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Influence of singularities on perturbation theory for the effective Hamiltonian

C. M. Vincent*
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
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The energy-independent effective Hamiltonian $\mathcal{H}(z)$ is considered as an analytic function of the coupling parameter z. It is shown that a point z_b is not a singularity of $\mathcal{H}(z)$ unless the energy of some state that is selected for representation in the model space (L_P) coincides, at $z = z_b$, with the energy of a state that is excluded from representation in L_P. This result establishes the correctness of previous conjectures by Schucan and Weidenmüller, and implies that perturbation theory for $\mathcal{H}(z)$ will generally have a larger radius of convergence than perturbation theory for the individual energies. For the case of a cut ("intruder-state cut") joining an isolated pair of branch points close to the real axis, the singular behavior of $\mathcal{H}(z)$ is examined in detail. The residue of the cut is expressed in terms of quantities that can be calculated by diagonalization of a real, symmetric modification ("minimal smoothing") of the Hamiltonian matrix. A formula is given for the contribution of an intruder-state cut to the error incurred by nth order perturbation theory for the physical quantity $\mathcal{H}(1)$. Consideration of a numerical example shows that if the values of sufficiently high orders of perturbation theory are known, the residues of intruder-state cuts may be evaluated. This allows estimation of the errors that intruder-state cuts produce in perturbation theory summed to finite order, and yields a criterion for the optimal truncation of divergent perturbation series.

[NUCLEAR STRUCTURE Effective Hamiltonian for ^{18}O $J^\pi = 0^+$; estimated errors of perturbation theory produced by intruder state.]

I. INTRODUCTION

Rayleigh-Schrödinger perturbation theory (PT) is a powerful and systematic method for solving the time-independent Schrödinger equation for a many-body system. However, if PT is applied directly to the energies of a system with several valence particles, the set of energies corresponding to the simplest configurations (which span the "model space") is degenerate—or nearly degenerate—in zero order. Consequently, small energy denominators occur, and result in poor convergence. A possible cure for this difficulty is to use PT only to construct an effective Hamiltonian $\mathcal{H}$, which then gives the desired energies when it is diagonalized in the model space. This approach turns out to eliminate all small energy denominators. Unlike traditional degenerate PT, PT for $\mathcal{H}$ also lends itself to a systematic description in terms of many-body diagrams.[1]

The promise of diagrammatic PT has not yet found realization in satisfactorily accurate numerical calculations of $\mathcal{H}$ for nuclear problems. The amount of arithmetic involved is not the only difficulty, though the capacity of available computers is a severe limitation. It is found necessary to include very large numbers of intermediate states in each diagram[2] and third-order terms are often larger than second-order terms.[3] These observations, especially the second, have motivated discussion[4] of the theoretical basis of PT for $\mathcal{H}$. A preliminary question is whether PT for $\mathcal{H}$ does indeed converge better than the PT expansions of individual energies. This point is crucial, because on it depends the superiority of the effective-Hamiltonian strategy in practical computation of the energies. Although Schucan and Weidenmüller[5] (SW) have previously addressed this point, their conclusions are tentative, and it seems worthwhile to decide the question with greater certainty, before proceeding with the present discussion of PT for $\mathcal{H}$.

The effective Hamiltonian $\mathcal{H}$ can also be used to derive an effective *interaction*, which can be used to relate problems with different numbers of valence particles, provided that the effective interaction is dominated by its two-body part.[6,7] However, the present work is concerned with the problem of computing $\mathcal{H}$, rather than with the question of the dominance of the two-body part of the effective interaction. Therefore, it will not be necessary to bring the many-body nature of the system into the discussion.

More definite notations are now needed to discuss an uncertainty remaining in the SW analysis, and to introduce the main subjects of the present paper. Let H_0 (assumed Hermitian) be the unperturbed Hamiltonian, whose eigenvalues ϵ_j and

eigenvectors ϕ_j are assumed to be known:

$$H_0\phi_j = \epsilon_j\phi_j . \tag{1.1}$$

In most cases H_0 will be chosen as a sum of one-body Hamiltonians, although this is not a formal necessity. The full Hamiltonian H (assumed Hermitian) for the problem can be separated into a zero-order Hamiltonian and a perturbation, as follows:

$$H = H_0 + zV . \tag{1.2}$$

Here the parameter z is the strength of the perturbation. By convention, we take $z = 1$ as corresponding to the physical value of the perturbation strength. Perturbation theory consists in expanding various quantities in powers of z; for this reason we regard these quantities as functions of z.

Let E_j be the eigenvalues of H, and ψ_j the corresponding eigenvectors, so that

$$H\psi_j = E_j\psi_j . \tag{1.3}$$

A subset $\{E_m\}$ of energies and a corresponding subset $\{\psi_m\}$ of eigenvectors are selected for representation in a model space L_P. They will be referred to as the "represented" energies and eigenvectors. All other E_i and ψ_i will be called "excluded" energies and eigenvectors. The model space is spanned by a chosen set of unperturbed eigenvectors $\{\phi_m\}$ that correspond to simple configurations. The criterion for selecting the sets $\{E_m\}$ and $\{\psi_m\}$ is that each represented ψ_m should have a large component in L_P. By convention, we label the eigenvalues and eigenvectors so that the represented eigenvalues and eigenvectors are the first M:

$$E_m, \psi_m \quad (m = 1, \ldots, M) . \tag{1.4}$$

The unperturbed states selected to span L_P are

$$\phi_m \quad (m = 1, \ldots, M) . \tag{1.5}$$

There is no implication that the full set of eigenvalues $\{E_j \ (j = 1, 2, \ldots)\}$ is arranged in order of ascending values.

Two orthogonal projection operators can be defined as follows:

$$P = \sum_{m=1}^{M} |\phi_m\rangle\langle\phi_m| , \tag{1.6}$$

and

$$\mathcal{P} = \sum_{m=1}^{M} |\psi_m\rangle\langle\psi_m| . \tag{1.7}$$

By convention, script capitals will always denote formal quantities (i.e., those whose evaluation is tantamount to solution of the complete problem), while italic capitals denote quantities that can be constructed from zero-order quantities. The formal quantities, e.g., E_j, ψ_j, and $\mathcal{P}$, are always functions of z, while ϵ_j, ϕ_j, and P are independent of z.

A particular energy-dependent effective Hamiltonian[8] $\mathcal{H}(z)$ is defined as an operator on L_P, whose eigenvalues are the represented eigenvalues E_m of H [Eq. (1.4)], and whose eigenvectors χ_m are the projections of the corresponding eigenvectors of H onto L_P, defined by

$$\chi_m = P\psi_m \quad (m = 1, \ldots, M) . \tag{1.8}$$

Thus the defining property of $\mathcal{H}(z)$ is

$$\mathcal{H}\chi_m = E_m\chi_m \quad (m = 1, \ldots, M) . \tag{1.9}$$

It is shown in Sec. II that the only operator with this property is

$$\mathcal{H} = PH\mathcal{P}P(\mathcal{P}_{PP})^{-1} , \tag{1.10}$$

where $\mathcal{P}_{PP}$ is the restriction of $\mathcal{P}$ to the model space, and its inverse $(\mathcal{P}_{PP})^{-1}$ is assumed to exist.

PT for $\mathcal{H}(z)$ is formally an expansion of Eq. (1.10) in powers of z. If z is regarded as a complex variable,

$$z = x + iy , \tag{1.11}$$

$\mathcal{H}$ can be shown to be an analytic function of z, in some domain including the origin. According to the theory of operator-valued functions of a complex variable,[9] the radius of convergence of PT is the distance R from the origin to the nearest singularity of $\mathcal{H}$, i.e.,

$$R = \min\{|z_b|\} , \tag{1.12}$$

where $\{z_b\}$ is the set of points at which $\mathcal{H}(z)$ is singular. For the physical problem ($z = 1$), PT converges if

$$R > 1 \tag{1.13}$$

[i.e., if $\mathcal{H}$ has no singularity inside the unit circle], and diverges if $R < 1$.

In practice, the question of mathematical convergence may not be decisive, because a convergent series may be numerically useless and a divergent series may be useful if truncated appropriately. (Asymptotic series[10] are only one possible type of useful divergent series. We shall encounter another type.) Nevertheless, for the moment we accept convergence as a criterion of utility and ask whether the PT series for $\mathcal{H}$ has a larger radius of convergence than the series for an individual represented energy.

As will be shown, a singularity of $\mathcal{H}$ can occur only at a point where one (or more) individual represented energy E_m is singular. The singularities of E_m are discussed by Kato,[9] and compactly reviewed by SW. Here we assume that H and H_0

act on a space of finite dimensionality, thereby excluding several pathologies that can occur only in spaces of infinite dimensionality (for example, the entire spectrum of H may become continuous for some values of z). This limitation to finite (though large) spaces agrees well with the spirit of the double-partitioning approach of Barrett.[11] He assumes that a suitable Brueckner reaction matrix is an adequate approximation to the effective interaction in a large finite space. If so, the only problem remaining is to construct an effective interaction for a second model space that is small enough to allow shell-model diagonalizations. Our discussion then applies directly to the calculation of the effective Hamiltonian for the second model space.

Following SW, we agree to disregard some types of singularity because they are statistically unlikely. Only one type of singularity occurs systematically: a first-order branch point at a value $z = z_b$ such that two eigenvalues of H coincide (i.e., a "biexceptional point"). We disregard the possibility of permanent degeneracy, and ignore branch points of second and higher orders, because these would require accidental coincidence of two or more biexceptional points. Thus, by the term "singularity" we shall always mean "first-order branch point."

