padé approximants from the corresponding exact energies for ^{18}O.

	STD		DEG	
$[N/L]$	[2/1]	[1/2]	[2/1]	[1/2]
$E_1 - E_1[N/L]$	−0.382	−0.084	−0.383	−0.120
$E_2 - E_2[N/L]$	−0.261	−0.017	−0.240	−0.009
$E_3 - E_3[N/L]$	−0.747	−0.293	−0.452	−0.079

V. CONCLUSIONS

From the present study of solvable test problems, we see that low orders of Bloch-Horowitz PT (especially $n=4$) can provide satisfactory approximations to the energies and the effective interaction. This holds even in the presence of intruder states, which cause the PT expansion to diverge. Experience with Brandow PT, applied to the same Hamiltonians, has previously led[2,11] to similar conclusions for that method, except that the optimal order of PT was $n=3$, rather than $n=4$.

In even orders, Bloch-Horowitz PT seems to be much less affected by intruders than in Brandow PT. Although odd orders of Bloch-Horowitz PT do slightly improve the approximation, even orders provide more marked improvements. No general reasons for this are known.

The model-space projections of the PT and exact represented wave functions have overlaps better than 0.99, even in first-order PT. This suggests that diagonalization of H_{PP}, followed by nondegenerate Brillouin-Wigner PT, may be a successful approach. It also means that the pseudo-Padé approximants discussed in Sec. IV E are close to true Padé approximants, because the model-space vector $\chi^{(n)}$ can be regarded as the same in all orders. Thus, some theoretical basis might be found for the success of the [1/2] pseudo-Padé approximants.

Two varieties of upper bounds are available: the MT upper bounds E^{MU}, and the variational bounds $\bar{E}$. Both types are rigorous when no *physical* intruder states are present. They are unaffected by back-door intruders. The third-order E^{MU} bounds, which require only the terms of PT through third order, are better than the second-order bounds $\bar{E}$; both involve two intermediate state sums. When either the E^{MU} bound or the $\bar{E}$ bound is applied to a state that lies above an intruder state, the result is only a quasibound, in the sense that the conditions of the derivation are not satisfied. Nevertheless, E^{MU} and $\bar{E}$ give satisfactory bounds in our test cases.

Lower bounds are more difficult to calculate than upper bounds, and tend to be looser, though, again, they are unaffected by back-door intruders. The MT lower bounds require at least fourth-order PT. They can be derived rigorously, but because

they require estimation of the parameter $\hat{k}$, in practice they are only quasibounds. In the same way, the lower bounds of the form $\overline{E}-\sigma^2/\epsilon$ are in practice only quasibounds, because ϵ must be estimated. Nevertheless, the E^{ML} and $\overline{E}-\sigma^2/\epsilon$ lower quasibounds are both quite reliable, because they are not very sensitive to the estimated information. They are tight enough to be useful, though they are noticably looser for the third energy in the STD case, which is influenced by an intruder state.

The behavior of the quasibounds suggests that physical intruder states have more effect on the tightness of the bounds than on the accuracy of the simple fourth-order Bloch-Horowitz results. The sensitivity of the quasibounds to intruder states is a real difficulty that remains to be solved.

It is desirable to have lower bounds as well as upper bounds. We have seen, however, that MT lower bounds require at least fourth-order PT, and useful norm lower bounds require calculation of σ with eigenvectors correct to first order, at least. Both types of bounds require threefold intermediate-state sums. Nevertheless, the results of the present study should encourage calculation of the lower bounds, wherever possible.

Finally, we consider some of the inevitable limitations of our investigation. Our solvable test problems involve at most only 168 intermediate states; realistic problems are much larger. Therefore, it is possible that the errors will be much larger in realistic problems. Some idea of how the errors depend on the size of the problem can be gained by considering Table IV, which shows results for ^{16}O, with only nine intermediate states. The third-order error is 0.079 MeV for ^{16}O, whereas the largest corresponding error is 0.755 MeV for ^{18}O, a large increase. The errors of the effective interaction υ, displayed in Table V, are considerably smaller than the errors of the ^{18}O energies; this must be due to cancellation of errors in Eq. (2.29). To use our methods to estimate the errors in υ, upper and lower bounds for all the quantities on the right hand side of Eq. (2.29) would have to be combined in the most pessimistic possible way. The resulting bounds would inevitably be discouraging, because they would neglect the tendency of the errors to cancel.

This last difficulty is avoided in the standard linked-cluster methods, which formally exploit the cancellation of the separated core energies, to obtain direct approximations to υ. Unfortunately, the linked-cluster methods obscure the vector-space properties that make our error analysis possible. A task for the future will be to combine the linked-cluster approach with sufficient vector-space concepts to permit analysis of the errors.

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APPENDIX A: PROOF OF THE THEOREM IN SEC. II C

As a preliminary, we state the following three lemmas and a corollary.

