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Effective and intermediate Hamiltonians obtained by similarity transformations

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A simple similarity transformation is used to derive equations for effective and intermediate Hamiltonians in a lucid way. Effective and intermediate Hamiltonians based on the wave operator formalism provide only a subset of all eigenvalues while the similarity transform technique divides the eigenvalue problem into two subproblems that can be solved separately. This means that the complete spectrum of the Hamiltonian remains well defined and this proves to be advantageous in the formal analysis and may be useful in many applications. Moreover both left and right hand eigenvectors of the transformed Hamiltonian can be obtained and this allows a convenient evaluation of properties. Rayleigh–Schrödinger and Brillouin–Wigner perturbation expansions of the intermediate Hamiltonians are discussed and a comparison is made of the various possible schemes. © *1995 American Institute of Physics.*

I. INTRODUCTION

Effective Hamiltonians play a fundamental role in the quantum theory of matter. Several reviews have been written on the subject and specific references may be found there.[1–4] The basic idea of effective Hamiltonians H^{eff} is to isolate the problem of obtaining a few eigenvalues from the total eigenvalue problem given by the Schrödinger equation. Most of the derivations are based on a mapping of the set of exact eigenfunctions corresponding to eigenvalues we are interested in onto the set of zeroth-order functions. Then, the so-called wave operator[5–8] is assumed to give the exact eigenfunctions corresponding to the eigenvalues of interest while acting on the model space (space spanned by selected zeroth-order functions). The resulting equation for the wave operator gives a necessary condition to have the above mentioned mapping, but it does not determine the mapping uniquely. That is reflected by the possibility of obtaining multiple solutions in a coupled cluster framework[9] and relatedly the intruder state problem (for discussion see Ref. 10). In spite of the fact that we are interested only in some subproblem of the total eigenvalue problem of the Hamiltonian H it is convenient to keep track of the rest of the problem. That can be important in the case when one would like to get some additional eigenvalues or the left eigenvectors which would be required for some further calculations. An example of such a situation is given by the equation of motion coupled cluster method,[11–15] where the excitation energy calculation is preceded by the ground state calculation. The latter can be considered as an effective Hamiltonian implementation with a one-dimensional model space.

A promising remedy for the problem of intruder states is provided by the concept of intermediate Hamiltonians introduced by Malrieu *et al.*[10] The effective Hamiltonian formalism includes the correlation effects in two ways; contributions from the orthogonal space are provided by the wave operator while the impact of model space functions is given by diagonalization of the effective Hamiltonian. The intermediate Hamiltonian approach is based on the idea of taking into account contributions from the states that potentially can strongly interact with the model space not through the wave operator but also by diagonalization. In this way the intermediate Hamiltonian acts in an extended space consisting of the main model and intermediate spaces. The inclusion of the intermediate space does not provide extra eigenvalues but permits to deal with the problem of intruder states in a more efficient way. The equations that determine the intermediate Hamiltonian are not uniquely defined by a specification of only the main and full model spaces and some additional conditions have to be imposed to arrive at a well-defined computational scheme. Different strategies can be followed here (for an overview see Ref. 16) and it is a matter of ongoing research to find an optimal scheme that is relatively simple, well convergent and size-extensive.[17,18] Other desiderata might be Hermiticity of the intermediate Hamiltonian[19,20] and a relatively high accuracy of the phony solutions that are obtained from a diagonalization of the intermediate Hamiltonian.[10,21]

Previous formulations of effective and intermediate Hamiltonian schemes have been mainly based on the wave operator formalism. In this work we will show how alternatively a simple similarity transformation can be used to arrive at effective and intermediate Hamiltonian formulations in a transparent way. In the derivation of effective Hamiltonians the similarity transformation divides the eigenvalue problem of H into two subproblems allowing to deal with each of them separately. This has been also observed while analyzing extra solutions obtained within the Fock-space coupled cluster method for ionization potentials.[13] In order to define this similarity transformation we do not need a mapping of any kind but only a simple partitioning of the vectorial space in which H acts into two subspaces. A similar technique of employing similarity transformations is used in the more complicated case of intermediate Hamiltonians. Applying a sequence of two similarity transformations it is relatively easy to see how the desired structure of the transformed Hamiltonian can be obtained. In general, at the start-

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ing point the number of the parameters to be determined will be greater than the number of initial equations, so some additional conditions must be imposed to determine the transformation. As a consequence the same structure of the transformed Hamiltonian can be obtained in a variety of ways yielding different intermediate Hamiltonians.

The question of imposing additional conditions to define a set of equations that determines the similarity transformation is intimately tied to the means of solving the equations. One possibility is to work in the coupled cluster framework.[17,18,22] We will restrict ourselves here to the use of perturbation theory to determine the transformation coefficients that couple to the orthogonal space. Both Rayleigh–Schrödinger (R–S) and Brillouin–Wigner (B–W) perturbation expansions are discussed. In the final section of this paper we apply a variety of possible schemes to a simple model problem introduced by Malrieu *et al.*[10] Our main goal is to obtain a first impression of the performance of the different schemes. We have also found this model very useful to gain some insight in the plethora of possibilities that arises in the domain of the intermediate Hamiltonian formalism.

II. SIMPLE HILBERT-SPACE SIMILARITY TRANSFORMATIONS

Most of the recent derivations of the effective Hamiltonian equations are based on a mapping that connects a space spanned by some selected eigenfunctions of the Hamiltonian with a subspace of the same dimension constructed from eigenfunctions of a suitably chosen zeroth-order Hamiltonian H_0.[4] This is usually called the wave operator formalism.[1–4] Such an approach provides equations for a subset of the eigenvalues but leaves the problem of others undetermined. We find it convenient to employ a very simple similarity transformation and introduce the effective Hamiltonian as a particular block of the transformed Hamiltonian. Within this approach we can either consider the full eigenvalue problem or a subset of eigenvalues and this facilitates the analysis. Denoting by P and Q projection operators onto some subspace M of the Hilbert space and its orthogonal complement M', respectively, we introduce the operator X,

$$X=QXP. \tag{1}$$

The Hilbert-space transformation operator takes the form

$$U=e^{X}, \tag{2}$$

and therefore the inverse operator is

$$U^{-1}=e^{-X}. \tag{3}$$

Because P and Q are projection operators onto disconnected subspaces we have

$$X^2=0, \tag{4}$$

so

$$\begin{aligned} U&=1+X,\\ U^{-1}&=1-X. \end{aligned} \tag{5}$$

Although the expansion of U and U^{-1} terminate after the first two terms it is convenient to formally introduce the exponential form of U to have an immediate form of the inverse operator. Using the transformation U the transformed Hamiltonian reads

$$\tilde{H}=(1-X)H(1+X)=H+HX-XH-XHX. \tag{6}$$

We want to consider the similarity transformation that fulfills the condition that the off-diagonal block $Q\tilde{H}P$ of the transformed Hamiltonian vanishes. That is sufficient to split the eigenvalue problem of H into two subproblems. Hence we require

$$Q\tilde{H}P=0, \tag{7}$$

and X contains a sufficient number of parameters to satisfy this condition. The expressions for the various blocks of the transformed Hamiltonian $\tilde{H}$ can be obtained in the form

$$\begin{aligned} P\tilde{H}P&=PH(1+X)P,\\ Q\tilde{H}P&=Q(1-X)H(1+X)P,\\ P\tilde{H}Q&=PHQ,\\ Q\tilde{H}Q&=Q(1-X)HQ. \end{aligned} \tag{8}$$