We now outline some conclusions of SW regarding the effect of singularities in the energies E_m on $\mathcal{K}$. From Eq. (1.10) it is clear that $\mathcal{K}$ is analytic for all z such that (1) $\mathcal{P}$ is analytic and (2) $(\mathcal{P}_{PP})^{-1}$ exists. By contour integration methods, SW show that $\mathcal{P}$ is analytic even at points where two represented energies coincide, and they remark that $(\mathcal{P}_{PP})^{-1}$ exists provided that the set of projections $\{\chi_m \ (m = 1, \ldots, M)\}$ is linearly independent. They then state that linear dependence of $\{\chi_m \ (m = 1, \ldots, M)\}$ for reasonably complicated physical systems is unlikely (assumption 2.22, p. 490 of Ref. 5). It is indeed unlikely that the set $\{\chi_m \ (m = 1, \ldots, M)\}$ would be dependent if the set $\{\psi_m \ (m = 1, \ldots, M)\}$ is linearly independent; it would require a special relationship between P (or H_0), and $\mathcal{P}$ (or H). And for *real* z, the Hermiticity of H guarantees that the ψ_m can be chosen to be linearly independent (in fact, mutually orthogonal). However, in discussing convergence, *complex* z must be allowed; this introduces the new possibility that two of the represented energies may coincide at a complex point z_p. The eigenvectors corresponding to two energies that become degenerate at a complex point z_p always become parallel. Mathematically, $H_0 + z_p V$ is then not diagonalizable, because its eigenvectors no longer form a complete set. This point is illustrated by the analysis of the 2×2 matrix defined by Eq. (4.16) of Sec. IV.

Fortunately, as will be shown in Sec. III, the linear dependence of two represented eigenvectors (at a point z_p where two represented energies coincide) *does not produce any singularity in* $\mathcal{K}$. Since such points z_p will usually be the nearest singularities of the represented energies, this result implies that the radius of convergence of $\mathcal{K}$ will usually be larger than that of the individual represented energies. In agreement with SW, we shall conclude that only a coincidence of a represented and an excluded energy produces a singularity in $\mathcal{K}$. It follows that PT for $\mathcal{K}$ will generally have a larger radius of convergence than PT for the individual E_m.

The rules governing the location of the singularities of $\mathcal{K}$ are proved in Secs. II and III. They are a necessary preparation for the newer and perhaps more practically significant Secs. IV and V, which deal with methods of estimating the contributions of individual singularities. In Sec. IV the form of an intruder singularity in $\mathcal{K}$ is expressed in terms of quantities that can be calculated by diagonalizing real symmetric matrices. This result, Eq. (4.49), enables one to estimate the influence of an intruder-state singularity on perturbation theory for $\mathcal{K}$, at least in studies of solvable models. In Sec. V, some results of Sec. IV are applied to interpret the results of a previous calculation[12] of high orders of perturbation theory. This example shows that the contribution of a singularity can sometimes be accurately estimated solely from perturbation theory, without any matrix diagonalizations being needed. Section VI summarizes the conclusions.

II. FORMAL EXPRESSIONS

Many formal expressions for $\mathcal{K}$ can be derived. Those selected here are not claimed to have special merit for computational purposes. Rather, they are presented for use in Sec. III, in which relevant analytic properties are deduced. Questions regarding the existence of certain operator inverses are also deferred to Sec. III.

A fundamental formal quantity is the operator $\mathfrak{U}$ that diagonalizes H:

$$\mathfrak{U} = \sum_j |\psi_j\rangle\langle\phi_j| \,. \tag{2.1}$$

In this equation, the sum is over all eigenstates ψ_j (and ϕ_j) of H (and H_0). From the orthonormality of the bases $\{\psi_j\}$ and $\{\phi_j\}$ it follows that $\mathfrak{U}$ is unitary, so that

$$\mathfrak{U}^\dagger \mathfrak{U} = 1 \,, \tag{2.2a}$$

$$\mathfrak{U}\,\mathfrak{U}^\dagger = 1 \,. \tag{2.2b}$$

In terms of $\mathfrak{U}$, a valid expression for the effective Hamiltonian is

$$\mathcal{H} = PH\mathfrak{U}P(\mathfrak{U}_{PP})^{-1}. \tag{2.3}$$

Here, and everywhere, symbols such as $\mathfrak{U}_{PP}$ and $\mathfrak{U}_{PQ}$ will have the meanings

$$\mathfrak{U}_{PP} = P\mathfrak{U}P, \quad \mathfrak{U}_{PQ} = P\mathfrak{U}Q, \text{ etc.} \tag{2.4}$$

Also, the expression $(\mathfrak{U}_{PP})^{-1}$, for example, refers to the inverse of $\mathfrak{U}_{PP}$ regarded as an operator on the model space L_P, i.e., the space onto which P projects. It is easy to verify that (2.3) has the property [Eq. (1.9)] that defines $\mathcal{H}$. First, from Eq. (2.1),

$$\mathfrak{U}_{PP}\phi_m = P\psi_m = \chi_m, \tag{2.5}$$

so that

$$\phi_m = (\mathfrak{U}_{PP})^{-1}\chi_m \tag{2.6}$$

if the required inverse exists. Then

$$PH\mathfrak{U}P(\mathfrak{U}_{PP})^{-1}\chi_m = PH\mathfrak{U}P\phi_m = PH\psi_m = E_m\chi_m,$$

which is Eq. (1.9).

Another useful operator is $\mathcal{P}$, the projection on the space spanned by the set of represented states $\{\psi_m \ (m = 1, \ldots, M)\}$ [see Eq. (1.7)]. This operator is related to $\mathfrak{U}$ by

$$\mathcal{P} = \mathfrak{U}P\mathfrak{U}^{\dagger}, \tag{2.7}$$

so that

$$\mathcal{P}_{PP} = \mathfrak{U}_{PP}\mathfrak{U}_{PP}^{\dagger}. \tag{2.8}$$

The operator $\mathcal{P}_{PP}$ is central to the discussion. A certain set of vectors $\{\tilde{\chi}_m \ (m = 1, \ldots, M)\}$, said to be "dual" to the set $\{\chi_m \ (m = 1, \ldots, M)\}$, can be defined by

$$\tilde{\chi}_m = (\mathcal{P}_{PP})^{-1}\chi_m \quad (m = 1, \ldots, M). \tag{2.9}$$

The dual set is biorthonormal with respect to the original set, because [by Eqs. (2.6), (2.8), and (2.9)]

$$\begin{aligned}\langle\chi_m|\tilde{\chi}_{m'}\rangle &= \langle P\psi_m|(\mathfrak{U}_{PP}^{\dagger})^{-1}(\mathfrak{U}_{PP})^{-1}|P\psi_{m'}\rangle \\ &= \langle\phi_m|\phi_{m'}\rangle,\end{aligned}$$

so that, by the orthonormality of the set $\{\phi_m\}$,

$$\langle\chi_m|\tilde{\chi}_{m'}\rangle = \delta_{mm'}. \tag{2.10}$$

With the aid of the $\{\tilde{\chi}_m\}$ we can define an individual oblique projection operator for each represented state:

$$\tilde{\mathcal{P}}_m = |\chi_m\rangle\langle\tilde{\chi}_m|. \tag{2.11}$$

These operators are idempotent (but not Hermitian) and annihilate one another, so that

$$\tilde{\mathcal{P}}_m\tilde{\mathcal{P}}_{m'} = \delta_{mm'}\tilde{\mathcal{P}}_m. \tag{2.12}$$

In terms of these projections, it is easy to see that

$$\mathcal{H} = \sum_{m=1}^{M} E_m\tilde{\mathcal{P}}_m, \tag{2.13}$$

because

$$\left(\sum_{m=1}^{M} E_m\tilde{\mathcal{P}}_m\right)\chi_{m'} = E_{m'}\chi_{m'} \quad (m' = 1, \ldots, M).$$

The effective Hamiltonian can be expressed in terms of $\mathcal{P}$, in a form not containing the energies explicitly, as follows:

$$\mathcal{H} = PH\mathcal{P}P(\mathcal{P}_{PP})^{-1}. \tag{2.14}$$

This result, which is Eq. (1.10) of the Introduction, is seen to be equivalent to Eq. (2.3) by applying Eqs. (2.7) and (2.8).

