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Rigorous bounds on the energy-averaged effective Hamiltonian

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Best possible bounds on expectation values of the energy-averaged Bloch-Horowitz effective Hamiltonian are derived, assuming knowledge of only moments $m_0, \ldots, m_n$ of the intermediate-state Hamiltonian. These bounds are independent of the presence of intruder states. The simplest case that leads to nontrivial bounds is $n=2$. Explicit formulas are given for the $n=2$ upper and lower bounds for the Lorentzian averaging width Γ. There exists an intermediate range of Γ values, within which the bounds depend weakly on Γ. For $n=2$, the intermediate Γ values are of the order of the width of the strength function of the intermediate-state excitation. For larger n, the intermediate Γ values decrease, permitting finer resolution at the price of increased computation. A universal graph is given to aid in estimating the effect of Bloch-Horowitz self-consistency on the $n=2$ bounds. For a low-lying state with moments typical of those suggested by statistical spectroscopic theory, the upper and lower bounds differ from their average by about 25% of the virtual excitation contribution. Finally, an iterative method for approximating the model-space wave function is described.

[NUCLEAR STRUCTURE Energy averaged effective interactions, Lorentzian averaging. Moments, best possible bounds, inclusion region, moment cone, bounding polynomial, self-consistency.]

I. INTRODUCTION

It is well known[1] that the calculation of low-lying states of a nucleus can be formulated in terms of an effective Hamiltonian $\mathscr{H}$ for a finite subspace, called the model space, defined by an orthogonal projection operator P. The definition of the energy dependent (Bloch-Horowitz) $\mathscr{H}$ is

$$\mathscr{H}(\omega)=H_{PP}+H_{PQ}(\omega-H_{QQ})^{-1}H_{QP}\ , \tag{1.1}$$

where ω is an energy parameter, $Q=1-P$, H is the full Hamiltonian, and $H_{PQ}\equiv PHQ$, etc. We use Eq. (1.1) because it is easier to analyze than the energy-independent effective Hamiltonian. However it does suffer from the complication of requiring "self-consistent solutions." This means that one must find a value of ω such that the corresponding eigenvalue $E(\omega)$, defined by

$$\mathscr{H}(\omega)\chi(\omega)=E(\omega)\chi(\omega)\ , \tag{1.2}$$

also satisfies

$$E(\omega)=\omega\ . \tag{1.3}$$

In realistic cases of physical interest, the second term of (1.1) cannot be calculated exactly. Therefore, estimates of the errors of approximation are of interest. The present work gives methods for using Hamiltonian moments to obtain bounds on any arbitrary expectation value of $\mathscr{H}$. The set of such bounds for all model-space states in a sense gives bounds on the operator $\mathscr{H}$. In particular, bounds on off-diagonal matrix elements (and hence bounds on eigenvalues) can be calculated from the bounds on expectation values. (This can be seen by expanding out the expectation with respect to a linear combination of states, say $\phi_1+\phi_2$.)

Our moment-based bounds on expectation values are best possible bounds, in a sense to be defined in Sec. IV. However, we have not been able to solve the problem of constructing best possible bounds on the eigenvalues of $\mathscr{H}$. Fortunately, it has emerged from previous work[2] that the major source of error in eigenvalues is usually the uncertainty in the operator $\mathscr{H}$, not the uncertainty in its eigenvectors. Consequently, our expectation bounds may, for practical purposes, be interpreted as best possible bounds on eigenvalues.

The effective Hamiltonian method is particularly useful for cases where those eigenstates of H that have large overlap with the model space ("the

represented states") lie close together in energy. In nuclei, pure examples of such behavior are rare; instead one usually finds that the represented states are separated by several so called "intruder states." In any case, the main application of effective Hamiltonians is in the construction of an effective interaction $\mathscr{V}$ for shell-model calculations. This is done by calculating effective Hamiltonians for $n=0$, 1, and 2 valence particles, and performing appropriate subtractions[2,3] to extract $\mathscr{V}$ from them. Then assuming $\mathscr{V}$ to be a two-body operator, $\mathscr{H}$ can be calculated for systems of three or more valence particles by properly combining core and single-particle contributions with the two-body interaction $\mathscr{V}$.

Evidently, this is a kind of extrapolation procedure in which values of the effective Hamiltonian $\mathscr{H}$ for $n=0$, 1, and 2 are used to predict values of $\mathscr{H}$ for $n \geq 3$. Like all extrapolations, it is vulnerable to noise in the input data. Such noise is produced by the intruder-state singularities[2-4] which appear in the one- and two-particle effective Hamiltonians. These have usually attracted interest because of their role in preventing convergence of perturbative expansions.[4] One can see, however, that the intruder state singularities would cause difficulties for the $\mathscr{V}$ extrapolation procedure, even if it were possible to compute exact values of $\mathscr{H}$ for 0, 1, and 2 valence particles. Obviously, the singularities of the three-particle $\mathscr{H}$ cannot be predicted from those of the two-body $\mathscr{H}$. Therefore, including the exact two-particle intruder state singularities will not improve the extrapolated three-particle $\mathscr{H}$. Instead misinformation from the two-particle singularities will propagate into the extrapolated $n \geq 3$ effective Hamiltonians. The unitary scalar part[5] of each singularity will actually be amplified in the $n \geq 3$ effective Hamiltonians, because these contain interactions between more than one pair of particles.

Experience with ordinary numerical extrapolation suggests an analogous treatment of the intruder state difficulty. Faced with noisy input data, one gives up the attempt to predict extrapolated values with unlimited accuracy. Instead, one extrapolates only after first smoothing the input data, perhaps by fitting a low-order polynomial to them. The result is a "trend line" which should predict at least the average behavior, although of course it cannot reproduce the fluctuations.

There are several ways of applying the idea of smoothing to the effective Hamiltonian. The smoothing does not have to be with respect to the same variable n in which the extrapolation is being done. One still gains the needed stability by smoothing with respect to some other variable with respect to which $\mathscr{H}$ fluctuates. For example, one may smooth $\mathscr{H}_n(\omega)$ with respect to ω, rather than n. Assuming for the moment that ω smoothing has been decided on, it can still be done in different ways. One may expand $\mathscr{H}(\omega)$ in a Fourier series or integral, and filter out (or only attenuate) Fourier components above a certain limit to get a smoothed quantity $\langle \mathscr{H}(\omega) \rangle$. This is easily seen to be equivalent to a convolution or moving average with respect to a suitable function f:

$$\langle \mathscr{H}(\omega) \rangle = \int_{-\infty}^{\infty} \mathscr{H}(\omega') f(\omega-\omega') d\omega' , \tag{1.4}$$

where

$$\int_{-\infty}^{\infty} f(\omega) d\omega = 1 . \tag{1.5}$$

This method is invariant under translation in ω and in a sense weights all values of ω equally. One can instead use an expansion in polynomials which are orthogonal with respect to some reference density $\rho_R(\omega)$, and then truncate the expansion or attenuate the higher coefficients. The truncated orthogonal polynomial expansion method[6] can thus be interpreted as an exact calculation of an effective Hamiltonian that has been smoothed in a particular way. All that is lacking in the orthogonal polynomial expansion method is some means of assessing the accuracy and deciding whether the amount of smoothing is appropriate. And these concerns are, in fact, the main motivation of the present work.