Requirement (7) combined with the second expression in Eq. (8) leads to an equation for X,

$$Q(1-X)H(1+X)P=0. \tag{9}$$

If X satisfies Eq. (9) then the whole spectrum of eigenvalues of H is given by the separate diagonalizations of the diagonal $P\tilde{H}P$ and $Q\tilde{H}Q$ blocks. To see this one can consider a subsequent transformation of $\tilde{H}$ given by

$$W=1+S, \tag{10}$$

where

$$S=PSQ. \tag{11}$$

The doubly transformed Hamiltonian then reads

$$\tilde{\tilde{H}}=(1-S)\tilde{H}(1+S)=\tilde{H}-S\tilde{H}+\tilde{H}S \tag{12}$$

and we require S to satisfy

$$P\tilde{\tilde{H}}Q=P\tilde{H}Q-S\tilde{H}Q+P\tilde{H}S=0. \tag{13}$$

It is easy to see that because of Eq. (7) we have

$$\begin{aligned} P\tilde{\tilde{H}}P&=P\tilde{H}P,\\ Q\tilde{\tilde{H}}P&=Q\tilde{H}P=0,\\ Q\tilde{\tilde{H}}Q&=Q\tilde{H}Q, \end{aligned} \tag{14}$$

thus the second transformation changes only the $P\tilde{H}Q$ part by putting it equal to zero. Now the relation

$$\tilde{\tilde{H}}=P\tilde{H}P+Q\tilde{H}Q, \tag{15}$$

shows that indeed all eigenvalues of H can be obtained by separate diagonalizations of the $P\tilde{H}P$ and $Q\tilde{H}Q$ blocks. A similar idea of splitting a Fock-space-type similarity transformation leading to a block diagonal structure of the transformed Hamiltonian into two transformations has been presented by Stolarczyk and Monkhorst[23] in their version of the Fock space coupled cluster method. Obtaining a block-

diagonal structure in one step is troublesome, especially finding an explicit form for the inverse operator can be difficult.[24]

The doubly transformed Hamiltonian in which the sequence of transformations is reversed:

$$U^{-1}W^{-1}HWU, \tag{16}$$

where W and U satisfy analogous conditions

$$\begin{aligned} &PW^{-1}HWQ=0, \\ &QU^{-1}W^{-1}HWUP=0, \end{aligned} \tag{17}$$

has the same block diagonal structure as $\tilde{\tilde{H}}$ but is different in general. If H is Hermitian these two transformed Hamiltonians are Hermitian conjugates.

The equation for X, Eq. (9), is nonlinear. This indicates that the transformation U cannot be uniquely determined from the condition (7) and there are many transformations that satisfy this condition. Different solutions of Eq. (9) and hence different transformations of the Hamiltonian lead to exchange of eigenvalues of H between the $P\tilde{H}P$ and $Q\tilde{H}Q$ blocks. Multiple solutions obtained within an effective Hamiltonian formalism have been recently found and discussed within the Hilbert-space and Fock-space multireference coupled cluster methods.[9,13,25] This phenomenon of multiple solutions may pose problems, particularly if the calculation of the transformation is based on a perturbation expansion. The perturbation expansion may be ill behaved and it may be very difficult or impossible to converge to any particular solution. This is referred to as the intruder state problem.[10]

While the transformation U Eq. (2) leads to the separation of the eigenvalue problem into two subproblems it does not do the same for the eigenvector problem. To have the left and right eigenvectors correctly described the nonvanishing off-diagonal block of the transformed Hamiltonian $\tilde{H}$ has to be considered along with the diagonal blocks. Let the $\mathbf{A}$ and $\mathbf{B}$ matrices contain the eigenvectors of the $\tilde{\mathbf{H}}_{\mathbf{PP}}$ and $\tilde{\mathbf{H}}_{\mathbf{QQ}}$ matrices, respectively, so

$$\begin{aligned} &\tilde{\mathbf{H}}_{\mathbf{PP}}\mathbf{A}=\mathbf{A}\mathbf{D}, \\ &\tilde{\mathbf{H}}_{\mathbf{QQ}}\mathbf{B}=\mathbf{B}\mathbf{D}', \end{aligned} \tag{18}$$

where $\mathbf{D}$ and $\mathbf{D}'$ are diagonal matrices containing eigenvalues of $\tilde{\mathbf{H}}_{\mathbf{PP}}$ and $\tilde{\mathbf{H}}_{\mathbf{QQ}}$, respectively. Assuming a general form of the matrix containing the right eigenvectors of $\tilde{\mathbf{H}}$ one has

$$\begin{bmatrix} \tilde{\mathbf{H}}_{\mathbf{PP}} & \tilde{\mathbf{H}}_{\mathbf{PQ}} \\ \mathbf{0} & \tilde{\mathbf{H}}_{\mathbf{QQ}} \end{bmatrix} \begin{bmatrix} \mathbf{a} & \mathbf{c} \\ \mathbf{d} & \mathbf{b} \end{bmatrix} = \begin{bmatrix} \mathbf{a} & \mathbf{c} \\ \mathbf{d} & \mathbf{b} \end{bmatrix} \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}' \end{bmatrix}. \tag{19}$$

That leads to the set of equations

$$\begin{aligned} &\tilde{\mathbf{H}}_{\mathbf{PP}}\mathbf{a}+\tilde{\mathbf{H}}_{\mathbf{PQ}}\mathbf{d}=\mathbf{a}\mathbf{D}, \\ &\tilde{\mathbf{H}}_{\mathbf{QQ}}\mathbf{d}=\mathbf{d}\mathbf{D}, \\ &\tilde{\mathbf{H}}_{\mathbf{PP}}\mathbf{c}+\tilde{\mathbf{H}}_{\mathbf{PQ}}\mathbf{b}=\mathbf{c}\mathbf{D}', \\ &\tilde{\mathbf{H}}_{\mathbf{QQ}}\mathbf{b}=\mathbf{b}\mathbf{D}'. \end{aligned} \tag{20}$$

If all eigenvalues contained in $\mathbf{D}$ are different from those in $\mathbf{D}'$, so none of them is a solution of characteristic equation of $\tilde{\mathbf{H}}_{\mathbf{QQ}}$ then the second equation in (20) has only trivial solutions so $\mathbf{d}$ is equal to zero. In case when $\mathbf{D}$ and $\mathbf{D}'$ have at least one common eigenvalue then putting $\mathbf{d}=\mathbf{0}$ is a matter of choice. If $\mathbf{d}=\mathbf{0}$ then $\mathbf{a}=\mathbf{A}$ and $\mathbf{b}=\mathbf{B}$. Hence, the right eigenvectors of $\tilde{\mathbf{H}}$ form the matrix

$$\mathbf{R}=\begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{0} & \mathbf{B} \end{bmatrix}, \tag{21}$$

where $\mathbf{C}=\mathbf{c}$ has to satisfy the third equation in Eq. (20).