Lemma 1. If $\omega < \min(H_{0QQ})$, then the eigenvalues k_j of K have the property

$$(k_j)^{-1}dk_j/d\omega \geq 0\,. \tag{A1}$$

Corollary 1. If $k_j(\omega_0) > 0$ (or $k_j(\omega_0) < 0$) then $dk_j(\omega)/d\omega > 0$ (or $dk_j(\omega) < 0$) for $\omega > \omega_0$.

Lemma 2. The operator

$$\Lambda \equiv (\omega - H_{0QQ})^{-1}V_{QQ} = -GV_{QQ} \tag{A2}$$

has the same eigenvalues as $K \equiv -G^{1/2}V_{QQ}G^{1/2}$, if $G > 0$.

Lemma 3. The series $\mathcal{S} = 1 + zK + z^2K^2 + \cdots$ converges if all eigenvalues of K are less than 1 in absolute value; it diverges if any eigenvalue of K is greater than 1 in absolute value.

Proof of Condition (a): Given a fixed value of $\omega > w_1$, where $w_1 = \min(H_{QQ})$, let $|\lambda_j(\omega)\rangle$ be an eigenvector of $\Lambda(\omega)$ corresponding to an eigenvalue $k_j(\omega)$, so that

$$(\omega - H_{0QQ})^{-1}V_{QQ}\,|\lambda_j(\omega)\rangle = k_j(\omega)\,|\lambda_j(\omega)\rangle\,. \tag{A3}$$

Let $|\psi^Q_{w_1}\rangle$ be the eigenvector of H_{QQ} corresponding to the eigenvalue w_1:

$$(\omega_1 - H_{0QQ} - V_{QQ})\,|\psi^Q_{w_1}\rangle = 0\,. \tag{A4}$$

Equation (A4) means that $\Lambda(w_1)$ has an eigenvalue $k_j(w_1) = 1$. Then according to Corollary 1, since $\omega > w_1$ it follows that $k_i(\omega) > k_i(w_1)$, i.e., $k_i(\omega) > 1$. Since Λ and K have the same set of eigenvalues, it follows that $K(\omega)$ has at least one eigenvalue larger than 1. Let $k_1 > 1$ be such an eigenvalue and $|k_1(\omega)\rangle$ be the corresponding eigenvector. Then by Lemma 3, the power series $\mathcal{S}$ will diverge at $z = 1$. [The proof for the case $\omega > \min(\overline{H}_{QQ})$ is similar.]

Proof of Condition (b): Let w_i be an eigenvalue of H_{QQ} and $\overline{w}_i$ be an eigenvalue of $\overline{H}_{QQ}$, where w_i and $\overline{w}_i$ are less than $\min(H_{QQ})$. Then from

$$(w_i - H_{0QQ} - V_{QQ})\,|\psi^Q_{w_i}\rangle = 0 \tag{A5}$$

and

$$(\overline{w}_i - H_{0QQ} + V_{QQ})\,|\psi^Q_{w_i}\rangle = 0\,, \tag{A6}$$

it follows that $\Lambda(\omega)$ and $K(\omega)$ have an eigenvalue equal to 1 (or -1) for $\omega = w_i$ (or $\omega = \overline{w}_i$). These values are the points (A, B, C) of intersection of the curves $k(\omega)$ with the lines $k = 1$ (or -1) as is

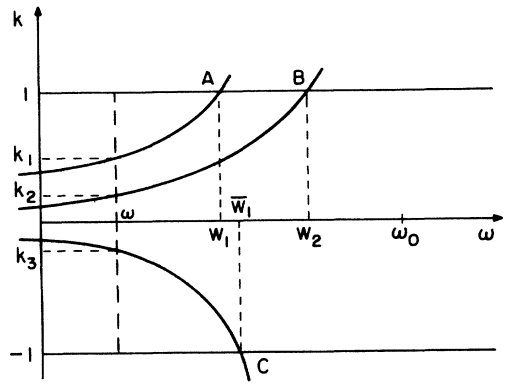

FIG. 3. Schematic graph of the eigenvalues k_i of K [Eq. (2.25)], for a three-dimensional excluded space. Points A and B correspond to eigenvalues w_1 and w_2 of H_{QQ}; point C corresponds to an eigenvalue $\bar{w}_1$ of $\bar{H}_{QQ} = H_{0QQ} - V_{QQ}$. If $\omega < \min(w_1, \bar{w}_1)$, all eigenvalues k_i satisfy $|k_i| < 1$, so that PT converges. If $\omega > \omega_0 \equiv \min(H_{0QQ})$, Eq. (2.22) is not satisfied, and the analysis fails.

shown in Fig. 3, for the case of a three-dimensional Q space. The indicated behavior of the eigenvalues $k(\omega)$ is a consequence of Corollary 1. From this figure it is seen that if ω is less than both $\min(H_{QQ})$ and $\min(\bar{H}_{QQ})$, the eigenvalues of $K(\omega)$ will be within the interval $(-1, 1)$, and then by Lemma 3 the series 8 will converge at $z = 1$. Otherwise, the series diverges.