Before going on to discuss the details involved in ω averaging, we mention another kind of motivation for averaging. In the large problems we have in mind, the amount of information that can be computed is far less than is needed to determine $\mathscr{H}$ completely. It is well known that the amount of information contained in $\mathscr{H}(\omega)$ is sufficient to determine all eigenvalues of H whose corresponding eigenvectors have nonzero P-space projections. In contrast, $\langle \mathscr{H} \rangle$ determines only a small number of energies, as will be seen in Sec. III. Therefore, the averaged $\langle \mathscr{H} \rangle$ contains much less information than the original $\mathscr{H}$. This allows the possibility that $\langle \mathscr{H} \rangle$ can be accurately computed, and such a calculation would constitute significant progress. If we then want to calculate the effect of an intruder state, we can still do so, by combining an appropriate model of the intruder state with a zero-order wave function generated from $\langle \mathscr{H} \rangle$. It

is reasonable to hope that $\langle \mathscr{H} \rangle$ will include most of the dynamics, and that the intruder state can therefore be treated as a small perturbation in some sense. This strategy recalls the separation of nuclear reaction amplitudes into direct and compound parts, where the direct part provides a background for the study of the compound part.

As we shall see in Sec. IV, ω averaging reduces the effect of intruder states on the bounds. Moreover, smoothing out the intruder-state singularities filters out their "noise" and so actually improves the accuracy of the resulting effective interaction. Motivated by these considerations, we proceed in Sec. II to discuss specific methods of ω averaging.

II. METHODS OF ω AVERAGING

To avoid dealing with operators which may not commute, we confine our attention to an arbitrary expectation of the effective Hamiltonian, with respect to a model space state ξ, say. Thus we write

$$\langle \xi \mid \mathscr{H}(\omega) \mid \xi \rangle = \langle \xi \mid H_{PP} \mid \xi \rangle + D(\omega) , \tag{2.1}$$

where

$$D(\omega) = \langle \xi \mid H_{PQ}(\omega - H_{QQ})^{-1} H_{QP} \mid \xi \rangle . \tag{2.2}$$

In principle, ξ should be an eigenvector of $\mathscr{H}(\omega)$. In practice, errors due to approximation of ξ are often unimportant.[2] We defer until Sec. VI the discussion of procedures for self-consistent approximation of ξ, and assume for now that ξ is known. Equation (2.2) can be rewritten

$$D(\omega) = \int (\omega - E)^{-1} \rho(E) dE , \tag{2.3}$$

where

$$\rho(E) = \sum_i | \langle \xi \mid H_{PQ} \mid \psi_{QE_i} \rangle |^2 \delta(E - E_i) . \tag{2.4}$$

Here the vectors ψ_{QE_i} are a complete set of eigenstates of H_{QQ}. The range of integration will be understood to be $(-\infty, \infty)$.

Let us now consider averaging of the type described by Eqs. (1.4) and (1.5), expressed by the notation

$$\langle Q(\omega) \rangle_\omega = \int Q(\omega') w(\omega - \omega') d\omega' \tag{2.5}$$

for the average of any quantity $Q(\omega)$ with respect to ω, where w is a normalized weighting function,

$$\int w(s) ds = 1 . \tag{2.6}$$

If w is an even function, it is easy to show that

$$\int \langle (\omega - E)^{-1} \rangle_E \rho(E) dE = \int (\omega - E)^{-1} \langle \rho(E) \rangle_E dE . \tag{2.7}$$

Also,

$$\langle (\omega - E)^{-1} \rangle_E = \langle (\omega - E)^{-1} \rangle_\omega . \tag{2.8}$$

Here, and in the following, all singular integrals are understood in the principal value sense. Combining Eqs. (2.7) and (2.8), we see that

$$\langle D(\omega) \rangle_\omega = \int dE \langle (\omega - E)^{-1} \rangle_\omega \rho(E) \tag{2.9}$$

$$= \int dE (\omega - E)^{-1} \langle \rho(E) \rangle_E , \tag{2.10}$$

that is, averaging D with respect to ω is equivalent to averaging ρ with respect to E.

Up to now we have left open the choice of the weighting function w. It is desirable that it should be positive and go to zero smoothly yet rapidly outside an interval of width Γ, say. On these grounds, the Gaussian of width Γ,

$$w(s) = (2\pi)^{-1/2} \Gamma^{-1} \exp(-s^2/2\Gamma^2) , \tag{2.11}$$

would be a good choice. However, the Lorentzian function

$$w(s) = \Gamma / \pi (s^2 + \Gamma^2) \tag{2.12}$$

has advantages of analytic convenience which outweigh the disadvantage of its long tail. One important advantage is that for Lorentzian averaging

$$\langle D(\omega) \rangle_\omega = \mathrm{Re} D(\omega + i\Gamma) , \tag{2.13}$$

as may be verified by contour integration. Consequently, Lorentzian averaging of $D(\omega)$ may be accomplished by evaluating it for a complex value of its argument, say

$$z = \omega + i\Gamma . \tag{2.14}$$

III. AVERAGING AND SELF-CONSISTENCY

Averaging will be successful in removing fluctuations only if there is a range of values of Γ in which the result depends weakly on Γ. When we have expressions for $D(\omega)$ in hand it will become easier to discuss more completely the limits on Γ. However, we can anticipate, in general terms, how averaging will affect practical applications of $\mathscr{H}$.