One can see that the $\tilde{\mathbf{H}}_{\mathbf{PQ}}$ submatrix which does not contribute to the determination of the eigenvalues, now is necessary to determine the right eigenvectors corresponding to $\mathbf{D}'$. The biorthogonal set of left eigenvectors is given by

$$\mathbf{L}=\begin{bmatrix} \mathbf{A^{-1}} & \mathbf{-A^{-1}CB^{-1}} \\ \mathbf{0} & \mathbf{B^{-1}} \end{bmatrix}. \tag{22}$$

One can also see that the right eigenvectors $\mathbf{A}$ given by diagonalization of $\tilde{\mathbf{H}}_{\mathbf{PP}}$ allow the determination of the right eigenvectors of $\mathbf{H}$ corresponding to $\mathbf{D}$,

$$\mathbf{V}_{\mathbf{D}}=\begin{bmatrix} \mathbf{A} \\ \mathbf{XA} \end{bmatrix}, \tag{23}$$

while the left eigenvectors $\mathbf{B^{-1}}$ given by diagonalization of $\tilde{\mathbf{H}}_{\mathbf{QQ}}$ allow the determination of the left eigenvectors of $\mathbf{H}$ corresponding to $\mathbf{D}'$,

$${}_{\mathbf{D}'}\mathbf{V}=[\mathbf{-B^{-1}X} \quad \mathbf{B^{-1}}]. \tag{24}$$

However, determination of the left eigenvectors of $\mathbf{H}$ corresponding to eigenvalues $\mathbf{D}$ as well as the right eigenvectors corresponding to $\mathbf{D}'$ requires to obtain the $\mathbf{C}$ matrix or the $\mathbf{S}$ matrix that relates to $\mathbf{C}$ through

$$\mathbf{S}=\mathbf{BC}^{-\mathbf{1}}. \tag{25}$$

The right eigenvectors corresponding to $\mathbf{D}$ are

$${}_{\mathbf{D}}\mathbf{V}=[\mathbf{A^{-1}+A^{-1}SX} \quad \mathbf{-A^{-1}S}], \tag{26}$$

while the left eigenvectors corresponding to $\mathbf{D}'$ are given by

$$\mathbf{V}_{\mathbf{D}'}=\begin{bmatrix} \mathbf{SB} \\ \mathbf{B+XSB} \end{bmatrix}. \tag{27}$$

Thus, to calculate eigenvalues, $\mathbf{V_D}$ and ${}_{\mathbf{D}'}\mathbf{V}$ the $\tilde{\mathbf{H}}_{\mathbf{PQ}}$ part of the transformed Hamiltonian is not necessary and can be ignored while to obtain ${}_{\mathbf{D}}\mathbf{V}$ and $\mathbf{V}_{\mathbf{D}'}$ it is indispensable. Having the eigenvectors of the transformed Hamiltonian determined properties other than energy can be calculated. It must be stressed here that while the equation for X, Eq. (9), is quadratic in X and can give many solutions corresponding to exchange of eigenvalues between $\mathbf{D}$ and $\mathbf{D}'$ the equation for S, Eq. (13), is linear in S. This is quite understandable, since once one of the possible solutions for X is determined and the corresponding partitioning of the eigenvalues of H between $\mathbf{D}$ and $\mathbf{D}'$ is established then there should not be any ambiguity in the determination of the remaining eigenvectors ${}_{\mathbf{D}}\mathbf{V}$ and $\mathbf{V}_{\mathbf{D}'}$ for which $\mathbf{S}$ is necessary. The linear character of Eq. (13) guarantees that.

Let us mention here an example of the formalism that implicitly uses the above technique. We would like to refer here to the single-reference coupled cluster method that has

been found a very powerful tool in describing the correlation effects of the ground state.[26] It is based on the Fock-space similarity transformation

$$\bar{H}=e^{-T}He^{T}, \tag{28}$$

where T is a second-quantized excitation operator defined with respect to the ground state determinant, usually the Hartree–Fock function Φ. Similarity transformation (28) is different from the Hilbert-space transformation described by Eq. (6), however, the transformed Hamiltonian is required to fulfill a relation analogous to Eq. (7),

$$Q\bar{H}P=0, \tag{29}$$

where

$$P=|\Phi\rangle\langle\Phi|, \quad Q=I-P. \tag{30}$$

Equation (29) allows to determine the cluster operator T. As discussed, more than one solution can be obtained from Eq. (29),[27,28] however, usually there is no problem with finding the solution corresponding to the ground state. Then

$$P\bar{H}P=E_0P, \tag{31}$$

where E_0 is the ground state energy. The similarity transformation (28) gives the right eigenvector corresponding to E_0 while the the left eigenvector is still to be determined. One can employ the Hilbert-space similarity transformation to find it:

$$P(1+\Lambda)\bar{H}(1-\Lambda)Q=0, \tag{32}$$

where Λ is used to denote the operator

$$\Lambda=P\Lambda Q. \tag{33}$$

This leads immediately to the well known linear equation for the Λ coefficients[29] that parameterize the left eigenfunction

$$P(1+\Lambda)(\bar{H}-E_0)Q=0. \tag{34}$$

Even if one uses a more complicated parameterization of the left eigenvector of $\bar{H}$ corresponding to E_0 like, e.g., employing an exponential expansion instead of a linear one

$$P(1+\Lambda)=Pe^{S}, \tag{35}$$

where S is a second-quantized deexcitation operator, the resulting equations for the S amplitudes are again linear as has been found by Jeziorski and Moszyński.[30] This is not surprising since the left eigenfunction corresponding to some particular eigenvalue must be uniquely determined while Eq. (29) in general has many solutions.

III. EFFECTIVE HAMILTONIANS

The purpose of using the similarity transformation described above is obviously the reduction of the problem of finding all eigenvalues of H to the problem of finding some of them. We assume that we have some small model space M and we are able to determine such a similarity transformation that all eigenvalues we are interested in are given by **D**. We start with the most common effective Hamiltonian given by the transformation U, Eq. (2) fulfilling Eq. (7) defined as[31]

$$H_B^{\mathrm{eff}}=P\tilde{H}P=PH(1+X)P, \tag{36}$$

where the subscript B means the Bloch effective Hamiltonian. Usually the appropriate X can be determined relatively easily if diagonalization of H within the model space M gives a reasonable approximation to the exact eigenvalues we are interested in and thus X can be considered as giving a relatively small correction. Another form for the effective Hamiltonian can be obtained by applying transformation W, Eqs. (10) and (11), and require

$$PW^{-1}HWQ=0. \tag{37}$$

This leads to an equation for S and the Hermitian conjugate of this equation is given by

$$Q(1+S^{\dagger})H(1-S^{\dagger})P=0. \tag{38}$$

Comparing this with the equation for X, Eq. (9), one can see that

$$S=-X^{\dagger}. \tag{39}$$

The effective Hamiltonian given by this transformation is

$$H_{\hat{O}}^{\mathrm{eff}}=P(1-S)HP, \tag{40}$$

where the subscript $\hat{O}$ refers to the Ôkubo effective Hamiltonian.[3,32] Using the correspondence between S and X one can find the relation between both effective Hamiltonians,[3]

$$H_{\hat{O}}^{\mathrm{eff}}=P(1+X^{\dagger})HP=(H_B^{\mathrm{eff}})^{\dagger}. \tag{41}$$