Further relations can be obtained by introducing Q, the projection complementary to P, which satisfies

$$Q = 1 - P, \quad Q^2 = Q, \quad PQ = QP = 0. \tag{2.15}$$

By inserting Eq. (2.2a) between P and Q, and using the relations (2.15), we obtain

$$0 = QP = Q\mathfrak{U}^{\dagger}\mathfrak{U}P = \mathfrak{U}_{QP}^{\dagger}\mathfrak{U}_{PP} + \mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QP},$$

so that

$$\mathfrak{U}_{QP}(\mathfrak{U}_{PP})^{-1} = -(\mathfrak{U}_{QQ}^{\dagger})^{-1}\mathfrak{U}_{QP}^{\dagger}. \tag{2.16}$$

Note that, for example,

$$\mathfrak{U}_{QP}^{\dagger} = Q\mathfrak{U}^{\dagger}P. \tag{2.17}$$

Equation (2.16) can be used to transform expressions into "complementary" forms, since it allows inverses in L_P (the space onto which P projects) to be replaced by inverses in L_Q (the space onto which Q projects). The most interesting application is an expression for $(\mathcal{P}_{PP})^{-1}$ in terms of inverses in L_Q. By developing the right-hand side of Eq. (2.16), using Eqs. (2.16), (2.2a), and (2.15), we find

$$\begin{aligned}\mathfrak{U}_{QP}(\mathfrak{U}_{PP})^{-1} &= -(\mathfrak{U}_{QQ}^{\dagger})^{-1}\mathfrak{U}_{QP}^{\dagger} \\ &= -\mathfrak{U}_{QQ}(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ})^{-1}\mathfrak{U}_{QP}^{\dagger} \\ &= -\mathfrak{U}_{QQ}(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ} + \mathfrak{U}_{QP}^{\dagger}\mathfrak{U}_{PQ})(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ})^{-1}\mathfrak{U}_{QP}^{\dagger} \\ &= -\mathfrak{U}_{QQ}\mathfrak{U}_{QP}^{\dagger}[P + \mathfrak{U}_{PQ}(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ})^{-1}\mathfrak{U}_{QP}^{\dagger}].\end{aligned} \tag{2.18}$$

Alternatively, from Eq. (2.2b),

$$Q\mathfrak{U}\mathfrak{U}^{\dagger}P = QP = 0, \tag{2.19}$$

so that by applying Eq. (2.8) we find

$$\begin{aligned}\mathfrak{U}_{QP}(\mathfrak{U}_{PP})^{-1} &= (\mathfrak{U}_{QP}\mathfrak{U}_{PP}^{\dagger})(\mathfrak{U}_{PP}\mathfrak{U}_{PP}^{\dagger})^{-1} \\ &= -\mathfrak{U}_{QQ}\mathfrak{U}_{QP}^{\dagger}(\mathcal{P}_{PP})^{-1}.\end{aligned} \tag{2.20}$$

Multiplying Eqs. (2.18) and (2.20) by

$$(\mathfrak{U}_{PQ}\mathfrak{U}_{QP}^{\dagger})^{-1}\mathfrak{U}_{PQ}(\mathfrak{U}_{QQ})^{-1} \tag{2.21}$$

finally yields the identity

$$(\mathcal{P}_{PP})^{-1} = P + \mathfrak{U}_{PQ}(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ})^{-1}\mathfrak{U}_{QP}^{\dagger}. \tag{2.22}$$

The operations involved in Eq. (2.22) require the existence of the inverses of the operators $\mathfrak{U}_{QQ}$, $\mathfrak{U}_{QQ}^{\dagger}$ and

$$\mathfrak{Q}_{PP} \equiv \mathfrak{U}_{PQ}\mathfrak{U}_{QP}^{\dagger} = P(1-\mathcal{P})P. \tag{2.23}$$

The expression (2.22) for $(\mathcal{P}_{PP})^{-1}$ can be inserted in Eq. (2.14) to give a new expression for $\mathcal{H}$:

$$\mathcal{H} = PH\mathcal{P}[P + \mathfrak{U}_{PQ}(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ})^{-1}\mathfrak{U}_{QP}^{\dagger}]. \tag{2.24}$$

As formal expressions for $\mathcal{H}$ we now have several equations: (2.3), (2.13), (2.14), and (2.24). The result (2.22) will also be of particular interest because of its implications for analytic properties. Finally, we shall find it convenient to introduce the model operator[13] (or wave operator) $\mathcal{F}$, defined by

$$\mathcal{F} = \mathfrak{U}P(\mathfrak{U}_{PP})^{-1}. \tag{2.25}$$

From Eqs. (2.25), (2.7), and (2.10) the following characteristic property of $\mathcal{F}$ can be derived:

$$\mathcal{F}\chi_m = \psi_m \quad (m = 1, \ldots, M). \tag{2.26}$$

In terms of $\mathcal{F}$, Eq. (2.3) becomes

$$\mathcal{H} = PH\mathcal{F}, \tag{2.27}$$

while Eqs. (2.14) and (2.24) are respectively equivalent to

$$\mathcal{F} = \mathcal{P}P(\mathcal{P}_{PP})^{-1} \tag{2.28}$$

and

$$\mathcal{F} = \mathcal{P}[P + \mathfrak{U}_{PQ}(\mathfrak{U}_{QQ}^{\dagger}\mathfrak{U}_{QQ})^{-1}\mathfrak{U}_{QP}^{\dagger}]. \tag{2.29}$$

Other effective operators, besides the effective Hamiltonian, can be expressed in terms of $\mathcal{F}$.

III. POSITIONS OF THE SINGULARITIES OF $\mathcal{H}(z)$

The method of this section depends on analytic continuation of operator-valued functions to complex values of z. In considering such analytic continuations, it is convenient to assume that H_0 and H are time-reversal invariant,[14] and that the basis $\{\phi_j\}$ is such that their matrices are real (for real z). Then the Hermitian conjugation (denoted with a dagger) (which appears in some of the expressions of Sec. II) can always be interpreted as a transpose. Thus, discussion of analytic properties is not obscured by the appearance of the nonanalytic function z^*, the complex conjugate of z.

The derivations of Sec. II can fail at most for a discrete set of z values. In particular, they are certainly valid at least for some finite continuous segment of the real axis, including the origin. Therefore, if all the operators appearing in one of these algebraic relations are analytically continued to complex z, the analytic continuations of the operators will still satisfy the relation. It is only the singularities of the *analytic continuations* of the operators that determine the radius of convergence; it does not matter if the original definitions of the operators fail at some value of z. Much use will be made of the fact that all singularities of operators can be referred to singularities in the energies, $\{E_j\}$. In fact, Kato[15] shows that the projection operator on an eigenstate,

$$\mathcal{P}_j = |\psi_j\rangle\langle\psi_j| \tag{3.1}$$

is analytic everwhere except possibly at points z where at least one other energy coincides with E_j. We can see that ψ_j has similar properties, if its overall phase is appropriately chosen. Let f be some arbitrary vector, independent of z. Then one can choose the overall phase of ψ_j so that, for real z,

$$\psi_j = [\langle f|\mathcal{P}_j|f\rangle]^{-1/2}\mathcal{P}_j f, \tag{3.2}$$

where the square root is interpreted as positive. Note that Eq. (3.2) determines the phase of ψ_j, because the definition of $\mathcal{P}_j$ in terms of ψ_j does not depend on the phase of ψ_j. Because $\mathcal{P}_j$ is analytic (away from exceptional points), $[\langle f|\mathcal{P}_j|f\rangle]^{-1/2}$ is also analytic, provided that $\mathcal{P}_j f \neq 0$, which can be ensured by a suitable choice of f. Therefore ψ_j is analytic everywhere—except possibly at those values of z where another energy coincides with E_j. Since $\mathfrak{U}$ depends on z only through the eigenvectors ψ_j [see Eq. (2.1)], all singularities of $\mathfrak{U}$ must also be at the branch points of the energies.

Every branch point is either (1) a "P-P singularity," defined as a point where two represented energies are the only energies that coincide; (2) a "Q-Q singularity," defined as a point where only two excluded energies coincide; or (3) a "P-Q singularity," defined as a point where one represented energy and one excluded energy coincide.

Theorems regarding the location of singularities can now be stated and proved.

Theorem 1. $\mathcal{P}(z)$ is analytic except possibly at P-Q singularities. (Kato[15] gives a proof of this theorem, using contour-integral methods.)

Proof. From Eq. (1.7), $\mathcal{P}$ depends on z only through the represented eigenvectors ψ_m. Hence only P-P and P-Q singularities can appear in $\mathcal{P}$. To see that a P-P singularity, say z_p, cannot appear in $\mathcal{P}$, write $\mathcal{P}$ in the form

$$\mathcal{P} = 1 - \sum_{i>M} |\psi_i\rangle\langle\psi_i|. \tag{3.3}$$

Now the right-hand side of Eq. (3.3) is manifestly analytic at a P-P singularity, because none of the excluded eigenvectors $\{\psi_i\ (i>M)\}$ has a P-P singu-

larity. Therefore $\mathcal{P}$ is analytic except at P-Q singularities.

The use of the "manifest" analyticity of $\mathcal{P}$ as expressed by Eq. (3.3) is typical of the methods of this section. Several of the formulas in Sec. II display manifest analyticity of this kind, in that either represented or excluded states are absent from the right-hand side.

Theorem 2. $(\mathcal{P}_{PP})^{-1}$ *is analytic except possibly at* P-Q *singularities.*

Proof. From Eq. (2.22), $(\mathcal{P}_{PP})^{-1}$ is manifestly analytic at P-P singularities because the operators $\mathfrak{U}_{PQ}$, $\mathfrak{U}_{QP}^{\dagger}$, $\mathfrak{U}_{QQ}$, and $\mathfrak{U}_{QQ}^{\dagger}$ do not contain represented eigenvectors. From Eq. (1.7), $(\mathcal{P}_{PP})^{-1}$ is manifestly analytic at Q-Q singularities. Hence $(\mathcal{P}_{PP})^{-1}$ is analytic except possibly at P-Q singularities.

Theorem 3. The model operator $\mathcal{F}(z)$ *and the effective Hamiltonian* $\mathcal{K}(z)$ *are analytic, except possibly at* P-Q *singularities.*

Proof. These results follow at once from Eqs. (2.25) and (2.27), because the product of analytic operators is analytic.