First consider self-consistent solutions of Eqs. (1.2) and (1.3). Figure 1 shows a plot of a typical

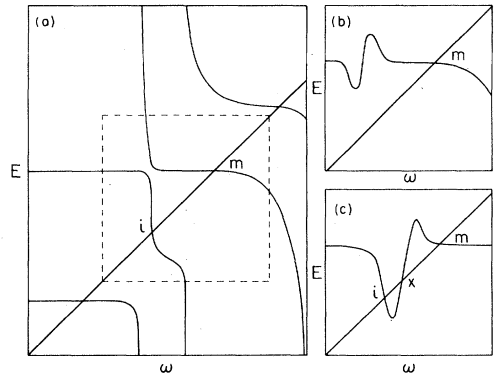

FIG. 1. Schematic graph to show some of the effects of averaging. Two eigenvalues $E_i(\omega)$ and $E_m(\omega)$ of $\mathscr{H}(\omega)$ are plotted against ω. Their self-consistent solutions are at i and m, the points of intersection with the line $\omega=E$. Part (a), before averaging, shows that i is an intruder state and that m is a represented state. In (b), i is shown to be removed without much affecting the solution of m after averaging. Part (c) shows the possibility of a ghost solution x.

eigenvalue $E(\omega)$, in accordance with qualitative properties of $\mathscr{H}(\omega)$ described in Ref. 2. In Fig. 1(a) we see that in addition to solutions, such as m, which have large model space overlaps so that $dE/d\omega$ is small, there are solutions, such as i, corresponding to intruder states near the positions of eigenvalues of H_{QQ}. In Fig. 1(b) we see that averaging removes the intruder solution without much affecting the model solution. This is a great advantage, because without averaging *every* eigenvalue of H will be a solution of (1.2) and (1.3), unless some eigenvector has no P space part.[4] Averaging, therefore, can eliminate an embarrasing excess of solutions. Figure 1(c) shows the possibility of a "ghost" solution x being produced by averaging. The positivity of $dE/d\omega$ at x identifies x as a "state of negative norm" because of the relation[4]

$$(dE/d\omega)_{\omega=E}=-\langle\psi_E\,|\,Q\,|\,\psi_E\rangle/\langle\psi_E\,|\,P\,|\,\psi_E\rangle, \quad (3.1)$$

where ψ_E is an eigenvector of H. Such solutions can be identified and discarded. However, if the averaging width Γ is chosen large enough, the curve of E against ω will have negative slope over a wide range of ω values. Sufficient averaging is therefore expected to eliminate the ghost states. This automatic removal of unwanted solutions of both types is a strong motivation for averaging over a sufficiently wide ω interval.

IV. BOUNDS BASED ON MOMENTS

Let us assume that the computed information about D consists of a finite number of moments m_k of the density $\rho(E)$ given by Eq. (2.4), defined by

$$m_k=\int dE\,\rho(E)E^k\,. \quad (4.1)$$

In practice these would be calculated from the equivalent expression

$$m_k=\langle\xi\,|\,H_{PQ}(H_{QQ})^kH_{QP}\,|\,\xi\rangle\,. \quad (4.2)$$

For convenience in later developments we also introduce the normalized moments

$$\bar{m}_k=m_k/m_0\quad(k=1,\,2,\ldots)\,. \quad (4.3)$$

The final estimates of D based on these moments will have the ω dependence explicit, because m_k itself is independent of ω. This is an advantage over expressions based on terms of Brillouin-Wigner perturbation theory,[3] which depend on ω and must be recomputed for each iteration in solving the self-consistency equations (1.2) and (1.3).

Comparison with experiment cannot decide the accuracy of a dynamical calculation in nuclear physics, because the interaction is not known. Therefore, we need bounds on D. Only from such bounds can we tell whether a change in procedure leads to an improved approximation. Moreover, the moments m_k are expensive to compute. Therefore, it is highly desirable that the bounds be the *best possible* bounds that can be proved on the basis of the given information. A bound is said to be "best possible" when one can find for the unknown density ρ a choice ρ_B that reproduces the known moments, and yields a value of D *equal* to the bound. Then ρ_B provides a counterexample to the possibility that the bound can be improved without introducing additional information. We proceed to derive such bounds by an inclusion region method.

Let $\beta_0\,|\,f_0\,\rangle=H_{QP}\,|\,\xi\rangle$, where $f_0\in Q$ and $\langle f_0\,|\,f_0\rangle=1$. The complex value $D(z)$ in Eq. (2.13) can be written as

$$D(z)=\beta_0^2\langle f_0\,|\,(z-H_{QQ})^{-1}\,|\,f_0\rangle\,. \quad (4.4)$$

If we divide the space Q into a space $P_1=|\,f_0\rangle\times\langle f_0\,|$ and a space $Q_1=Q-P_1$, the familiar operator identity used in the theory of the optical potential[7]

$$P_1(z-H_{QQ})^{-1}P_1=P_1[z-H_{P_1P_1}-H_{P_1Q_1}(z-H_{Q_1Q_1})^{-1}H_{Q_1P_1}]^{-1}P_1 \quad (4.5)$$

gives

$$\langle f_0 | (z-H_{QQ})^{-1} | f_0 \rangle = [z-\alpha_1-\beta_1{}^2\langle f_1 | (z-H_{Q_1Q_1})^{-1} | f_1 \rangle]^{-1} , \tag{4.6}$$

where

$$\begin{aligned} &\alpha_1=\langle f_0 | H | f_0 \rangle , \\ &\beta_1 | f_1 \rangle = Q_1 H | f_0 \rangle , \\ &\langle f_1 | f_1 \rangle = 1 . \end{aligned} \tag{4.7}$$

The space Q_1 can be subsequently divided into spaces $P_2=|f_1\rangle\langle f_1|$ and $Q_2=Q_1-P_2$; Q_2 in turn can be divided into spaces P_3 and Q_3; and so on. Therefore, in general, we will have

$$\langle f_p | (z-H_{Q_pQ_p})^{-1} | f_p \rangle = [z-\alpha_{p+1}-\beta_{p+1}{}^2\langle f_{p+1} | (z-H_{Q_{p+1}Q_{p+1}})^{-1} | f_{p+1} \rangle]^{-1} \tag{4.8}$$

for $p=0,1,\ldots,$ where

$$\begin{aligned} &Q_{p+1}=Q_p-|f_p\rangle\langle f_p| , \\ &\alpha_{p+1}=\langle f_p | H | f_p \rangle , \\ &\beta_{p+1} | f_{p+1} \rangle = Q_{p+1} H | f_p \rangle , \\ &\langle f_{p+1} | f_{p+1} \rangle = 1 . \end{aligned} \tag{4.9}$$

Using identity (4.8) repeatedly for $p=0,1,\ldots,n$, Eq. (4.4) can be written in the form of a continued fraction,

$$D(z)=\cfrac{\beta_0{}^2}{z-\alpha_1-\cfrac{\beta_1{}^2}{z-\alpha_2-\cdots-\cfrac{\beta_n{}^2}{z-D_{n+1}(z)}}} , \tag{4.10}$$

where

$$D_{n+1}(z)=\alpha_{n+1}+\beta_{n+1}{}^2\langle f_{n+1} | (z-H_{Q_{n+1}Q_{n+1}})^{-1} | f_{n+1} \rangle . \tag{4.11}$$