The Bloch and Ôkubo effective Hamiltonians are the basic ones that can be derived within the scheme described in the previous section. These formulations are completely equivalent (Hermitian conjugate) also if approximations are introduced. The other effective Hamiltonian that is well known is the des Cloizeaux effective Hamiltonian[33]

$$H_{\mathrm{dC}}^{\mathrm{eff}}=P(1+X^{\dagger}X)^{-(1/2)}(1+X^{\dagger})H(1+X)(1+X^{\dagger}X)^{-(1/2)}P, \tag{42}$$

where again X is determined by Eq. (7). The characteristic feature of this effective Hamiltonian is that it is Hermitian unlike both previous formulations:

$$H_{\mathrm{dC}}^{\mathrm{eff}}=(H_{\mathrm{dC}}^{\mathrm{eff}})^{\dagger}. \tag{43}$$

Of course, all these effective Hamiltonians that furnish the exact eigenvalues of H must be related by similarity transformations within the model space. Let us show now similarity transformations that relate all these effective Hamiltonians. We start with the des Cloizeaux effective Hamiltonian that can be cast into the form

$$\begin{aligned}H_{\mathrm{dC}}^{\mathrm{eff}}=&P(1+X^{\dagger}X)^{-1/2}(1+X^{\dagger})(1+X)(P+Q)\\&\times(1-X)H(1+X)(1+X^{\dagger}X)^{-1/2}P.\end{aligned} \tag{44}$$

Using Eq. (9) that is satisfied by X one can get

$$\begin{aligned}H_{\mathrm{dC}}^{\mathrm{eff}}=&P(1+X^{\dagger}X)^{-(1/2)}(1+X^{\dagger}X)PH(1+X)\\&\times P(1+X^{\dagger}X)^{-(1/2)}P\\=&P(1+X^{\dagger}X)^{1/2}H_B^{\mathrm{eff}}(1+X^{\dagger}X)^{-1/2}P.\end{aligned} \tag{45}$$

Using Eqs. (43) and (41) we also have

$$H_{\mathrm{dC}}^{\mathrm{eff}}=(H_{\mathrm{dC}}^{\mathrm{eff}})^{\dagger}=P(1+X^{\dagger}X)^{-1/2}H_{\hat{O}}^{\mathrm{eff}}(1+X^{\dagger}X)^{1/2}P. \quad (46)$$

Finally, from Eqs. (45) and (46) we get

$$H_{B}^{\mathrm{eff}}=P(1+X^{\dagger}X)^{-1}H_{\hat{O}}^{\mathrm{eff}}(1+X^{\dagger}X)P. \quad (47)$$

Equations (45)–(47) show similarity transformations within the model space relating all discussed effective Hamiltonians. Of course, there are many similarity transformations leading to many different effective Hamiltonians but all of them can be expressed through the basic similarity transformation U (or W) and an additional similarity transformation within the model space. However, it is important to realize that results using the des Cloizeaux effective Hamiltonian will be different from those obtained in the Bloch or Ôkubo formalisms if approximations are introduced.

For the purpose of the next section we would like to introduce now the most basic perturbation expansions for X. As mentioned before we can expect to obtain all eigenvalues of interest in a relatively easy way if X can be considered to give a small correction to the eigenvalues obtained with the first-order approximation (diagonalization of H within the model space). If X is relatively small then a perturbation expansion can be used for X and thus the effective Hamiltonian can be obtained in terms of a perturbation expansion. We assume that the Hamiltonian is divided into a zeroth-order part H_0 and a perturbation V. The basis functions Φ_k are assumed to be eigenfunctions of H_0,

$$H=H_0+V, \quad H_0\Phi_k=E_0^k\Phi_k, \quad (48)$$

where E_0^k is the zeroth-order energy. Using this zeroth-order description of the system the projector operator P can be expressed as

$$P=\sum_{i\in I}|\Phi_i\rangle\langle\Phi_i|=\sum_{i\in I}P_i, \quad (49)$$

where I contains indices of the zeroth-order functions spanning the model space M. Equation (9) can be written in the form

$$Q[V+(H_0+V)X-XH_0-XV(1+X)]P=0 \quad (50)$$

or

$$QVP_i-Q(E_0^i-H_0-V)XP_i-XV(1+X)P_i=0. \quad (51)$$

One can see that a formal expression for XP_i can be extracted from Eq. (51) if one is able to find the inverse operators of $(E_0^i-H_0-V)$ within the orthogonal space M'. This can be done be using the geometric expansion if V is assumed to be small:

$$[Q(E_0^i-H_0-V)Q]^{-1}=R_i(1-VR_i)^{-1}=\sum_{n=0}^{\infty}R_i(VR_i)^n, \quad (52)$$

where all inversions are considered within the M' space only. R_i is the inverse of the diagonal operator $(E_0^i-H_0)$ within M',

$$R_i=\frac{Q}{E_0^i-H_0}. \quad (53)$$

That gives the recursive formula for X,

$$X=\sum_{i\in I}\sum_{n=0}^{\infty}R_i(VR_i)^n[V-XV(1+X)]P_i, \quad (54)$$

that can be used to build the order-by-order Rayleigh–Schrödinger expansion for the effective Hamiltonians. It is seen that the various components XP_i are coupled in the above equation by the occurrence of XV.

Closer inspection of Eq. (8) shows that Eq. (7) can be also written in the form

$$QVP+QHX-XP\tilde{H}P=0, \quad (55)$$

that can be used to obtain a Brillouin–Wigner-type of expansion. To do so we will use the eigenvectors **A** and eigenvalues **D** of the effective Hamiltonian and multiply the above equation from the right by the associated operator A acting in M to obtain

$$QVA+QHXA-XAD=0, \quad (56)$$

where D is the diagonal operator containing the exact energies. Operator A can be expressed in the form

$$A=\sum_{i\in I}A_i, \quad (57)$$

where

$$H_B^{\mathrm{eff}}A_i=A_iE_i, \quad (58)$$

so we have

$$Q[V-(E_i-H_0-V)X]A_i=0. \quad (59)$$

In a similar way as Eq. (52) the B–W perturbation expansion can be obtained for XA_i,

$$XA_i=\sum_{n=0}^{\infty}R(E_i)[VR(E_i)]^nVA_i, \quad (60)$$

where

$$R(E_i)=\frac{Q}{E_i-H_0}. \quad (61)$$

Interestingly, if we would know the eigenvectors of the effective Hamiltonian as well as the eigenvalue the individual components XA_i satisfy completely decoupled sets of equations. This indicates that the Brillouin–Wigner scheme has potential for a self-consistent scheme, where each eigenvector is calculated individually. We will return to this topic later on. The complete operator X can be obtained by summing over the various components