Theorems 2 and 3 do not seem to have been proved before. That $(\mathcal{P}_{PP})^{-1}$ should have the same domain of analyticity as $\mathcal{P}$ seems quite unexpected, for the following reason. The inverse of $\mathcal{P}_{PP}$ cannot be constructed from normalized eigenvectors at a point z_p where two represented eigenvalues coincide, because the corresponding eigenvectors, ψ_1 and ψ_2, say, become parallel at z_p. Consequently, their projections $\chi_1 = P\psi_1$ and $\chi_2 = P\psi_2$ become parallel, so that the determinant of the matrix whose (i,j)th element is

$$(\mathcal{P}_{PP})_{ij} = \sum_{m=1}^{M} \langle \phi_i | \psi_m \rangle \langle \psi_m | \phi_j \rangle \quad (i,j = 1, \ldots, M) \tag{3.4}$$

vanishes at z_p. In fact, this is the Gram matrix[16] of the set of vectors $\{\chi_m\ (m = 1, \ldots, M)\}$, and its vanishing is a standard test for linear dependence. The failure of $(\mathcal{P}_{PP})^{-1}$ to have P-P singularities becomes easier to understand when it is appreciated that the analytic continuation of $\mathcal{P}_m$ always has an *infinity*[17] at a branch point of E_m. This infinity essentially cancels the zero of the determinant that would occur in constructing $(\mathcal{P}_{PP})^{-1}$ from normalized eigenvectors. Equation (3.2) shows that the eigenvector ψ_m will also be infinite at a branch point of E_m.

Because its eigenvalues are all real, $\mathcal{K}$ can be converted into a Hermitian operator by a similarity transformation. In particular, we easily see that the operator defined by

$$\mathcal{K}_{\text{sym}} \equiv (\mathcal{P}_{PP})^{-1/2} \mathcal{K} (\mathcal{P}_{PP})^{1/2} \tag{3.5}$$

has the same eigenvalues as $\mathcal{K}$, because

$$(\mathcal{K}_{\text{sym}} - E_m)(\mathcal{P}_{PP})^{-1/2} \chi_m = 0 \quad (m = 1, \ldots, M) \tag{3.6}$$

and is Hermitian because [by Eqs. (2.9), (2.11), and (2.13)] it can be written in the form

$$\mathcal{K}_{\text{sym}} = (\mathcal{P}_{PP})^{-1/2} \left(\sum_{m=1}^{M} |\chi_m\rangle E_m \langle \chi_m | \right) (\mathcal{P}_{PP})^{-1/2}. \tag{3.7}$$

The practical advantage of this symmetrized effective Hamiltonian is that it can be diagonalized using standard methods. However, its analytic properties are not so transparent as those of $\mathcal{K}$, because of the possibility that $(\mathcal{P}_{PP})^{1/2}$ may introduce singularities that are not present in $\mathcal{K}$.

The main result of Sec. III is that only P-Q singularities appear in $\mathcal{K}$ (Theorem 3). This means that the radius of convergence of PT for $\mathcal{K}$ is not limited by the P-P singularities. Since these are usually the nearest singularities, we conclude that PT for $\mathcal{K}$ will usually converge better than PT for the individual represented energies. Section IV discusses the effect of P-Q singularities on PT for $\mathcal{K}$.

IV. STRUCTURE OF AN ISOLATED SINGULARITY OF $\mathcal{K}(z)$

A. Minimal smoothing adjustment of an isolated singularity

According to Theorem 3, every singularity of $\mathcal{K}(z)$ is located at a P-Q branch point. Therefore consider a complex-conjugate pair of P-Q branch points $z_b = x_b + iy_b$ and $z_b^* = x_b - iy_b$ (where by convention $y_b > 0$). Two such branch points will be described as *isolated* if their separation $\lambda_b = 2y_b$ is much smaller than the distance from z_b to any other branch point. Then it can be assumed that in the neighborhood of an isolated pair of branch points, the influence of all other singularities can be neglected. The notion of an isolated pair of branch points is an idealization. Though it can only be realized approximately in practice, it is very useful in theory. In this respect it is analogous to the idea of an isolated resonance pole in scattering theory.

Now consider the z dependence of the energies and eigenvectors near an isolated pair of branch points. Suppose E_m (represented) and E_i (excluded) are the energies that coincide at z_b, and let ψ_m and ψ_i be the corresponding eigenvectors. Regarded as a function of real z, the difference $E_i - E_m$ will be a minimum at some value $z = x_{b0}$, near $x_b \equiv \text{Re} z_b$, so that

$$\frac{\partial}{\partial z} \{E_i(z) - E_m(z)\}_{z = x_{b0}} = 0. \tag{4.1}$$

The eigenvectors evaluated at $z = x_{b0}$ can be used to define a basis (called "the x_b basis") for the perturbation problem:

$$\psi_{jb} \equiv \psi_j(x_{b0}) \quad (j = 1, 2, \ldots). \tag{4.2}$$

Similarly, we denote the expectations of $H(x_{b0})$ in the x_b basis by

$$E_{jb} \equiv E_j(x_{b0}) \quad (j = 1, 2, \ldots). \tag{4.3}$$

We now construct an *adjusted perturbation problem* with the same H_0, but with V replaced by

$$V_b = V - V_{\text{adj}}, \tag{4.4}$$

where the adjustment V_{adj} is defined by

$$V_{\text{adj}} \equiv \tfrac{1}{2} m_b [\, |\psi_{ib}\rangle\langle\psi_{ib}| - |\psi_{mb}\rangle\langle\psi_{mb}| \,], \tag{4.5}$$

with

$$m_b = \tfrac{1}{2}(E_{ib} - E_{mb})/x_{b0}. \tag{4.6}$$

Note that V_b is Hermitian and independent of z.

Theorem 4. The energies of the adjusted perturbation problem

$$H^a(z) = H_0 + z V_b$$

are analytic functions of z, at and near z_b and z_b^*.

Proof. Consider the adjusted problem in the x_b basis. We have

$$\begin{aligned} H^a &= H_0 + z V_b \\ &= (H_0 + x_{b0} V_b) + (z - x_{b0}) V_b, \end{aligned} \tag{4.7}$$

where $H_0 + x_{b0} V_b$ is diagonal, so that H^a can be regarded as a zero-order Hamiltonian $H^a(x_{b0})$, perturbed by $(z - x_{b0}) V_b$. It can be shown directly from Eqs. (4.4)–(4.6) that ψ_{ib} and ψ_{mb} are eigenvectors of $H^a(x_{b0})$, belonging to a common eigenvalue $\bar{E}_b$ defined by

$$\bar{E}_b = \tfrac{1}{2}(E_{ib} + E_{mb}). \tag{4.8}$$

The perturbation $(z - x_{b0}) V_b$ splits these degenerate eigenvalues in first order, and—as usual—the expansion of the energies in powers of $(z - x_{b0})$ has a nonzero radius of convergence. This radius of convergence is of the same order as the distance from z_b to the nearest singularity (other than z_b), so that the energies are analytic at and near z_b and z_b^*. (For a more rigorous treatment of analyticity near a degeneracy at real z, see Theorem 6.1 of Ref. 9.)

Because of Theorem 4, V_b can appropriately be called a *smoothed perturbation,* to indicate that the singularities of the original problem at z_b and z_b^* are absent from the adjusted problem. Other smoothed perturbations can be constructed. An example is $V_{PP} + V_{QQ}$, for which the P-Q biexceptional points are always on the real axis (because there is no coupling between L_P and L_Q), so that crossing between represented and excluded eigenvalues of $H_0 + z(V_{PP} + V_{QQ})$ is always smooth. However, the replacement $V \to V_{PP} + V_{QQ}$ is much more drastic than is necessary to remove singularities within the unit circle. Replacing V by $V_{PP} + V_{QQ}$ involves large changes in the energies, and consequently the crossing points of represented and excluded eigenvalues may be shifted from the values of x_b that hold for the original H, by distances much greater than the values of y_b. An example of this effect is shown in Fig. 1, where replacement of V by $V_{PP} + V_{QQ}$ shifts a biexceptional point much closer to the origin because the important effect of the excluded space in depressing the represented eigenvalue E_m is removed, while the effect of the model space on the intruder eigenvalue E_i remains very small. In contrast to $V_{PQ} + V_{QP}$, V_{adj} defined by (4.5) has the valuable advantage of being a *minimal* smoothing adjustment of V. This is because the eigenvalues of $x_{b0} V_{\text{adj}}$ are

$$\pm m_b x_{b0} = \pm \tfrac{1}{2}(E_{ib} - E_{mb}),$$

which is clearly the smallest shift that will produce degeneracy, and by Eq. (4.1) this difference is itself minimized at $z = x_b$. Thus, of all possible smoothing adjustments, V_{adj} has the smallest norm. By a well-known theorem quoted by Wilkinson,[18]

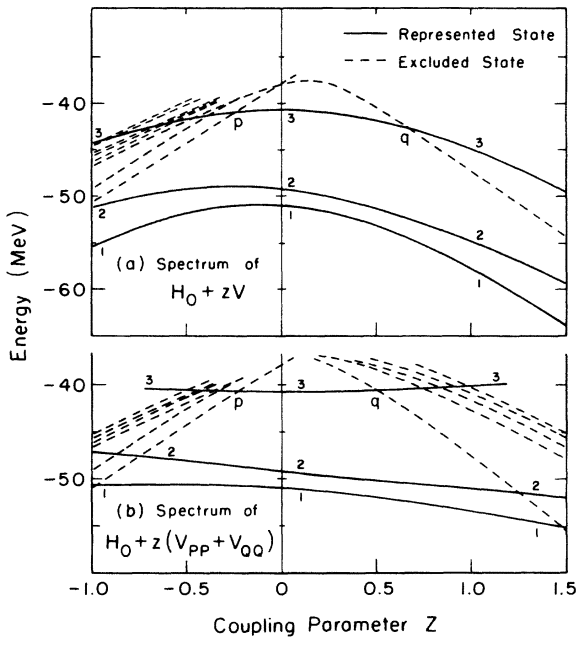

FIG. 1. Spectra of (a) H and (b) $H_{PP} + H_{QQ}$ for the calculation described in Ref. 12. The represented states are labeled by their main configurations: $1 \equiv d_{5/2}{}^2$, $2 \equiv s_{1/2}{}^2$, and $3 \equiv d_{3/2}{}^2$. Note that the P-Q singularity labeled p is only slightly shifted by the smoothing replacement $H \to H_{PP} + H_{QQ}$; however, the singularity q is considerably shifted, and $H_{PP} + H_{QQ}$ has five intruder states at $z = 1$, while H has only one. This illustrates the rather drastic effect of this type of smoothing.

every eigenvalue of the physical smoothed Hamiltonian $H^a(1)$ lies within a distance m_b of the corresponding eigenvalue of $H(1)$. This already provides an absolute bound on the effect of the singularity on eigenvalues of $\mathcal{H}$; however, closer estimates are often possible.