Furthermore, Eq. (4.10) can be expressed as a rational fraction[8]

$$D(z)=\frac{[z-D_{n+1}(z)]p_n(z)-\beta_n{}^2 p_{n-1}(z)}{[z-D_{n+1}(z)]q_n(z)-\beta_n{}^2 q_{n-1}(z)} , \tag{4.12}$$

where $p_n(z)$ and $q_n(z)$ are the polynomials of degree $n-1$ and n, respectively, that satisfy the recurrence relations

$$\left.\begin{aligned} p_n(z)&=(z-\alpha_n)p_{n-1}(z)-\beta_{n-1}{}^2 p_{n-2}(z) \\ q_n(z)&=(z-\alpha_n)q_{n-1}(z)-\beta_{n-1}{}^2 q_{n-2}(z) \end{aligned}\right\} , \quad n=1,2,\ldots , \tag{4.13}$$

with

$$\begin{aligned} &q_0(z)=1 , \quad q_{-1}(z)=0 , \\ &p_0(z)=0 , \quad p_{-1}(z)=-1 . \end{aligned} \tag{4.14}$$

Knowledge of the moment $m_0,\ldots,m_{2n}$ is necessary and sufficient to calculate the polynomials p and q and the coefficient β_n appearing in Eq. (4.12). For example, using Eq. (4.9) and (4.13),

$$\begin{aligned} &\beta_0{}^2=m_0 , \\ &\alpha_1=\bar{m}_1 , \\ &\beta_1=(\bar{m}_2-\bar{m}_1{}^2)^{1/2} , \\ &p_1(z)=\beta_0{}^2 , \\ &q_1(z)=z-\alpha_1 . \end{aligned} \tag{4.15}$$

If we assume that these moments are known, Eq. (4.12) relates D to the unknown quantity D_{n+1} through a linear fractional transformation. Because $\mathrm{Im}(z)=\Gamma>0$, Eq. (4.11) implies that $\mathrm{Im}(D_{n+1})\leq 0$. From the general properties of linear fractional transformations,[9] Eq. (4.12) maps the half plane $\mathrm{Im}(D_{n+1})<0$ onto the interior of a certain circle C_{n+1} in the D plane. This circle is the image of the real axis $\mathrm{Im}(D_{n+1})=0$ under the transformation Eq. (4.12). Therefore, $D(z)$ will lie inside the circle C_{n+1}. Because the unknown real coefficients α_{n+1} and β_{n+1} in Eq. (4.11) can be adjusted to make D_{n+1} lie as near as desired to any point on the real axis, $D(z)$ can arbitrarily closely approach any point on the perimeter of C_{n+1}. Therefore, the *best possible* bounds on $D(z)$, given only moments through order $2n$, are determined by the perimeter of C_{n+1}.

From Eq. (4.12) we can show that the equation of the circle C_{n+1} is

$$a_{n+1}D^*D+b_{n+1}D^*+b_{n+1}^*D+d_{n+1}=0\ , \tag{4.16}$$

where

$$\begin{aligned} a_{n+1}&=2\Gamma q_n q_n^*+i\beta_n{}^2(q_n^*q_{n-1}-q_n q_{n-1}^*)\ ,\\ b_{n+1}&=-2\Gamma p_n q_n^*+i\beta_n{}^2(p_n q_{n-1}^*-q_n^*p_{n-1})\ ,\\ d_{n+1}&=2\Gamma p_n p_n^*+i\beta_n{}^2(p_{n-1}p_n^*-p_{n-1}^*p_n)\ , \end{aligned} \tag{4.17}$$

and the notation p^* represents the complex conjugate of p. The center and radius of the circle C_{n+1} are just

$$\begin{aligned} c_{n+1}&=-b_{n+1}/a_{n+1}\ ,\\ r_{n+1}&=\beta_n{}^2\,|\,(p_n q_{n-1}-p_{n-1}q_n)/a_{n+1}\,|\ . \end{aligned} \tag{4.18}$$

The best possible bounds for the real part of $D(z)$ are then given by the two extreme points of the projection of the circle C_{n+1} on the real axis. They are

$$\begin{aligned} I_U&=\mathrm{Re}(c_{n+1})+r_{n+1}\ ,\\ I_L&=\mathrm{Re}(c_{n+1})-r_{n+1}\ . \end{aligned} \tag{4.19}$$

Let us consider the $n=1$ case in detail. Here only m_0, m_1, and m_2 are known. We eliminate m_1 and m_2 in favor of the centroid $\bar{m}_1$ and the variance $\sigma^2=\bar{m}_2-\bar{m}_1{}^2$. Substituting Eq. (4.15) into Eq. (4.17) we have

$$\begin{aligned} a_2&=2\Gamma[(\omega-\bar{m}_1)^2+\sigma^2+\Gamma^2]\ ,\\ b_2&=m_0[2\Gamma(\bar{m}_1-\omega)+i(\sigma^2+2\Gamma^2)]\ ,\\ d_2&=2\Gamma m_0{}^2\ . \end{aligned} \tag{4.20}$$

Equation (4.18) then gives us

$$\begin{aligned} c_2&=\frac{-\frac{1}{2}m_0[2\Gamma(\bar{m}_1-\omega)+i(\sigma^2+2\Gamma^2)]}{\Gamma[(\omega-\bar{m}_1)^2+\sigma^2+\Gamma^2]}\ ,\\ r_2&=\tfrac{1}{2}m_0\sigma^2/\Gamma[(\omega-\bar{m}_1)^2+\sigma^2+\Gamma^2]\ . \end{aligned} \tag{4.21}$$

The best possible upper and lower bounds of $\langle D(\omega)\rangle_\omega$ are then

$$D_-\leq\langle D(\omega)\rangle_\omega\leq D_+\ , \tag{4.22}$$

where

$$D_\pm=\frac{m_0[(\omega-\bar{m}_1)\pm\sigma^2/2\Gamma]}{[(\omega-\bar{m}_1)^2+\sigma^2+\Gamma^2]}\ . \tag{4.23}$$

An alternative approach is to use the general Theorem 2.1 given by Karlin and Studden.[10] We call this the bounding polynomial method. For convenience let us first write the real part of $D(z)$ as

$$I\equiv\langle D(\omega)\rangle_\omega=\int F(t)\sigma(t)dt\ , \tag{4.24}$$

where

$$\begin{aligned} t&=(E-\omega)/\Gamma\ ,\\ F(t)&=-t/(1+t^2)\ ,\\ \sigma(t)&=\rho(\Gamma t+\omega)\ . \end{aligned} \tag{4.25}$$

The theorem simply says that knowing only the lowest N moments of σ, the best possible upper and lower bounds of the integral I are, respectively, the maximum and minimum of the integral $\mathcal{I}=\int u(t)\sigma(t)dt$ when $u(t)$ ranges over the set of all polynomials of order N that bound $F(t)$ from above or below. Because an odd order polynomial ranges from $+\infty$ to $-\infty$, it is immediately clear that, in order to bound $F(t)$ for all t, N must be even. It can also be shown that only the polynomials that touch $F(t)$ [but do not intersect $F(t)$] can possibly attain the best possible bounds. Consequently, only even-order touching polynomials need to be considered. We shall see that these polynomials are conveniently parametrized in terms of their touching points.