$$XA=\sum_{i\in I}XA_i=\sum_{i\in I}\sum_{n=0}^{\infty}R(E_i)[VR(E_i)]^nVA_i, \quad (62)$$

and finally

$$X=\sum_{i\in I}\sum_{n=0}^{\infty} R(E_i)[VR(E_i)]^n VA_iA^{-1}. \tag{63}$$

IV. INTERMEDIATE HAMILTONIANS

The idea of intermediate Hamiltonians has been introduced by Malrieu *et al.*[10] The formalism introduces two kinds of model spaces; the main model space M_0 and the intermediate model space M_I. Let us denote the projection operator on these spaces by P_0 and P_I, respectively. The rest of the space is called the orthogonal space M' with the projection operator Q. The idea of intermediate Hamiltonians was motivated by the problem of intruder states that is faced in many practical implementations of the effective Hamiltonian theory. This is especially important when a perturbation expansion is applied since in this case one can expect divergency problems or alternatively the perturbation expansion may converge to an undesired solution. In such a case the use of an intermediate Hamiltonian appears to be a promising solution to the problem. The situation is often different when the multireference coupled cluster theories are employed within the effective Hamiltonian framework because it may be possible to converge to a number of different solutions using different starting points or different convergence procedures. This phenomenon has recently been found and discussed in both the Hilbert-space[9] and Fock-space[25] versions of the multireference CC method. Although the CC theories within the effective Hamiltonian framework seem more efficient in dealing with the intruder state problem, the intermediate Hamiltonians can be useful in many situations like for example when the proper description of some low-lying states requires the inclusion of many reference functions in the model space. Then those essential for all geometries can be included in the main model space while the rest of them span the intermediate model space. Coupled cluster theories based on the intermediate Hamiltonian formalism have been recently proposed by Koch[17] and Mukhopadhyay *et al.*[18] In some cases intermediate Hamiltonians are convenient to use also for formal reasons to simplify the formalism like in the coupled electron pair approximation (CEPA) type methods[34] or in a recently proposed dressing for the matrix elements of equation of motion coupled cluster method (EOM-CC).[35]

In the following we will present a way of obtaining intermediate effective Hamiltonians based on the idea of the simple similarity transformation presented in the second section. This approach shows properties and structure of the transformed Hamiltonian. One can get a variety of intermediate Hamiltonians since we split one transformation like that used in the effective Hamiltonian scheme [Eq. (2)] into two similarity transformations and that can be done in many different ways. Extra conditions have to be imposed in order to make the equations unique and there are different possibilities. Therefore, only some of the possible schemes that can be obtained are considered explicitly.

We will first consider the general formalism of intermediate Hamiltonians from the point of view of similarity transforms. Let us define Y and Z operators as

$$\begin{aligned} Y&=QYP,\\ Z&=P_IZP_0, \end{aligned} \tag{64}$$

where

$$P=P_0+P_I, \tag{65}$$

while the transformed Hamiltonian is assumed to be

$$\tilde{H}=(1-Z)(1-Y)H(1+Y)(1+Z). \tag{66}$$

To have the eigenvalue problem corresponding to the main model space M_0 separated we have to require

$$(Q+P_I)\tilde{H}P_0=0, \tag{67}$$

so that the diagonalization of $P_0\tilde{H}P_0$ gives the desired eigenvalues of H. One can see that at this moment the number of parameters to determine is greater than the number of equations in Eq. (67). That gives an extra degree of freedom and it will be necessary to impose additional conditions on the transformation to determine it uniquely. Inserting Eq. (66) into Eq. (67) and using Eq. (65) we get

$$Q[H(1+Y)(1+Z)-YPH(1+Y)(1+Z)]P_0=0 \tag{68}$$

and

$$P_I(1-Z)H(1+Y)(1+Z)P_0=0, \tag{69}$$

while

$$P_0\tilde{H}P_0=P_0H(1+Y)(1+Z)P_0 \tag{70}$$

plays the role of the effective Hamiltonian. Using the identity

$$P=(1+Z)P(1-Z) \tag{71}$$

in Eq. (68) one has

$$\begin{aligned} &Q[H(1+Y)(1+Z)-Y(1+Z)P(1-Z)\\ &\times H(1+Y)(1+Z)]P_0=0. \end{aligned} \tag{72}$$

Now making use of Eq. (69) we get

$$Q[H(1+Y)-Y(1+Z)P_0H(1+Y)](1+Z)P_0=0. \tag{73}$$

Now to make the number of equations sufficient to determine all unknown components of Y one can impose the condition

$$Q[H(1+Y)-Y(1+Z)P_0H(1+Y)]P=0. \tag{74}$$

This condition leads to satisfying Eq. (73) but must be seen as only one of the possible ways to do so. It corresponds to the so-called simplest generalization of the wave operator formalism by Malrieu *et al.*[10]

Diagonalization of $P_0\tilde{H}P_0$ yields a subset of the exact eigenvalues of H. The number of eigenvalues is equal to the dimension of the main model space but one can also notice that this set of eigenvalues along with some other set of numbers that are not, in general, eigenvalues of H can be obtained by diagonalization of

$$H_I^{\text{eff}}=P(1-Y)H(1+Y)P=PH(1+Y)P, \tag{75}$$

since the same eigenvalues are furnished by

$$P\tilde{H}P=P(1-Z)(1-Y)H(1+Y)(1+Z)P. \tag{76}$$

The operator $P\tilde{H}P$ and the intermediate Hamiltonian H_I^{eff} are related by a similarity transformation within the model space by the operator $P(1+Z)P$ and hence have the same eigenvalues. However, due to Eq. (67) part of the eigenvalues of $P\tilde{H}P$ (and H_I^{eff}) is a set of eigenvalues of the Hamiltonian H. The rest of eigenvalues of H_I^{eff} are phony ones in the sense that in general they are not eigenvalues of H.

It can be seen from Eq. (75) that Z can be directly obtained from the diagonalization of the intermediate Hamiltonian if the eigenvectors corresponding to the main model space are expressed in the intermediate normalization. It can be viewed as a particular way of solving Eq. (69). Another way of solving Eq. (69) is to develop into a perturbation expansion, and this choice has been implicit in most of the work on intermediate Hamiltonians using R–S perturbation expansions. However, in suitable applications of the intermediate Hamiltonian formalism there will be a fairly strong coupling between the main and the intermediate model space and therefore a perturbation expansion can be expected to be at best slowly converging. In the following we will explore the possibility of obtaining Z by diagonalization of the intermediate Hamiltonian. The equation for Y (or approximations to it) in most cases depends on Z. This suggests an iterative solution to the problem. We can solve for Z, given Y and then for Y with fixed Z and iterate this sequence until self-consistency.