B. Eigenvalue problem in the x_b basis

If the pair of branch points z_b, z_b^* is isolated, then, near $z = x_{b0}$, E_i and E_m are the only eigenvalues of $H(z)$ that are closely spaced, and the doubly-degenerate eigenvalue $\overline{E}_{im}$ of $H_b(z)$ is also isolated from other eigenvalues. Therefore, the eigenvectors and eigenvalues of the original Hamiltonian $H(z)$ can consistently be approximated by working within a truncated x_b basis consisting of the two vectors ψ_{mb} and ψ_{ib}. In this basis,

$$H(z) = \begin{pmatrix} \overline{E}_b & 0 \\ 0 & \overline{E}_b \end{pmatrix} + \begin{pmatrix} -m_b x_{b0} & 0 \\ 0 & +m_b x_{b0} \end{pmatrix} + (z - x_{b0}) \begin{pmatrix} V_{mm} & V_{mi} \\ V_{im} & V_{ii} \end{pmatrix}, \tag{4.9}$$

where

$$V_{jj'} \equiv \langle \psi_{jb} \mid V \mid \psi_{j'b} \rangle \quad (j, j' = m \text{ or } i). \tag{4.10}$$

Because E_{mb} and E_{ib} are not degenerate, perturbation theory to first order in $(z - x_{b0})$ gives

$$\frac{\partial E_m}{\partial z} = V_{mm}, \quad \frac{\partial E_i}{\partial z} = V_{ii} \tag{4.11}$$

when applied to Eq. (4.9). Equations (4.1) and (4.11) together now require that

$$V_{mm} = V_{ii}. \tag{4.12}$$

For convenience, and to conform with the notation of Ref. 12, we can therefore describe the matrix defined by Eq. (4.10) in terms of only two independent parameters

$$D \equiv V_{mm} = V_{ii}, \quad d = 2V_{mi} = 2V_{im}, \tag{4.13}$$

so that Eq. (4.9) becomes

$$H(z) = \begin{pmatrix} \overline{E}_b + D(z - x_{b0}) & 0 \\ 0 & \overline{E}_b + D(z - x_{b0}) \end{pmatrix} + \begin{pmatrix} -m_b x_{b0} & \frac{1}{2} d(z - x_{b0}) \\ \frac{1}{2} d(z - x_{b0}) & m_b x_{b0} \end{pmatrix}. \tag{4.14}$$

The work of diagonalizing $H(z)$ can be streamlined by realizing that the first term is a scalar and does not influence the eigenvectors. The eigenvalues of Eq. (4.14) are found to be

$$E_m = \overline{E}_b + D(z - x_{b0}) - \epsilon, \tag{4.15a}$$

$$E_i = \overline{E}_b + D(z - x_{b0}) + \epsilon, \tag{4.15b}$$

where

$$\epsilon = [(m_b x_{b0})^2 + \tfrac{1}{4} d^2 (z - x_{b0})^2]^{1/2}. \tag{4.16}$$

The term ϵ contains branch points at

$$z_b = x_{b0} + 2im_b/d, \quad z_b^* = x_{b0} - 2im_b/d. \tag{4.17}$$

Thus, for an isolated pair of branch points,

$$x_b = x_{b0}, \tag{4.18}$$

that is, the real part of z_b is equal to the value of z that corresponds to closest approach of the eigenvalues. In terms of the branch points, Eq. (4.17), ϵ can be written in the form

$$\epsilon = \tfrac{1}{2} d [(z - z_b)(z - z_b^*)]^{1/2}. \tag{4.19}$$

The eigenvectors, corresponding to E_m and E_i given by Eq. (4.15) and normalized to unity, are

$$\psi_m = (1 + c^2)^{-1/2} (\psi_{mb} + c\psi_{ib}), \qquad \psi_i = (1 + c^2)^{-1/2} (-c\psi_{mb} + \psi_{ib}), \tag{4.20}$$

where

$$c = \frac{m + \epsilon}{\frac{1}{2} d (z - x_b)}. \tag{4.21}$$

At $z = z_b$, and at $z = z_b^*$, we have

$$c(z_b) = -i, \quad c(z_b^*) = +i, \tag{4.22}$$

respectively. From Eq. (4.22) it follows that ψ_m and ψ_i [given by Eq. (4.20)] both become infinite at z_b and z_b^*. Also, ψ_i and ψ_m become parallel, so that the eigenvectors of $H(z_b)$ no longer form a complete set, and $H(z_b)$ cannot be diagonalized. In considering behavior near these singularities, it is therefore convenient to make use of unnormalized eigenvectors, e.g.,

$$\psi_m^u(z) = \psi_{mb} + c\psi_{ib}, \tag{4.23}$$

which for $z = z_b$ takes on the value

$$\psi_m^u(z_b) = \psi_{mb} - i\psi_b. \tag{4.24}$$

Near $z = z_b$, we can simplify $\psi_m^u(z)$ by expanding c in powers of $(z - z_b)^{1/2}$ as

$$c(z) = c(z_b) - 2(i\lambda_b)^{-1/2} (z - z_b)^{1/2} + \cdots, \tag{4.25}$$

and neglecting higher powers. Here we have introduced a convenient notation:

$$\lambda_b = 2\,\mathrm{Im}(z_b) = 4m_b/d \tag{4.26}$$

for the distance between the conjugate singularities. We find

$$\psi_m^u(z) = \psi_m^u(z_b) - 2(i\lambda_b)^{-1/2}(z - z_b)^{1/2}\psi_{ib} + \cdots . \tag{4.27}$$

The square root in Eq. (4.27) causes ψ_m^u and ψ_i^u to undergo very rapid rotations near the singular points.

The results of this eigenvalue problem [especially Eqs. (4.15), (4.16), (4.19), (4.20), (4.21), (4.25), and (4.27)] will be used in Sec. IV D to construct the form of $\mathcal{H}(z)$ near z_b and z_b^*.

C. Step and gap singularities; branch cuts

We now discuss the branch cuts of $\mathcal{H}$. The branch points are determined solely by H_0 and V, but the way in which the branch cuts connect them is entirely a matter of choice, which determines what is being conventionally taken as the first sheet of $\mathcal{H}(z)$. Consider an isolated pair of branch points with $|x_b| \gg y_b$. Then, as discussed by SW, the model-space probability, defined by

$$p(x) \equiv \langle \psi_m(x) | P | \psi_m(x) \rangle , \tag{4.28}$$

changes abruptly near x_b. It is appropriate to select ψ_m for representation in the model space only if $p(x)$ is fairly close to unity. If $\psi_m(x)$ is analytically continued from $z = 0$ [where $p(x) = 1$] to $x > x_b$ along the real axis, then near x_b, $p(x)$ will abruptly fall to a small value characteristic of the excluded eigenvector ψ_i. If, instead, $\psi_m(z)$ is analytically continued *around* the branch point z_b, $p(x)$ will remain large for real $x > x_b$. Therefore, if the first sheet of $\mathcal{H}$ is to correspond to eigenvectors with large model-space probabilities, a cut should be drawn from z_b to z_b^*. The exact shape of the cut is unimportant; for simplicity, a straight line can be used. The presence of the cut implies that $E_m(x)$ will not be continuous at x_b; it will have a finite discontinuity, that is a "step," of height $2m_b x_b$. Accordingly, we say that a pair of branch points with $y_b \ll |x_b|$ leads to a *step singularity*. This is the type of singularity associated with a so-called intruder state,[19] defined as any state belonging mainly to L_Q that is depressed below the uppermost represented state by the action of the perturbation.

On the other hand, if $|x_b| \ll y_b$, then $p(x)$ varies slowly even near x_b, and it is appropriate to analytically continue E_m and ψ_m by passing through the gap between z_b and z_b^*. This corresponds to drawing two cuts from z_b and z_b^* to infinity, away from the real axis. Such a gap would not usually be regarded as an intruder-state singularity, but rather as an effect of strong interaction between model and excluded spaces. If $|y_b| < 1$, then $p(x) < \frac{1}{2}$ at $x = 1$, so that the model space can at best represent only a small part of ψ_m. Existence of such a gap singularity with $|y_b| < 1$ would suggest that the model space has been chosen inappropriately, rather than simply indicating that PT diverges. Accordingly, we do not treat gap singularities. However, their possible importance in realistic problems remains an open question.