Each touching point (t_i, say) imposes two conditions on $u(t)$:

$$\begin{aligned} u(t_i)&=F(t_i)\ ,\\ [du(t)/dt]_{t=t_i}&=[dF(t)/dt]_{t=t_i}\ . \end{aligned} \tag{4.26}$$

Therefore, a polynomial of degree $2n$ with only $2n+1$ coefficients can at most touch $F(t)$ at $n+1$ points. The $2n+2$ touching conditions then not only determine the $2n+1$ coefficients but also constrain the touching points; only n of them will be independent. These polynomials will not intersect $F(t)$ because $\Delta(t)\equiv F(t)-u(t)$ can have at most $2n+2$ real roots (a consequence of the choice of Lorentzian averaging) and the $n+1$ touching points, each a double root of $\Delta(t)$, are the $2n+2$ real solutions. These polynomials then necessarily bound $F(t)$ from one side.

A polynomial that touches $F(t)$ at $n+1$ touching points $t_1,\ldots,t_{n+1}$ can be written as

$$u(t)=\sum_{j=1}^{n+1}[A_j(t-t_j)+B_j]\prod_{i(i\neq j)}^{n+1}(t-t_i)^2\Big/\prod_{i(i\neq j)}^{n+1}(t_j-t_i)^2 , \tag{4.27}$$

where

$$B_j=F(t_j) ,$$
$$A_j=F'(t_j)-2F(t_j)\sum_{i(i\neq j)}^{n+1}(t_j-t_i)^{-1} . \tag{4.28}$$

This is a polynomial of degree $2n+1$. Our polynomial of even degree $2n$ can, however, be obtained from Eqs. (4.27) and (4.28) by simply demanding that the coefficient of t^{2n+1} equal zero. This then also gives us the constraint among the $n+1$ touching points. Again let us specialize to the $n=1$ case. Then $u(t)$ should be a quadratic polynomial. According to Eq. (4.27), however, we will first obtain a cubic polynomial. By demanding that the coefficient of t^3 equal zero a quadratic polynomial is obtained with a constraint connecting its two touching points. The constraint can be factorized as

$$(t_1t_2+t_1+t_2-1)(t_1t_2-t_1-t_2-1)=0 . \tag{4.29}$$

Upon substituting the root t_1 of the first factor into $u(t)$ to eliminate t_1, we have

$$u(t)=u_+(t)\equiv\tfrac{1}{2}[(t_2+1)^2t^2-2(t_2+1)(t_2^2+1)t+t_2^2(t_2-1)^2]/\Gamma(t_2^2+1)^2 . \tag{4.30}$$

Because the highest order coefficient of t is positive, this polynomial is positive at infinity. It then must bound $F(t)$ from above and provide upper bounds. The second factor in Eq. (4.29) will yield a quadratic polynomial

$$u(t)=u_-(t)\equiv\tfrac{1}{2}[-(t_2-1)^2t^2+2(t_2-1)(t_2^2+1)t-t_2^2(1+t_2)^2]/\Gamma(t_2^2+1)^2 . \tag{4.31}$$

Because the highest order coefficient of t is negative, the polynomial $u_-(t)$ provides lower bounds.

The best possible upper bound is then the minimum (with respect to t_2) of $\mathscr{I}_+$ defined by

$$\begin{aligned}\mathscr{I}_+&=\int u_+(t)\sigma(t)dt\\&=\tfrac{1}{2}M_0[(t_2+1)^2\overline{M}_2-2(t_2+1)(t_2^2+1)\overline{M}_1+t_2^2(t_2-1)^2]/\Gamma(t_2^2+1)^2 ,\end{aligned} \tag{4.32}$$

where $M_0=m_0/\Gamma$ and the quantities $\overline{M}_i$ are normalized moments of the density σ of Eq. (4.25), related to the moments of ρ through

$$\overline{M}_k=\Gamma^{-k}\sum_{p=0}^{k}(-1)^p\begin{bmatrix}k\\p\end{bmatrix}\omega^p\overline{m}_{k-p} . \tag{4.33}$$

The first derivative of $\mathscr{I}_+$ can be written in factorized form as

$$d\mathscr{I}_+/dt_2=\tfrac{1}{2}M_0(t_2^2+2t_2-1)[t_2^2(\overline{M}_1+1)-t_2(\overline{M}_2+1)+\overline{M}_1-\overline{M}_2]/\Gamma(t_2^2+1)^3 . \tag{4.34}$$

Because the second derivative of $\mathscr{I}_+$ at a value of t_2 satisfying $t_2^2+2t_2-1=0$ is

$$d^2\mathscr{I}_+/dt_2^2=-4[(t_2-\overline{M}_1)^2+(\overline{M}_2-\overline{M}_1^2)]/(t_2^2+1)^3<0 , \tag{4.35}$$

the roots of the first factor in Eq. (4.34) give relative maxima of $\mathcal{I}_+$. The best possible upper bound then must come from the second factor, which gives us

$$D_+ = \tfrac{1}{2}M_0(\bar{M}_2 - \bar{M}_1^2 - 2\bar{M}_1)/(\bar{M}_2+1) \ . \tag{4.36}$$

Similarly, we obtain the best possible lower bound from the polynomial u_- of Eq. (4.31):

$$D_- = -\tfrac{1}{2}M_0(\bar{M}_2 - \bar{M}_1^2 + 2\bar{M}_1)/(\bar{M}_2+1) \ . \tag{4.37}$$

Equations (4.36) and (4.37) can be shown to be identical to Eq. (4.23) with $\bar{M}_1 = (\bar{M}_1 - \omega)/\Gamma$ and $\sigma^2 = (\bar{M}_2 - \bar{M}_1^2)/\Gamma^2$.

The two methods of deriving bounds are to some extent complementary. The bounding polynomial method can be applied to other functions F, besides that defined in Eq. (4.25). Thus it could be used to study bounds on a convolution average with a non-Lorentzian weighting function—for example, the desirable Gaussian function defined in Eq. (2.11). Of course, it is then no longer obvious that $\Delta(t)$ will have at most $2n+2$ real roots, and the constraint Eq. (4.29) will be replaced by a transcendental equation. Therefore, it is probably impossible to give such an explicit result as Eqs. (4.36) and (4.37). Nevertheless, the bounding polynomials can still be parametrized by n independent touching points.