Another way of satisfying Eq. (73) can be found by employing the simplest decomposition of the similarity transformation leading to H^{eff} in which the Y and Z operators are defined as follows:

$$Y=QYP_0, \quad Z=P_IZP_0, \tag{77}$$

or alternatively we have imposed the extra conditions $QYP_I=0$, which imply $QYZP_0=0$. One can see that the number of parameters to determine is again equal to the number of equations. Y must satisfy

$$Q[H(1+Y)-YH(1+Y)](1+Z)P_0=0 \tag{78}$$

or

$$Q(1-Y)H(1+Y+Z)P_0=0, \tag{79}$$

and the intermediate Hamiltonian is traditionally given by Eq. (75). Equation (79) can be considered as an equation for Y that also depends on $(1+Z)P_0$ which corresponds to the set of eigenvectors of H_I^{eff} for the selected eigenvalues of H we want to obtain. Therefore the right eigenvectors of H_I^{eff} are necessary to determine Y. This scheme has been implemented to modify the equation of motion coupled cluster method with singles and doubles (EOM-CCSD) (Refs. 11 and 12) to include the effect of higher excitations and eliminate the extensivity error.[35]

Equation (79) can be cast in an iterative form using the partitioning $H=H_0+V$,

$$Q(YH_0-H_0Y)P_0=Q(1-Y)V(1+Y+Z)P_0, \tag{80}$$

and this allows for a convenient determination of Y. All energy denominators involve energy differences between the main model space and the Q-space and are therefore well behaved. This very simple scheme has the advantage that the number of Y parameters is minimal. Malrieu *et al.*[10] have discarded this possibility because the intermediate Hamiltonian can be rather nonsymmetric because the so-called dressing $PHYP_0$ modifies only the main model space columns of the intermediate effective Hamiltonian. However, the assumption in these schemes is always that Y can be obtained from a perturbation expansion and will hence be small. Therefore we consider this scheme perfectly viable for application to quantum chemical problems. Jolicard and Billing[36] have implemented a scheme that is based on the above parametrization and applied it successfully to some model problems relating to nuclear dynamics.

Another kind of condition that satisfies Eq. (73) can be found when the main model space is completely degenerate in the zeroth-order approximation

$$H_0P_0=E_0^0P_0. \tag{81}$$

Using the partitioning of the Hamiltonian into a zeroth order and perturbed part, Eq. (73) can be rewritten in the form

$$Q[H(1+Y)(1+Z)-Y(1+Z)P_0H_0 - Y(1+Z)P_0V(1+Y)(1+Z)]P_0=0. \tag{82}$$

Due to Eq. (81) we have

$$Y(1+Z)P_0H_0=YE_0^0(1+Z)P_0, \tag{83}$$

and Eq. (82) takes the form

$$Q[H(1+Y)-YE_0^0-Y(1+Z)P_0V(1+Y)](1+Z)P_0=0. \tag{84}$$

Equation (84) is satisfied if

$$Q[H(1+Y)-YE_0^0-Y(1+Z)P_0V(1+Y)]P=0. \tag{85}$$

The number of unknown parameters in Y and Z is now equal to the number of equations. The set of Eqs. (85), (69), and (75) may be developed completely into perturbation expansions to obtain the generalized degenerate perturbation expansion (GDPT).[10] We have immediately from Eq. (85),

$$Y=R_Q\sum_{n=0}^{\infty}(VR_Q)^n[V-Y(1+Z)P_0V(1+Y)]P, \tag{86}$$

where

$$R_Q=\frac{Q}{E_0^0-H_0}. \tag{87}$$

While the perturbation expansion for Z is given by

$$Z=R_I\sum_{n=0}^{\infty}(VR_I)^n[V(1+Y+YZ)-ZV(1+Z)(1+Y)]P_0, \tag{88}$$

where

$$R_I=\frac{P_I}{E_0^0-H_0}. \tag{89}$$

Equations (86)–(89) can be used to obtain an explicit order-by-order expansion for Y and hence for the intermediate

Hamiltonian [Eq. (75)]. One can see that because of use of the intermediate Hamiltonian scheme denominators appearing in R_I that may cause problems have been shifted from the second order in the H^{eff} expansion [multireference R–S PT (Sec. III), which under condition (81) is called degenerate perturbation theory (DPT)] to the fourth order in the H_I^{eff} expansion (GDPT).[10] Alternatively, the operator Z can be obtained from diagonalization of the intermediate Hamiltonian. This alleviates all problems arising from the strong coupling between the main and intermediate model spaces.

The above two schemes involving either QYP_0 or QYP and a degenerate main model space are closely related. Suppose the intermediate Hamiltonian is given by $PH(1+Y)P$ and Z is determined to satisfy Eq. (69), then one can alternatively use the intermediate Hamiltonian $PH[1+Y(1+Z)P_0]P$. This intermediate effective Hamiltonian provides the same eigenvalues for the main model space, because

$$P_I(1-Z)H[1+Y(1+Z)P_0](1+Z)P_0$$
$$=P_I(1-Z)H(1+Y)(1+Z)P_0=0 \tag{90}$$

and

$$P_0H[1+Y(1+Z)P_0](1+Z)P_0$$
$$=P_0H(1+Y)(1+Z)P_0=P_0H^{\text{eff}}P_0. \tag{91}$$

This shows that the vital information is provided by $QY(1+Z)P_0=QY'P_0$. The relation between the two approaches becomes even deeper if we compare the equations for Y and Y'. The explicit perturbation expansion for Y' is

$$Y'=R_Q\sum_{n=0}^{\infty}(VR_Q)^n[V-Y'V(1+Y')](1+Z)P_0. \tag{92}$$

Comparing Eqs. (86) and (92) we find that $QY'P_0=QY(1+Z)P_0$ in each order of the perturbation provided the same operator Z is used in both equations. It follows that both schemes yield exactly the same result in each order of the perturbation if and only if the operator Z is calculated up to self-consistency. The change in results due to self-consistency will usually be small and therefore we expect these two schemes to give very similar results, irrespective of the details of solution. Let us stress here that the number of parameters Y' is much less and this will be a distinct advantage.

The intermediate Hamiltonian schemes presented above are based on dependence of the Y operator on some eigenvectors of H_I^{eff}, through their dependence on $(1+Z)$. For the one-dimensional main model space M_0 (dim $M_0=1$) this dependence can be replaced by an eigenvalue dependence. For dim $M_0=1$ we have

$$P_0\tilde{H}P_0=P_0H(1+Y)(1+Z)P_0=EP_0, \tag{93}$$

and then Eq. (73) gives

$$Q[H(1+Y)-YE](1+Z)P_0=0. \tag{94}$$

Requiring

$$Q[(H_0+V-E)Y+V]P=0 \tag{95}$$

to determine the solution uniquely we have an equation for Y that is now not Z-dependent but energy dependent. The equation is linear in Y, which means that for a selected energy E there can be only one solution for Y,

$$Y=\sum_{n=0}^{\infty}R(E)[VR(E)]^nVP, \tag{96}$$

where $R(E)$ is given by Eq. (61). The intermediate Hamiltonian is again defined by Eq. (75) giving only one selected eigenvalue of H. The scheme presented above has been discussed by Lindgren as a version of B–W expansion of the effective Hamiltonian.[7] However, in the light of subsequent developments it is better to consider the scheme as an example of an intermediate Hamiltonian formulation. One can find many more implicit implementations of this idea like, for example, the partitioning technique by Löwdin[37] and the self-energy operator in the theory of propagators (see, e.g., Ref. 38). In all of these approaches an eigenvalue is determined by diagonalizing a matrix that depends on the eigenvalue. The final solution is obtained at self-consistency.