Figure 2 illustrates the difference between step and gap singularities, and shows examples of isolated step singularities.

D. Residue of a step singularity

If an isolated step singularity of $\mathcal{H}(z)$ is, in addition, distant from the origin $z = 0$ and the physical point $z = 1$, it can be well approximated by a pole[20] placed at the center of the step. As will be seen in Sec. V, this provides a useful way of estimating the effect of the step singularity on PT approximations. For quantitative estimates it is necessary to know the *residue* μ_b of the step; this is an operator equal to $(2\pi i)^{-1}$ times the integral of $\mathcal{H}(z)$ around a closed counterclockwise contour containing the step (but no other singularities).

We aim to express the residue in terms of quan-

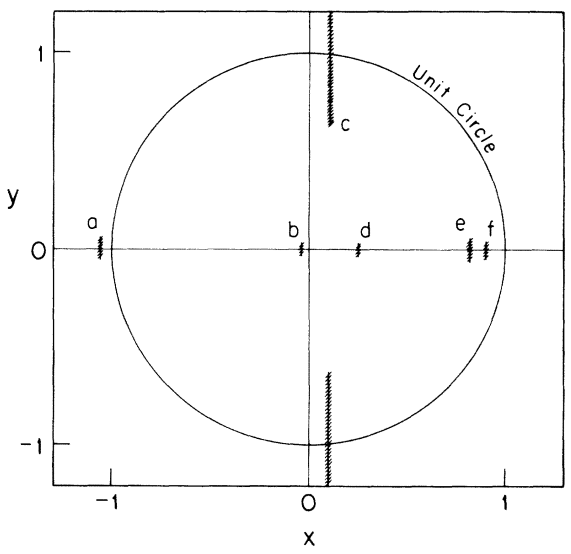

FIG. 2. Argand diagram showing gap and step singularities. For this hypothetical distribution of singularities, PT diverges at $z = 1$ because of the presence of the pairs of branch points b, c, d, e, and f inside the unit circle. Even in the absence of the step singularities (b, d, e, and f) the gap singularity c would still cause divergence. Of the step singularities, only a, b, and d are isolated, while e and f are not. The pole approximation of Sec. V would be appropriate for a and d, but not for b, c, e, or f.

tities that can be obtained by diagonalizing only real matrices. The major difficulty is the correct inclusion of background effects of terms that behave smoothly in the vicinity of the step. These influence the value of the residue, but not the form of the singularity. Analogously, background effects modify the energy and width of a scattering resonance, even in an approximation which retains the Breit-Wigner form.

Background effects correspond to a problem which has all singularities except the one under consideration. Therefore they are correctly described by the minimally adjusted Hamiltonian defined by Eqs. (4.4) and (4.5). All quantities derived from the minimally adjusted problem will be marked by a superscript a. From Eq. (2.3) it is clear that the operator $(\mathfrak{U}_{PP})^{-1}$ is central to the discussion. Let the background be described by the operator

$$\mathfrak{U}^a = \sum_{m'=1}^{M} |\psi^a_{m'}\rangle\langle\phi_{m'}| . \tag{4.29}$$

This operator is analytic near z_b and z_b^*, so it can be taken as constant and evaluated at $z = x_b$. Because the step singularity of the original problem involves only the eigenvectors ψ_m and ψ_i, it is consistent to assume that

$$\begin{aligned} \psi_{m'} &= \psi^a_{m'b} \quad (m' \neq m) , \\ \psi_{i'} &= \psi^a_{i'b} \quad (i' \neq i) , \end{aligned} \tag{4.30}$$

so that

$$\mathfrak{U} = \mathfrak{U}^a + |\zeta_m\rangle\langle\phi_m| , \tag{4.31}$$

with

$$\zeta_m = \psi_m - \psi^a_{mb} . \tag{4.32}$$

The separable form of the second term of Eq. (4.31) enables $(\mathfrak{U}_{PP})^{-1}$ to be expressed in terms of $(\mathfrak{U}^a_{PP})^{-1}$:

$$(\mathfrak{U}_{PP})^{-1} = (\mathfrak{U}^a_{PP})^{-1}\left[1 - \frac{P|\zeta_m\rangle\langle\phi_m|(\mathfrak{U}^a_{PP})^{-1}}{1 + \langle\phi_m|(\mathfrak{U}^a_{PP})^{-1}|\zeta_m\rangle}\right] . \tag{4.33}$$

By introducing the convenient notation

$$B \equiv (\mathfrak{U}^a_{PP})^{-1} \tag{4.34}$$

for the background matrix, and noticing that

$$\langle\phi_m|(\mathfrak{U}^a_{PP})^{-1} = \langle\tilde{\chi}^a_m| , \tag{4.35}$$

so that

$$1 + \langle\phi_m|(\mathfrak{U}^a_{PP})^{-1}|\zeta_m\rangle = \langle\tilde{\chi}^a_m|\psi_m\rangle , \tag{4.36}$$

Eq. (4.33) can be rewritten as

$$(\mathfrak{U}_{PP})^{-1} = B\left(1 - \frac{P|\zeta_m\rangle\langle\tilde{\chi}^a_m|}{\langle\tilde{\chi}^a_m|\psi_m\rangle}\right) . \tag{4.37}$$

Let us consider the step singularity in the model operator $\mathfrak{F}$. Because of the identity $P\mathfrak{F} = P$, only $Q\mathfrak{F}$ can contain a singularity. Equations (4.31) and (4.37), applied to Eq. (2.25), give

$$\begin{aligned} Q\mathfrak{F} &= \mathfrak{U}_{QP}(\mathfrak{U}_{PP})^{-1} \\ &= (\mathfrak{U}^a_{QP} + Q|\zeta_m\rangle\langle\phi_m|)B\left(1 - \frac{|\zeta_m\rangle\langle\tilde{\chi}^a_m|}{\Delta}\right) \\ &= \mathfrak{U}^a_{QP}B\left(1 - \frac{|\zeta_m\rangle\langle\tilde{\chi}^a_m|}{\Delta}\right) \\ &\quad + Q|\zeta_m\rangle\left(1 - \frac{\langle\tilde{\chi}^a_m|\zeta_m\rangle}{\Delta}\right)\langle\tilde{\chi}^a_m| \\ &= \mathfrak{F}^a_{QP} - \frac{\mathfrak{F}^a_{QP}}{\Delta}|\zeta_m\rangle\langle\tilde{\chi}^a_m| \\ &\quad + \frac{Q}{\Delta}|\zeta_m\rangle\langle\tilde{\chi}^a_m|\psi^a_m\rangle\langle\tilde{\chi}^a_m| , \\ \Delta &\equiv \langle\tilde{\chi}^a_m|\psi_m\rangle . \end{aligned} \tag{4.38}$$

Equations (2.25) and (4.34) have been used to introduce the operator $\mathfrak{F}^a_{QP}$, which is analytic near z_b, so that the first term of Eq. (4.38) can be disregarded. We also note that

$$\langle\tilde{\chi}^a_m|\psi^a_m\rangle = \langle\tilde{\chi}^a_m|\chi^a_m\rangle = 1 , \tag{4.39}$$

from the biorthonormal property of $\tilde{\chi}^a_m$ [Eq. (2.10)]. The singular part of Eq. (4.38) now becomes

$$Q\mathfrak{F}_{\text{sing}} = \frac{Q(1 - \mathfrak{F}^a_{QP})|\zeta_m\rangle\langle\tilde{\chi}^a_m|}{\langle\tilde{\chi}^a_m|\psi_m\rangle} . \tag{4.40}$$

Here $\zeta_m = \psi_m - \psi^a_m$ may be replaced by ψ_m, because

$$Q(1 - \mathfrak{F}^a_{QP})\psi^a_m = Q(\psi^a_m - \psi^a_m) = 0 , \tag{4.41}$$

from the characteristic property of $\mathfrak{F}^a$ [Eq. (2.26)]. Finally we obtain the quasiseparable form

$$Q\mathfrak{F}_{\text{sing}} = \frac{Q(1 - \mathfrak{F}^a)|\psi_m\rangle\langle\tilde{\chi}^a_m|}{\langle\tilde{\chi}^a_m|\psi_m\rangle} , \tag{4.42}$$

whose significance is not yet clear, because ψ_m is subject to violent changes of direction near z_b.