On the other hand, the inclusion region method based on Eq. (4.12) is more readily generalized to higher order. The required polynomials can be evaluated by means of simple recursion formulas. If higher-order moments are known one can easily apply this method, but one is obliged to use Lorentzian averaging.

The moment m_2 is hard to calculate, so one might ask if there exist bounds that require fewer moments, perhaps only m_0 and m_1. The answer is that the best bounds possible with knowledge of only m_0 are

$$-\tfrac{1}{2}m_0/\Gamma \le \langle D \rangle \le \tfrac{1}{2}m_0/\Gamma \ . \tag{4.38}$$

Knowledge of m_1 does not improve these bounds, as can most easily be seen by noting that the bounding polynomials u must be of even degree. The bounds [Eq. (4.38)] are in a sense trivial, because they are a direct consequence of the uniform bounds $\pm(2\Gamma)^{-1}$ on the energy averaged F, and could be derived by elementary techniques. They are also uninformative, being insufficient to determine even the sign of D, which is the least information that could be physically significant. The bounds [Eq. (4.23)] based on m_0, m_1, and m_2 are therefore the simplest nontrivial bounds of this type.

V. STABILITY WITH RESPECT TO VARIATION OF Γ

Let us now consider the choice of the averaging interval Γ that is appropriate for use in these bounds. As usual in averaging, we require that Γ be confined to a range within which the results are essentially stable with respect to variations of Γ. It is evident from Eq. (4.23) that this requirement will be satisfied if

$$|\omega - \bar{m}_1| >> \tfrac{1}{2}\sigma^2/\Gamma \tag{5.1}$$

and

$$\Gamma << [(\omega - \bar{m}_1)^2 + \sigma^2]^{1/2} \ , \tag{5.2}$$

because under these conditions one has, for example,

$$D_\pm \approx m_0(\omega - \bar{m}_1)/[(\omega - \bar{m}_1)^2 + \sigma^2] \ , \tag{5.3}$$

which is independent of Γ. [Interestingly, the right hand side of Eq. (5.3) can be interpreted as resulting from a *Lorentzian density* ρ, of width σ and centroid $\bar{m}_1$.] Now the conditions (5.1) and (5.2) imply

$$(\omega - \bar{m}_1)^2 + \sigma^2 > \sigma^4/4(\omega - \bar{m}_1)^2 \ . \tag{5.4}$$

Introducing the reduced energy variable

$$\delta = (\omega - \bar{m}_1)/\sigma \ , \tag{5.5}$$

this becomes

$$4\delta^4 + 4\delta^2 - 1 > 0 \ , \tag{5.6}$$

which requires

$$|\delta| > 0.455 \ . \tag{5.7}$$

Of course, if $|\delta|$ is much larger than this there will be a wider range of permissible values of Γ, defined by

$$\sigma(1+\delta^2)^{1/2} >> \Gamma >> \tfrac{1}{2}\sigma/|\delta| \ . \tag{5.8}$$

On the basis of the central limit theorem, averaged spectral densities are expected to have Gaussian form.[11] Let us assume that the density ρ in Eq. (2.4) and the spectral density of H are both Gaussian and (pessimistically) that they have the same centroid and width. Then we expect 2.3% of the levels to lie at energies low enough to satisfy

$|\delta| > 2$. (It would be quite normal in large shell model calculations to disregard the remaining 97.7% of the levels.) The range of permissible Γ values is then

$$\sqrt{5}\sigma >> \Gamma >> \sigma/4 \ . \tag{5.9}$$

This seems a satisfactorily wide range of stability. Clearly, less Γ stability is to be expected for higher lying levels, however.

One can investigate the relative separation between the upper and lower bounds, namely

$$(D_+ - D_-)/(D_+ + D_-) = \tfrac{1}{2}\sigma^2/\Gamma(\omega - \overline{m}_1) = \tfrac{1}{2}\sigma/\Gamma\delta \ . \tag{5.10}$$

For the largest permissible Γ, this is

$$(D_+ - D_-)/(D_+ + D_-) = \tfrac{1}{2}\delta^{-1}(1+\delta^2)^{-1/2} \ , \tag{5.11}$$

which is 0.11 for $\delta = 2$. This means that when only m_0, m_1, and m_2 are known and H_{PP} is such that $\delta = 2$, we can expect to evaluate $\langle D \rangle_\omega$ with $\Gamma = \sqrt{5}\sigma$ only correct to 11%. This shows the importance of choosing the model space to reduce the magnitude of D, perhaps by Hartree-Fock techniques, before embarking on higher order calculations of any kind. An interesting step in this direction is the "correlated core" formulation of Kuo and Krenciglowa.[12]

It seems surprising that the permissible values of Γ are so large. One would have expected that Γ should be much larger than the typical spacing of energy levels, and much *smaller* than σ. One might feel that even $\Gamma = \sigma/4$ is too large to be legitimate. But from another point of view it seems very natural. The densities that are considered in constructing bounds are constrained only to be positive. They may consist of a small number of very narrow peaks. But statistical considerations[11] suggest that the many delta function peaks of ρ are arranged so that the density is as well represented by a smooth function as it could be, and still contain the fluctuations inevitably associated with the discrete energy levels. Recall that $\langle D \rangle_\omega$ can be expressed as an integral involving an energy-averaged density $\langle \rho \rangle_E$, as in Eq. (2.10). The averaged density $\langle \rho \rangle_E$ is more constrained than ρ is, because the averaging excludes the possibility of δ functions tions in $\langle \rho \rangle_E$. Consider the problem of finding the upper and lower bounds of the integral $\int dE\, \overline{\rho}(E)(\omega - E)^{-1}$, given that $\overline{\rho}$ is a Lorentzian average of some positive density ρ, with only the 0th, 1st, and 2nd moments of ρ known. It is equivalent to the problem of bounding $\int dE\, \rho(E)\langle(\omega - E)^{-1}\rangle_E$, knowing only the same moments of ρ, and its solution is therefore the same. In fact, the extremal densities $\langle \rho \rangle_E$, which lead to the bounds D_+ and D_-, will be the sum of two Lorentzian functions of width Γ. As an example, assume $\delta = 2$ and $\Gamma = (0.646)\sigma$. Then the Lorentzians of the extremal density for D_+ will have equal strengths and separation 2σ. Now we ask if $\Gamma = (0.646)\sigma$ is a reasonable averaging interval. We can easily see that the sum of the two Lorentzians will exhibit two distinct maxima for this value of Γ, and indeed for all Γ satisfying

$$\Gamma < \sqrt{3}\sigma \ . \tag{5.12}$$

We may make a requirement that the average density should have only one maximum, as a way of expressing the conclusion of statistical theory that the averaged density is smooth. Then we see that $\Gamma = (0.646)\sigma$ is, from this point of view, too *small* an averaging interval.