The scheme introduced by Lindgren does not depend on the eigenvectors given by the diagonalization. This is a consequence of having a one-dimensional main model space. In the scheme proposed by Zaitsevskii and Dement'ev[21] based also on the B–W type expansion in which dim M_0 is greater than one the dependence on the eigenvectors of H_I^{eff} does appear. In the above scheme we used an operator QYP and included extra equations by replacing $(1+Z)P_0$ by P. As before we can construct an alternative scheme by equating the QYP_I components to zero. Let us for later convenience indicate this operator as Y'. In this case we have

$$P_0H(1+Y'+Z)P_0=EP_0, \tag{97}$$

and Eq. (73) takes the form

$$Q[H(1+Y'+Z)-EY']P_0=0. \tag{98}$$

Using the partitioning of the Hamiltonian we obtain

$$Q(H_0+V-E)Y'+QV(1+Z)P_0=0, \tag{99}$$

which leads to another B–W type expansion

$$Y'=R(E)\sum_{n=0}^{\infty}[VR(E)]^n[V(1+Z)]P_0, \tag{100}$$

where again $R(E)$ is defined by Eq. (61). In this way Y' becomes energy and eigenvector dependent.

The two B–W type of approaches described above lead to the same results in each order of the perturbation if Z is calculated self-consistently. This can be easily seen if we multiply Eq. (96) by $(1+Z)P_0$, and compare with Eq. (100). It follows that $Y'=Y(1+Z)P_0$. Given that Z is determined from $H_I^{\text{eff}}=PH(1+Y)P$ and the fact that $PH[1+Y(1+Z)P_0]P$ gives the same main eigenvalues and operator Z it follows that both approaches yield identical results if Z is calculated self-consistently. It seems therefore that the second scheme (using less parameters) is to be preferred over the first scheme. However, the first scheme does not explicitly depend on Z and therefore it is likely that self-

consistency can be achieved easier in the first approach. Therefore, if one aims at a self-consistent solution of the equations, the first scheme may be preferable.

Let us for the sake of completeness also consider the case of a multidimensional main model space within a Brillouin–Wigner framework. Substituting

$$P_0H(1+Y)(1+Z)P_0=H^{\mathrm{eff}} \tag{101}$$

into Eq. (72) we get

$$Q[H(1+Y)(1+Z)-Y(1+Z)H^{\mathrm{eff}}]P_0=0. \tag{102}$$

To arrive at a Brillouin–Wigner scheme we need the eigenvectors and eigenvalues of H^{eff}, denoted A and D, respectively,

$$H^{\mathrm{eff}}A=AD. \tag{103}$$

Multiplying Eq. (102) by A from the right we find

$$Q[H(1+Z)A+HY(1+Z)A-Y(1+Z)AD]=0. \tag{104}$$

Let us note that $(1+Z)A$ represent simply the eigenvectors of the intermediate Hamiltonian. If we now define a new quantity $Y'=QY(1+Z)A$ the working equations become

$$Q[H(1+Z)A+HY'-Y'D]=0. \tag{105}$$

This last equation can be cast into an iterative form as

$$(Y'D-H_0Y')=Q[V(1+Z)A+VY']. \tag{106}$$

As discussed before the intermediate Hamiltonian can be written as $PH[1+Y(1+Z)P_0]P$, if the operator Z is determined self-consistently. It follows that in terms of Y' the intermediate Hamiltonian is given by $PH(1+Y'A^{-1})P$. The parameters Z as well as A are obtained from a diagonalization of the intermediate effective Hamiltonian. An important feature of this general B–W scheme is that results are strictly independent of the size of the main model space in each order of the perturbation. From Eq. (106) it follows that each component Y_i' corresponding to a particular eigenvector A_i can be calculated individually. Moreover defining the intermediate Hamiltonian as $H(1+Y'P_0'A'^{-1}P_0')$, where P_0' is a model space smaller than P_0 yields the same eigenvalues corresponding to the eigenvectors Y_i' included in P_0' as $H(1+Y'P_0A^{-1}P_0)$. This adds a lot of flexibility to the general B–W scheme in actual applications.

All B–W schemes discussed in this section yield the same result in each order of the perturbation if the intermediate model space quantities (E, Z, and/or A) are iterated up to self-consistency. However, the convergence behavior in the self-consistency cycle may be quite different. The scheme proposed by Lindgren does not depend on Z and therefore one can expect this scheme to converge very rapidly. However, the number of Y parameters is larger than in the other two schemes and therefore we think that this scheme will be most useful (assuming a rather large intermediate space) if Y is calculated only up to first order (in first order the computational cost to incorporate QYP or QYP_0 is the same). The B–W scheme has the interesting property that results are independent of the size of the main model space and this provides a high flexibility in the application of the scheme.

V. NUMERICAL EXAMPLE

We have discussed a number of possible schemes within the framework of intermediate Hamiltonian theory. These schemes can be classified as follows. We consider either a full dressing QYP or a minimal dressing QYP_0. As mentioned before if the quantities determined from the intermediate Hamiltonian, Z and/or E, are calculated up to self-consistency the results from these schemes will be identical in each order of the perturbation with respect to Y. This is true in both the Rayleigh–Schrödinger (assuming H_0 is degenerate in the main model space) and Brillouin–Wigner formulations. The number of iterations required to achieve self-consistency does depend on the dressing, however. In order to get a first impression of the performance of these schemes we apply the various schemes to a well known model problem introduced by Malrieu.[10] The model is defined by a real symmetric matrix of dimension 20. Five of the eigenvalues of the matrix are centered around unity and five others are close to two. Therefore, the dimension of the full model space is 10.[10] The matrix is dominantly diagonal (the diagonal defining H_0) and the first five elements of H_0 are all unity, so that we can define a degenerate main model space of dimension 5. We have carried out self-consistent RSPT (SC-RSPT) and BWPT (SC-BWPT) calculations employing either a full or minimal dressing (giving identical results) and an iterative RSPT scheme in which Z and Y are not calculated self-consistently but we simply update Z and Y alternately. In all calculations presented the dimension of the main model space was 5. In Tables I and II we show the convergence behavior of the first and fourth eigenvalues as typical examples. We show the difference with exact eigenvalue as a function of the order of iteration in Y. Also included in the tables is the behavior of conventional degenerate perturbation theory (possibly suffering from intruder states) and generalized degenerate perturbation theory.[10] The results in Table II are most indicative of the performance of the various methods. It is seen that all schemes based on the intermediate Hamiltonian formulation exhibit a substantially more stable and smoother convergence behavior than DPT. It can also be seen that the convergence of GDPT slows down after the first few orders, and this is due to the slowly converging perturbation expansion for Z which involves small denominators. This problem is alleviated in the self-consistent schemes which show very similar convergence behavior. The convergence behavior of iterative RSPT is quite stable too, and this shows that self-consistency may not be very important. Let us note that the total number of iterations on Z is much larger in the self-consistent formulations and this most likely explains the slower convergence of iterative RSPT.