APPENDIX B: COUNTEREXAMPLE TO BOUNDS BASED ON μ_0, μ_1, AND μ_2 ONLY

Let us assume that three constants μ_0, μ_1, and μ_2 are given, with μ_0 and μ_2 positive. We first show that it is always possible to choose a vector. $|f\rangle$ and a Hermitian operator K such that

$$\mu_0 = \langle f | f \rangle , \tag{B1a}$$

$$\mu_1 = \langle f | K | f \rangle , \tag{B1b}$$

$$\mu_2 = \langle f | K^2 | f \rangle . \tag{B1c}$$

Then we show that this K, which satisfies Eqs. (B1), can always be chosen so that $g \equiv \langle f | (1-K)^{-1} | f \rangle$ is as large or as small as desired. This means that knowledge of only μ_0, μ_1, and μ_2 (for a given ω value) can never be sufficient to construct bounds on g.

The normalization of $|f\rangle$ can be chosen to satisfy $\mu_0 = \langle f | f \rangle$; $|f\rangle$ is otherwise undertermined (arbitrary). Define a normalized vector $|\phi_1\rangle = (\mu_0)^{-1/2} |f\rangle$ and choose any vector $|\phi_2\rangle$ such that $\langle \phi_2 | \phi_2 \rangle = 1$ and $\langle \phi_1 | \phi_2 \rangle = 0$. Then define a Hermitian operator K as follows:

$$K = K_{11} |\phi_1\rangle\langle\phi_1| + K_{21} |\phi_2\rangle\langle\phi_1| + K_{12} |\phi_1\rangle\langle\phi_2| + K_{22} |\phi_2\rangle\langle\phi_2| , \tag{B2a}$$

where

$$K_{11} = \mu_1/\mu_0 \tag{B2b}$$

and

$$K_{12} = K_{21} = \left[\frac{\mu_2}{\mu_0} - \left(\frac{\mu_1}{\mu_0} \right)^2 \right]^{1/2} . \tag{B2c}$$

The remaining matrix element K_{22} may be regarded as an unconstrained parameter. It is easily verified that Eqs. (B1) are satisfied, independent of the value of K_{22}. Now consider

$$g \equiv \langle f | (1-K)^{-1} | f \rangle = \mu_0 \langle \phi_1 | (1-K)^{-1} | \phi_1 \rangle = \frac{\mu_0 K_{22}}{K_{11} K_{22} - (K_{12})^2} . \tag{B3}$$

The denominator vanishes when

$$K_{22} = (K_{12})^2 / K_{11} . \tag{B4}$$

For slightly larger or slightly smaller values of K_{22}, $\langle f | (1-K)^{-1} | f \rangle$ can therefore be made arbitrarily large, and either positive or negative. Attempts to construct bounds to this quantity in terms of μ_0, μ_1, and μ_2 alone are therefore futile.

It is also impossible to bound the spectrum of K using only μ_0, μ_1, and μ_2. Taking $|\phi_2\rangle$ as an approximate eigenvector, we evaluate $\langle \phi_2 | K | \phi_2 \rangle = K_{22}$ and $\sigma_2^2 = \langle \phi_2 | K^2 - (K_{22})^2 | \phi_2 \rangle = (K_{12})^2$. It follows that K has an eigenvalue in the interval $(K_{22} - K_{12}, K_{22} + K_{12})$. However, because K_{22} can be made arbitrarily large or small without changing μ_0, μ_1, and μ_2, this eigenvalue can also be made arbitrarily large or small.

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[31]See Ref. 14, Theorem 15.2, p. 215.
[32]See Ref. 13, pp. 103–104.
[33]In the original, unperturbed basis.
[34]One could proceed by first Schmidt orthogonalizing the vectors. Instead, we used a method involving numerical inversion of the matrix of overlaps.
[35]See Ref. 15, p. 116.
[36]This means that the $\bar{E}_m$ are upper bounds to the *lowest* M energies. Intruder states could therefore invalidate the bounds; in practice they do not.
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[46]However, the derivation breaks down if $\hat{k} > 1$, in which case these bounds become only quasibounds.
[47]The equation for $\hat{k}$ is a quadratic; only the positive root was taken.
[48]In the notation of Appendix B, $\mathcal{K} = K_{11} + K_{12}$, which is the upper bound of the Gershgorin disk centered at K_{11}.
[49]We use the name "Bloch-Horowitz" to mean only self-consistent diagonalization of the energy-dependent $\mathcal{K}(\omega)$, as described in Sec. II. Unlike Ref. 1, we do not separate the core energy.
[50]We use the name "Brandow" to refer to an expansion of the energy-independent $\tilde{\mathcal{K}}$ in powers of the coupling strength, without the separation of core and single-particle energies that is also described in Ref. 22.