Smaller values of Γ become permissible when higher order bounds are used, because the average spacing of the delta functions of the extremal density will be less. For some order n, the smallest Γ permitted by the stability requirement on the nth order bound will become comparable with the average level spacing. Higher orders than this presumably improve the treatment of the fluctuations without affecting the trend line. This transition from smooth to fluctuating behavior deserves more detailed study.

So far, we have presented only bounds on $\langle D(\omega) \rangle_\omega$. To investigate the influence of ω consistency on the energy bounds, we can assume that we know $|\xi\rangle$, the self-consistent eigenvector of $\langle \mathscr{H} \rangle_\omega$, and write the self-consistency relation $E = \omega$ as

$$\langle \xi | H_{PP} | \xi \rangle + \langle D(\omega) \rangle_\omega = \omega \ . \tag{5.13}$$

To represent the solution of all equations of this type by means of a universal graph, we define additional reduced variables

$$\delta_1 = (\langle \xi | H_{PP} | \xi \rangle - \overline{m}_1)/\sigma \tag{5.14}$$

(the "first-order" value of δ) and

$$\gamma = \Gamma/\sigma \ . \tag{5.15}$$

Now, in Eq. (5.13), $\langle D(\omega) \rangle_\omega$ can be replaced by either of the bounds given in Eq. (4.23), to obtain corresponding bounds on the energy. In terms of the reduced energy variable δ, given by Eq. (5.5), and the energy-independent quantity δ_1, given by

(5.14), we have

$$\bar{m}_1+\sigma\delta_1+m_0\frac{\omega-\bar{m}_1\pm\sigma^2/2\Gamma}{(\omega-\bar{m}_1)^2+\sigma^2+\Gamma^2}$$
$$=\bar{m}_1+\sigma\delta\ , \quad (5.16)$$

so that, in terms of the reduced variables,

$$(\delta\pm 1/2\gamma)/(\delta^2+1+\gamma^2)$$
$$=\sigma^2(\delta-\delta_1)/m_0\ . \quad (5.17)$$

For a given value of γ, this equation can be written as a cubic in δ. We shall resort to a graphical method for solving it. We define a scaled quantity, $y_\pm\equiv\sigma D_\pm/m_0$, so that

$$y_\pm(\delta)=(\delta\pm 1/2\gamma)/(\delta^2+1+\gamma^2)\ . \quad (5.18)$$

Then the solutions $\delta_\pm$ of

$$y_\pm(\delta)=\sigma^2(\delta-\delta_1)/m_0 \quad (5.19)$$

give bounds on the self-consistent energy $\bar{E}_{\rm av}$ obtained from $\langle D(\omega)\rangle_\omega$,

$$\bar{m}_1+\sigma\delta_-\le\bar{E}_{\rm av}\le\bar{m}_1+\sigma\delta_+\ . \quad (5.20)$$

Of course, the results depend on γ. For a given negative value of δ, we find by differentiating Eq. (5.18) that y_+ has a minimum when γ is a positive root of the cubic equation

$$4\delta\gamma^3+3\gamma^2+(\delta^2+1)=0\ . \quad (5.21)$$

This value of γ gives optimal stability of the upper bound. Unfortunately, for $\delta<0$, y_- has no minimum in γ. We find that this optimal value of γ is quite near 1, for all $\delta<-0.5$.

Figure 2 shows graphs of $y_\pm$ versus δ. For each value of δ the corresponding optimal value of γ, satisfying Eq. (5.21), is used. To estimate the effect of self-consistency from the graph, one must calculate δ_1 and σ^2/m_0 and draw a straight line

$$y=\sigma^2(\delta-\delta_1)/m_0\ . \quad (5.22)$$

The intersections of this line with the curves $y_\pm$ give the desired solutions δ_+ and δ_-. The relative accuracy can be calculated even if one knows nothing more than δ_1 and δ; δ_1 is easy to calculate, while δ can be estimated from experiment. Clearly, the method fails if $\delta_1>0$. This implies a minimum standard for the quality of the model space. A weak interaction between model and excluded spaces would give a small value of m_0, and hence a large slope and tight bounds $\delta_\pm$.

It is difficult to quote typical values of m_0, m_1, σ, and $\langle\xi\,|\,H_{pp}\,|\,\xi\rangle$, because these quantities vary widely with the hardness of the interaction and the choice of P and Q spaces. Nevertheless, a statistical treatment can give useful orientation on the magnitudes of the reduced variables δ_1 and δ. For example, assume as before that ρ is Gaussian with centroid $\bar{m}_1=m_1/m_0$ and width σ, and that the density of states has the same distribution. Then the number of states that lie below energy ω can be estimated from the value of erf(δ). Conversely, one can see what values of δ are reasonable for low-lying states.

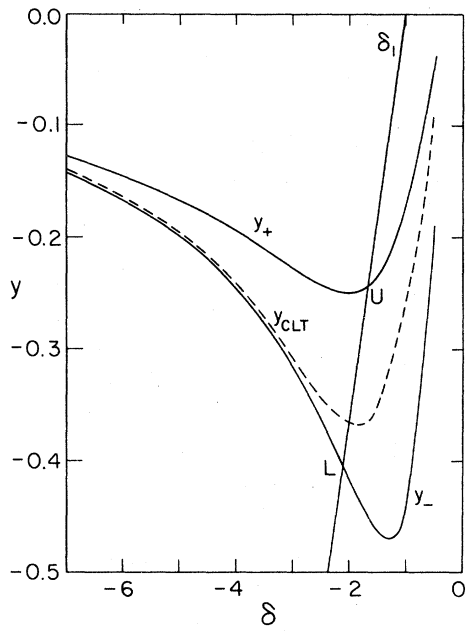

FIG. 2. Universal self-consistency graph. The intersection points U and L give solutions of Eq. (5.19). The corresponding energies are upper and lower bounds on the self-consistent energies. To illustrate, we assume $\delta_1=-1$ and draw a straight line that gives a self-consistent energy corresponding to $\delta\approx 2$. On the basis of statistical spectroscopy, $\delta=-2$ would correspond to a typical low-lying level. Our choice of $\delta_1=-1$ means that the model space is only good enough to give an unperturbed energy midway between the centroid ($\delta=0$) and the actual energy. For comparison with the bounds, the dashed curve labelled $y_{\rm CLT}$ shows the result of taking the unknown density ρ to have Gaussian form.