Equation (4.42) is independent of the normalization of ψ_m, so the unnormalized form, Eq. (4.23), may be used. The easiest method of obtaining the residue of Eq. (4.42) is to expand c, given by Eqs. (4.21) and (4.19), in a Laurent series in powers of $(z - x_b)^{-1}$, and hence generate the Laurent series of Eq. (4.42). We find

$$c = 1 + \frac{2m_b x_b}{d(z - x_b)} + O[(z - x_b)^{-2}] \tag{4.43}$$

so that, from Eq. (4.23),

$$\psi^u_m = 2^{1/2}\psi^a_m + \frac{2m_b x_b}{d(z - x_b)}\psi_{ib} + \cdots . \tag{4.44}$$

In writing this equation we have used the first of the following equations:

$$\psi_m^a = 2^{-1/2}(\psi_{mb} + \psi_{ib}), \quad \psi_i^a = 2^{-1/2}(\psi_{mb} - \psi_{ib}). \quad (4.45)$$

Equation (4.44) now gives

$$\frac{\psi_m}{\langle\tilde{\chi}_m^a|\psi_m\rangle} = \frac{\psi_m^u}{\langle\tilde{\chi}_m^a|\psi_m^u\rangle} = \frac{\psi_m^a}{\langle\tilde{\chi}_m^a|\psi_m^a\rangle} + \frac{m_b x_b}{d(z-x_b)}(\psi_i^a - \theta_b\psi_m^a) + \cdots . \quad (4.46)$$

We have defined the quantity

$$\theta_b \equiv \langle\tilde{\chi}_m^a|\psi_i^a\rangle \quad (4.47)$$

and made use of Eq. (4.39). Because of Eq. (4.41), the terms in ψ_m^a do not contribute to Eq. (4.42). Hence, by substituting Eq. (4.46) into Eq. (4.42), we find

$$Q\mathcal{F}_{sing} = \frac{m_b x_b}{d(z-x_b)} Q(1-\mathcal{F}^a)|\psi_i^a\rangle\langle\tilde{\chi}_m^a| \quad (4.48)$$

for the leading term in the Laurent series of $Q\mathcal{F}_{sing}$.

From Eq. (4.48), the residue of the step singularity can be derived for any desired effective operator. In particular, we find

$$\mathcal{H}_{sing} = PHQ\mathcal{F}_{sing} = \frac{m_b x_b}{d(z-x_b)} H_{PQ}(1-\mathcal{F}^a)|\psi_i^a\rangle\langle\tilde{\chi}_m^a|, \quad (4.49)$$

so that the residue is

$$\mu_b = \frac{m_b x_b}{d} H_{PQ}(1-\mathcal{F}^a)|\psi_i^a\rangle\langle\tilde{\chi}_m^a|. \quad (4.50)$$

A simple measure of the strength of μ_b is provided by its trace

$$\mathrm{tr}\mu_b = \frac{m_b x_b}{d}\langle\tilde{\chi}_m^a|H_{PQ}(1-\mathcal{F}^a)|\psi_i^a\rangle, \quad (4.51)$$

which is equal to the only nonzero eigenvalue of μ_b. Unfortunately, because μ_b is not Hermitian, some of its matrix elements may be larger than its trace, and so $\mathrm{tr}\mu_b$ is only a very crude measure. Under the assumption of weak mixing, Eqs. (4.50) and (4.51) can be simplified, because then

$$\mathcal{F}^a \approx P, \quad \tilde{\chi}_m^a \approx \chi_m^a \approx \psi_m^a, \quad Q\psi_i^a \approx \psi_i^a \quad (\textit{weak mixing}), \quad (4.52)$$

so that

$$\mu_b \approx \frac{m_b x_b}{d} H_{PQ}|\psi_i^a\rangle\langle\tilde{\chi}_m^a|, \quad (4.53a)$$

$$\mathrm{tr}\mu_b \approx (m_b x_b)^2/d. \quad (4.53b)$$

The second of these equations uses the relation

$$\langle\chi_m^a|H_{PQ}|\psi_i^a\rangle \approx \langle\psi_m^a|H|\psi_i^a\rangle = m_b x_b, \quad (4.54)$$

which applies if the mixing is weak, because of Eq. (4.52). Equations (4.53) and (4.54) have previously been suggested by Pittel,[21] with ψ_m^a and ψ_i^a replaced by eigenfunctions of $H_{PP}+H_{QQ}$, and Eq. (4.53b) has been tested in Ref. 12, where it is found to be quite successful—in a case with rather weak mixing. However, the result (4.50), which correctly takes background effects into account, is expected to be necessary for cases where the mixing is stronger.

Sometimes it may be interesting to know the form of the singularity of $\mathcal{F}$ near a branch point, say z_b, although it cannot have direct physical significance, because z_b is not real. The result is quoted without derivation:

$$\mathcal{F} \sim \mathcal{F}^a + \frac{2i(z-z_b)^{1/2}}{(i\lambda_b)^{1/2}(1+i\theta_b)^2} Q(1-\mathcal{F}^a)|\psi_i^a\rangle\langle\tilde{\chi}_m^a| \quad (z \to z_b). \quad (4.55)$$

It is interesting to make more explicit the connection between Eq. (4.49) and earlier work by Vincent and Pittel[20] and Pittel.[21] They conjectured that the location and residue of a step singularity can be estimated from an equivalent two-state problem in which m_b is the interaction matrix element between the states, and d is the difference between the slopes of the levels that coincide. Now in the basis ψ_m^a, ψ_i^a defined by the minimally smoothed Hamiltonian, we have

$$H(x) = \begin{pmatrix} \bar{E}_b & m_b x_b \\ m_b x_b & \bar{E}_b \end{pmatrix} + (z-x_b)\begin{pmatrix} D-\frac{1}{2}d & 0 \\ 0 & D+\frac{1}{2}d \end{pmatrix}. \quad (4.56)$$

The role of $m_b x_b$ as an interaction matrix element between ψ_m^a and ψ_i^a is now clear, and also the meaning of d as the difference of slopes for $|z-x_b| \gg \lambda_b$ (but small compared with the distance to the nearest other singularity). Thus the present discussion mathematically defines the parameters m_b and d, which previously[20] were only imprecisely identified. That only real z values enter these definitions is an important computational convenience.

Although d and m_b are no easier to calculate than the desired eigenvectors and eigenvalues of $H(1)$, the result (4.50) has possible applications in studies[12,22] in which H is diagonalized exactly, so that approximations to $\mathcal{H}$ can be compared with the exact result. It can be used to identify the contributions of particular singularities, allowing the reasons for success or failure of an approximation to be more sharply identified. Experience in such controlled numerical experiments may

then suggest improved approximation schemes. Even in cases where H cannot be diagonalized exactly, m_b and d can often be estimated from approximations to ψ^a_{ib} and ψ^a_{mb}. Pittel[23] has used this method to estimate the effect of a step singularity due to a deformed 4-particle, 2-hole intruder state on low orders of PT for the 0^+ states of ^{18}O.

V. INFLUENCE OF AN ISOLATED STEP SINGULARITY ON PT

Perturbation theory for the effective Hamiltonian is an expansion of $\mathcal{H}(z)$ in powers of z:

$$\mathcal{H}(z)=h_0+h_1(z)+h_2z^2+\cdots . \tag{5.1}$$

As remarked earlier, the series converges for the physical value $z=1$ if all singularities of $\mathcal{H}(z)$ are outside the unit circle. If there is an intruder state, there will be at least one step singularity inside the unit circle.

Often the step singularity produced by an intruder state satisfies the conditions assumed in Sec. IV D,

$$\lambda_b \ll |x_b|, \quad \lambda_b \ll |1-x_b| , \tag{5.2}$$

so that the singularity is distant from both $z=0$ and $z=1$, as well as isolated from other singularities. In this case, the cut can be replaced by a pole at x_b,

$$\mathcal{H}_{\text{step}} \approx \mathcal{H}_{\text{pole}} = \frac{\mu_b}{z-x_b} , \tag{5.3}$$

where μ_b is the residue of the cut, given by Eq. (4.50). At the physical value $z=1$, we have

$$\mathcal{H}_{\text{pole}}(1)=\frac{\mu_b}{1-x_b} . \tag{5.4}$$

However, the contribution of the pole to PT through nth order is

$$\sum_{\nu=0}^{n} h_\nu(\text{pole}) \tag{5.5a}$$

with

$$h_\nu(\text{pole}) = -\mu_b/x_b^{\nu+1} . \tag{5.5b}$$

The difference between Eq. (5.4) and Eq. (5.5) is $e_n(\text{pole})$, the contribution of the pole to the error e_n incurred by nth-order PT at $z=1$:

$$e_n(\text{trunc}) \equiv \mathcal{H} - \sum_{\nu=0}^{n} h_\nu . \tag{5.6}$$

In the pole approximation, the contribution to the error of nth-order PT is

$$\begin{aligned} e_n(\text{pole}) &= -(\mu_b/x_b)\left[(1-x_b^{-1}) - \sum_{\nu=0}^{n} x_b^{-\nu}\right] \\ &= \frac{-\mu_b/x_b^{n+1}}{x_b-1} \end{aligned} \tag{5.7}$$

exactly. For $|x_b|<1$, the norm $\|e_n(\text{pole})\|$ is an increasing function of n, so that the series diverges.

Truncation of the PT series at a finite order n always involves some error, $e_n(\text{trunc})$. It may happen that for this value of n, the contribution of the pole to the error is small compared with the intrinsic error of truncation. As long as

$$\|e_n(\text{pole})\| \ll \|e_n(\text{trunc})\| , \tag{5.8}$$

the series through order n is practically indistinguishable by its behavior from the series for $\mathcal{H}-\mathcal{H}_{\text{step}}$, which is convergent if the step at x_b is the only singularity inside the unit circle. In fact, if μ_b is known or can be estimated, Eq. (5.8) can be used as a rule for deciding the optimal truncation point n.

Thus, although the PT series is divergent, it can nevertheless give good approximations—if appropriately truncated. In this respect, PT resembles an asymptotic series. However, the PT series is actually not asymptotic, except in the trivial sense that every power series with nonzero radius of convergence is asymptotic. An asymptotic series[10] would have the defining property

$$\|e_n(\text{trunc})\|/|z|^n \to 0 \quad \text{as} \quad z \to 0 , \tag{5.9}$$

with z confined to some sector of the plane, and n fixed; this limiting property states that the approximation becomes arbitrarily close *for small enough* z. In contrast, we are interested in the magnitude of e_n only for $z=1$. It is often tacitly assumed that $\|e_n(\text{trunc})\|$ is always smaller than the norm of the $(n+1)$th term; this is not generally true, either for asymptotic or for convergent series. For computational purposes, it is, in any case, perhaps best to disregard questions of the convergence or asymptoticity of series, and simply concentrate on estimation of the errors of approximations of finite order.