The straight line chosen for illustration in Fig. 2 corresponds to $\delta_1=-1$ and $\sigma^2/m_0=0.2$. The choice of $\delta_1=-1$ means that the model space is only good enough to give an unperturbed energy midway between the centroid ($\delta=0$) and the actual energy, and thus implies a rather strong interaction between the model space and excluded space. The choice of $\sigma^2/m_0=0.2$ gives a self-consistent value

of δ at about -2. On the basis of statistical spectroscopy, $\delta=-2$ would correspond to a typical low-lying level having about 2.3% of the intruder strength ρ below the level. For comparison, Fig. 2 also shows $y_{\mathrm{CLT}}=\sigma D/m_0$, where D is the result of assuming that the density ρ of Eq. (2.3) is of Gaussian form, as implied[11] by the Central Limit Theorem (CLT). Remarkably, this curve is much closer to the lower bound than to the upper bound, in the interesting region $\delta<-2$.

VI. VARIATIONAL ESTIMATION OF THE MODEL-SPACE EIGENSTATE

For any given value of ω, the eigenvalue calculation involved in solving the self-consistent equations (1.2) and (1.3) could be viewed as a search for a vector ξ that makes the expectation $\langle\xi\,|\,\mathscr{H}\,|\,\xi\rangle$ stationary. To find ξ, we would expand it in a basis for the M-dimensional model space:

$$\xi=\sum_{l}^{M} a_n\phi_n \ , \tag{6.1}$$

and then require $\langle\xi\,|\,\mathscr{H}(\omega)\,|\,\xi\rangle$ to be stationary with respect to variation of the coefficients a_n, subject to the constraint

$$\sum_{l}^{M} a_n{}^2=1 \ . \tag{6.2}$$

In our search for bounds, let us similarly require the bounds on the eigenvalue of $\mathscr{H}(\omega)$ under consideration, namely

$$\langle\xi_{\pm}\,|\,H_{PP}\,|\,\xi_{\pm}\rangle+D_{\pm} \ , \tag{6.3}$$

to be stationary with respect to variation of a_n. Recall that $D_{\pm}$ depends on ω and on the moments m_0, m_1, and m_2. These moments are quadratic forms in a_n:

$$m_p=\sum_{mn} m_{pmn}a_m^*a_n \ , \tag{6.4}$$

where

$$m_{pmn}=\langle\phi_m\,|\,H_{PQ}(H_{QQ})^pH_{QP}\,|\,\phi_n\rangle \ . \tag{6.5}$$

In the same way,

$$\langle\xi\,|\,H_{PP}\,|\,\xi\rangle=\sum_{mn} h_{mn}a_m^*a_n \ , \tag{6.6}$$

where

$$h_{mn}=\langle\phi_m\,|\,H_{PP}\,|\,\phi_n\rangle \ . \tag{6.7}$$

The condition for Eq. (6.3) to be stationary is

$$\sum_{n} A_{mn}^{\pm}a_n=\lambda a_m \ , \tag{6.8}$$

where

$$A_{mn}^{\pm}=h_{mn}+\sum_{p=0}^{2}(\partial D_{\pm}/\partial m_p)m_{pmn} \ , \tag{6.9}$$

and λ is the Lagrange multiplier associated with the normalization constraint. Thus the desired coefficients form an eigenvector of the matrix $A^{\pm}$. Because $A^{\pm}$ depends on a_n through the derivatives $\partial D_{\pm}/\partial m_p$, however, iteration is required. One begins with some guess for $\xi_{\pm}$ and uses it to calculate m_0, m_1, m_2, and hence $\partial D_{\pm}/\partial m_p$. Then one obtains a new value for $\xi_{\pm}$ by solving the eigenvalue equation (6.8). If the initial guess is close enough, the process will converge.

Statistical reasoning and experience both suggest that the matrices m_{pmn} are dominated by scalar parts. If this is so, the convergence should be rapid, because m_0, m_1, and m_2 then depend weakly on $\xi_{\pm}$. On may also exploit the fact that the dependence on m_0 is linear, to speed up convergence. Finally, it is tempting to assume that m_{1mn} and m_{2mn} are scalar matrices, in which case they can be calculated from trace moments.

When $\xi_{\pm}$ has been found, for a given value of ω, the next value of ω is set equal to Eq. (6.3). The process should be continued until ω self-consistency is achieved. Fortunately, neither of these two kinds of iteration requires the quantities (6.5) to be recomputed.

The quantities (6.3) rigorously bound the expectations $\langle\xi_{\pm}\,|\,\langle\mathscr{H}\rangle_{\omega}\,|\,\xi_{\pm}\rangle$. This does not quite guarantee that they bound the self-consistent eigenvalue of $\langle\mathscr{H}\rangle_{\omega}$, which can be written $\langle\xi\,|\,\langle\mathscr{H}\rangle_{\omega}\,|\,\xi\rangle$, because $\xi_{\pm}\neq\xi$. However, the error in ξ, being of second order in $\xi_{\pm}-\xi$, is usually an unimportant source of error in the self-consistent energy. This point arises also in Ref. 2, and is analyzed there.

VII. CONCLUSIONS AND OUTLOOK

We have shown how to construct best possible bounds on the energy averaged effective Hamiltonian from a finite number of moments. The energy averaging makes these bounds independent of the presence of intruder states; at the same time, it stabilizes the extrapolation process that is involved in the construction and use of effective interactions.

We have found explicit formulas for the bounds

that result when only the integrated strength m_0, centroid $\bar{m}_1$, and width σ are known. If the energy is separated from the centroid by about $\frac{1}{2}\sigma$ or more, the bounds turn out to be stable over a range of values of the averaging width Γ. The absolute accuracy of the bounds is improved when m_0 is small. Because the formulas are so explicit, it is not necessary to illustrate the method by any elaborate numerical example. Indeed, from a universal graph one can predict the accuracy to be obtained from these bounds when the self-consistency condition is applied to the energy.

The fact that these are *best possible* bounds means that they can be interpreted negatively as well as positively. We can be sure that if nothing besides m_0, $\bar{m}_1$, and σ is known, it is impossible to obtain rigorous bounds that are any closer. A possible response to this negative statement is to reject rigorous bounds in favor of probabilistic bounds. These would require knowledge of the probability distribution of D, based on some suitable statistical assumption about the unknown function D_{n+1} of Eq. (4.11). This additional information would have to come from something like the statistical many-body theory of French and others.

If the Q space can be partitioned into eigenspaces of H_Q, the eigenspaces will contribute incoherently to D and to the moments M_p. Each contribution can then be bounded individually by the methods we have described, using moments related to the corresponding subspace. For moments through a given order, one would expect this partitioning to give increased accuracy, because for each subspace the strength m_0 and width σ are smaller, while the separation of the centroid from the model-space energy is larger. Unfortunately, exact eigenspaces of H_Q are not easy to construct, and it is not yet clear how to use approximate eigenspaces in this way.

Bounds can also be improved if additional information, such as a cutoff on the density, is known. Cutoff information is of particular interest because we can easily generalize either the inclusion region method or the bounding polynomial method to utilize this information and derive better bounds. This will be discussed in a forthcoming paper.

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