According to Eq. (5.5b), the contribution of the pole always dominates PT for sufficiently large n. This is illustrated by Table I, which shows various orders of PT for an effective Hamiltonian $\mathcal{H}$ suitable for describing the $T=1$, $J^\pi=0^+$ states of ^{18}O in an s-d shell model space. A preliminary report of this calculation appears in Ref. 24, and details are given in Ref. 12. The ratio h_9/h_{10} of corresponding matrix elements of the ninth and tenth orders is almost constant and equal to -0.252 on the average. This indicates that, for $n \geq 9$, $h_n(\text{pole})$ already dominates PT. By Eq. (5.5b), the pole is at approximately

$$x_b = -0.252. \tag{5.10}$$

The residual variations in h_9/h_{10}, especially for some smaller matrix elements such as (m,m')

TABLE I. Matrix elements $\langle i|h_n|j\rangle$ for PT of orders $n=2-10$. Notation: $1\equiv d_{5/2}{}^2$, $2\equiv s_{1/2}{}^2$, $3\equiv d_{3/2}{}^2$. All energies are in MeV.

i,j	3,3	3,2	3,1	2,3	2,2	2,1	1,3	1,2	1,1
h_2	−5.091	−0.033	−0.119	−0.051	−4.385	−0.199	−0.205	−0.220	−5.106
h_3	−0.332	−0.016	+0.382	−0.092	+0.184	−0.033	+0.844	−0.016	+0.714
h_4	+0.921	−0.042	+0.153	−0.371	−0.593	+0.053	−0.998	−0.071	+0.531
h_5	−0.115	−0.014	−0.168	−0.413	−0.079	+0.109	+1.708	+0.065	−0.158
h_6	−0.069	+0.041	−0.032	+0.327	−0.180	+0.086	−4.121	−0.130	−0.694
h_7	−0.959	−0.020	+0.007	−0.159	+0.026	−0.128	+11.891	+0.346	+1.578
h_8	+2.487	+0.056	+0.341	−0.248	+0.102	+0.067	−46.219	−0.979	−3.731
h_9	−9.318	−0.195	−0.798	−2.430	−0.025	+0.097	+180.352	−3.553	+14.223
h_{10}	36.376	0.726	2.868	5.042	0.116	0.709	−716.770	−13.795	−56.335
h_9/h_{10}	−0.256	−0.269	−0.278	−0.482	−0.216	+0.137	−0.252	−0.258	−0.252
h_{10}(sep)	36.513	0.698	2.864	5.015	0.096	0.393	−716.549	−13.703	−56.204
$\mu_b\times10^6$	9.504	0.182	0.746	1.305	0.025	0.102	−186.518	−3.567	−14.630
e_3 (pole)	0.002	0.000	0.000	0.000	0.000	0.000	−0.037	−0.001	−0.003
e_4 (pole)	−0.007	−0.000	−0.001	−0.001	−0.000	−0.000	0.147	0.003	0.011
e_3 (trunc)	0.761	−0.036	−0.017	0.020	0.386	0.030	−0.107	−0.060	0.152
e_4 (trunc)	−0.160	0.006	−0.170	0.391	0.979	−0.023	0.891	0.011	−0.379

$=(2,1)$ and $(2,3)$ shows the extent to which other singularities also have some influence. As required by Eq. (4.22), h_{10} is very nearly a separable matrix. This is verified by comparing with h_{10}(sep), a separable approximation to h_{10}. Equation (5.5b) permits identification of h_{10}(sep) with $-\mu_b/x_b{}^{11}$, so that μ_b can be calculated, and values of e_3(pole) and e_4(pole) are then obtained from Eq. (5.7). Comparing e_3(pole) and e_4(pole) with h_3 and h_4, we see that the singularity at $x_b=-0.252$ has little effect on the behavior of PT through fourth order. Since the exact value of $\mathcal{C}$ is also known for this case, the values of e_3(trunc) and e_4(trunc) can be calculated. (This would not be true for realistic cases, where PT is being used for the very reason that an exact solution is not available.) Again we see that $|e_n(\text{trunc})|\gg|e_n(\text{pole})|$ for $n=3$ and 4. The largest matrix element of e_4(pole) is $\langle 1|e_4(\text{pole})|3\rangle=0.147$; in fifth order the value would be ≈ 0.6, so that it is not appropriate to add terms beyond the fourth order.[25] Notice that this conclusion is reached without any phenomenological assumptions. Only information obtained from PT is used.

Further details regarding the singularity can be obtained by factorizing the matrix h_{10}(sep) as follows:

$$h_{10}(\text{sep})=-19.60\,|f\rangle\langle\tilde{\chi}_m^a|\,, \tag{5.11}$$

where the factors (evaluated at x_b) are

$$f=(36.67,-0.257,-1.869), \tag{5.12a}$$

$$\tilde{\chi}_m=(0.078,0.019,0.997)\,. \tag{5.12b}$$

The normalization of f has been chosen so that

$$\langle\tilde{\chi}_m^a|f\rangle=1\,. \tag{5.13}$$

However, no information on the individual normalizations of f and $\tilde{\chi}_m^a$ is contained in PT for $\mathcal{C}$. Equation (5.13) implies that the separable operator $|f\rangle\langle\tilde{\chi}_m^a|$ has 1 and 0 as its only eigenvalues. However, $|f\rangle\langle\tilde{\chi}_m^a$ [and h_{10}(sep)] have both positive and negative diagonal elements, because they are far from being Hermitian. Thus the positive (or negative) semidefinite property of μ_b does not extend to individual matrix elements, even on the diagonal.

Lastly, the constant 19.60 in Eq. (5.11) can be identified with $\mathrm{tr}\mu_b/x_b{}^{11}$, by Eqs. (5.5b) and (5.13). The value of d, obtained by comparing spectra for at $z=0$ and $z=-0.252$, is

$$d=-10\,. \tag{5.14}$$

From these estimates applied to Eq. (4.53b), we get

$$m_b{}^2=51.4\times10^{-6}\,, \tag{5.15}$$

so that

$$m_b=\pm0.0071\,. \tag{5.16}$$

The pole approximation, Eq. (5.3), depends on the initial assumption that λ_b is small. From Eq. (4.26), with Eqs. (5.14) and (5.16),

$$\lambda_b=4m_b/d=0.003\,,$$

which indeed satisfies Eq. (5.2). (Should this check fail because λ_b is not negligible, the analysis could be improved by taking the finite value of λ_b into account.)

The choice of H_0 and V that led to the quoted PT

results is seen from Fig. 1 to produce several other step singularities inside the unit circle, in addition to that at $z = -0.252$. Among them is one near $z = +0.7$. High-order PT is always dominated by the singularity nearest the origin, which can therefore be studied accurately. However, other singularities may be more important in determining $\mathcal{H}$ at $z = 1$, so it is not unexpected that removal of the singularity nearest the origin (in this case, at $z = -0.252$) does not succeed in substantially improving third- and fourth-order approximations. The more difficult task of allowing for several singularities simultaneously will not be attempted here.

VI. CONCLUSIONS

The model operator $\mathcal{F}(z)$ and the effective Hamiltonian $\mathcal{H}(z)$ have been shown to have singularities only at values of the coupling constant z where represented and excluded eigenvalues coincide ("P-Q singularities"), in agreement with the conclusions of SW. A P-Q singularity is a pair of complex conjugate branch points which may be either close to the real axis (corresponding to a "step singularity") or close to the imaginary axis (corresponding to a "gap singularity"). The general form of an isolated step singularity has been derived, and a method of evaluating its residue by diagonalizing only real matrices has been given; the residue is a separable operator. This development converts the heuristic two-state model of Vincent and Pittel[20] into a precise instrument. For any solvable model it becomes possible to calculate the residues of all step singularities that lie in or near the unit circle, and hence remove them from $\mathcal{H}(z)$. Study of the behavior of the PT series for the remaining step-free part of $\mathcal{H}(z)$ [compared with PT for the full $\mathcal{H}(z)$] could then decide the relative importance of step and gap singularities in spoiling perturbative approximations. This knowledge would be useful in guiding the search for improved methods.

To the extent that isolated step singularities are responsible for the errors of low-order PT, estimates of their contributions can help in assessing its reliability. The location and residue of the step singularity that is nearest to the origin can actually be calculated quite accurately by using only information derived from the PT series. For other step singularities (at greater distances from the origin), the locations and residues may in turn be estimated by first calculating and removing the nearer singularities. However, it is not clear that this process would be stable enough for practical use. Moreover, high orders of PT would be needed to ensure sufficient dominance of the nearest singularity. The number of diagrams required rises so quickly with order that diagrammatic methods would become impossible.

In computer experiments with large many-body Hamiltonian matrices, it is often found that the step singularities are isolated and have small residues, so that the analysis described above is applicable. However, better understanding of the reasons for these tendencies is needed before they can be generally relied on in practice. The same is true of the question of the relative importance of gap singularities. In view of these reservations, it is clearly desirable for any proposed calculation scheme to supply internal rules for estimating the errors.

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