The self-consistent SC-RSPT and SC-BWPT calculations have been carried out using both a full dressing QYP and a minimal dressing QYP_0. The use of a minimal dressing requires most iterations to achieve self-consistency. Typically we need 12–14 iterations to find the energies stable up to 11 decimal places. Reducing the dimension of the main model space to one reduces the required number of iterations to 10–12. The reduction of the dimension of the main model space has hardly any effect on the order by order conver-

TABLE I. Convergence behavior of first energy eigenvalue of the Malrieu model problem using various schemes based on the intermediate Hamiltonian formalism. The main model space has dimension 5 in all schemes and the full model space has dimension 10. DPT is the standard effective Hamiltonian scheme, GDPT is the generalized degenerate perturbation theory (Malrieu, 1985). In the self-consistent schemes (SC-RSPT and SC-BWPT) the operator Z is optimized in each order of the perturbation until it does not change anymore. In the iterative RSPT scheme operators Z and Y are calculated alternately. For more details see the text.

Order of PT	DPT	GDPT	SC-RSPT	SC-BWPT	Iterative RSPT
1	$0.13e-2$	$0.13e-2$	$0.13e-2$	$0.13e-2$	$0.13e-2$
2	$-0.26e-2$	$0.29e-3$	$0.29e-3$	$0.34e-3$	$0.35e-3$
3	$0.83e-3$	$0.11e-3$	$0.76e-4$	$0.99e-4$	$0.11e-3$
4	$-0.27e-3$	$0.25e-4$	$0.19e-4$	$0.29e-4$	$0.37e-4$
5	$0.10e-3$	$0.95e-5$	$0.51e-5$	$0.88e-5$	$0.13e-4$
6	$-0.46e-4$	$0.20e-5$	$0.13e-5$	$0.26e-5$	$0.43e-5$
7	$0.24e-4$	$0.72e-6$	$0.35e-6$	$0.79e-6$	$0.15e-5$
8	$-0.14e-4$	$0.10e-6$	$0.89e-7$	$0.24e-6$	$0.52e-6$
9	$0.82e-5$	$0.31e-7$	$0.25e-7$	$0.71e-7$	$0.18e-6$
10	$-0.49e-5$	$-0.71e-8$	$0.60e-8$	$0.21e-7$	$0.62e-7$
11	$0.30e-5$			$0.64e-8$	$0.21e-7$
12	$-0.18e-5$				$0.74e-8$
13	$0.11e-5$				
14	$-0.62e-6$				
15	$0.37e-6$				
16	$-0.21e-6$				

gence. Using the full dressing in the SC-RSPT scheme we still need about 10–12 iterations (reduced to 8–10 if the dimension of the main model space is taken to be unity). This slight reduction is not very useful considering the increase in the number of parameters Y. However, in the SC-BWPT scheme with a full dressing (and necessarily a one-dimensional main model space) self-consistency can be achieved in two to three iterations. This clearly shows the enormous improvement that is obtained by replacing the dependence on Z by an eigenvalue dependence.

Preliminary conclusions from these model calculations are that the full dressing shows promise in conjunction with the one-dimensional SC-BWPT scheme. This is true in particular if the perturbation expansion for Y can be restricted to first order. The full dressing shows hardly any advantages for the SC-RSPT scheme and we think therefore that the iterative RSPT scheme (in which Y and Z are determined alternately) in conjunction with a minimal dressing is probably most useful in the context of higher order (or coupled cluster based) intermediate Hamiltonian schemes.

VI. CONCLUSION

We have shown how effective and intermediate Hamiltonians can be derived from a simple similarity transformation. This scheme provides a necessary condition for the

TABLE II. Convergence behavior of the fourth eigenvalue of the Malrieu eigenvalue problem. The same computational schemes are used as in Table I.

Order of PT	DPT	GDPT	SC-RSPT	SC-BWPT	Iterative RSPT
1	$0.15e-2$	$0.15e-2$	$0.15e-2$	$0.15e-2$	$0.15e-2$
2	$-0.73e-3$	$-0.99e-4$	$-0.99e-4$	$-0.18e-3$	$0.14e-3$
3	$0.73e-3$	$0.61e-4$	$0.71e-4$	$0.86e-4$	$0.89e-4$
4	$-0.40e-4$	$0.21e-4$	$-0.13e-5$	$-0.11e-4$	$0.36e-4$
5	$0.13e-3$	$0.59e-5$	$0.61e-5$	$0.78e-5$	$0.17e-4$
6	$0.14e-4$	$0.86e-5$	$0.30e-6$	$-0.98e-6$	$0.81e-5$
7	$0.35e-4$	$0.17e-5$	$0.60e-6$	$0.80e-6$	$0.39e-5$
8	$0.10e-4$	$0.28e-5$	$0.65e-7$	$-0.99e-7$	$0.18e-5$
9	$0.10e-4$	$0.76e-6$	$0.63e-7$	$0.84e-7$	$0.87e-6$
10	$0.47e-6$	$0.86e-6$	$0.10e-7$	$-0.10e-7$	$0.42e-6$
11	$0.32e-5$	$0.34e-6$	$0.69e-8$	$0.89e-8$	$0.20e-6$
12	$0.19e-5$	$0.27e-6$			$0.95e-7$
13	$0.11e-5$	$0.14e-6$			$0.45e-7$
14	$0.72e-6$	$0.89e-7$			$0.22e-7$
15	$0.37e-6$	$0.52e-7$			$0.10e-7$
16	$0.26e-6$	$0.31e-7$			$0.49e-8$
17	$0.13e-6$				
18	$0.90e-7$				

separation of the eigenvalue problem of H into two subproblems and it allows the determination of all left and right eigenvectors in a straightforward manner. The separation leads to the definition of the effective Hamiltonian as an operator that acts in a small model space that has the same eigenvalues as the full Hamiltonian. Many different effective Hamiltonians can be defined but the construction of all of them can be based on the introduced similarity transformation. Obviously, all exact effective Hamiltonians are related by similarity transformations within the model space, so the difference between them becomes visible only when the necessary approximations are introduced. One of the criteria for such approximations can be perturbation expansions of either the Rayleigh–Schrödinger or Brillouin–Wigner-type and these are discussed throughout the paper as one of the possible ways to obtain effective as well as intermediate Hamiltonians.

Intermediate Hamiltonians have been introduced by splitting the similarity transformation that leads to the effective Hamiltonians into a sequence of two similarity transformations. The second similarity transformation is determined from the block-diagonalization within an extended model space of the Hamiltonian transformed by the first transformation, the so-called intermediate Hamiltonian. The mixing between main model and intermediate model space components is taken into account by diagonalization rather than a perturbative treatment and this allows the use of small main model spaces. In this way the problem of intruder states connected with the first similarity transformation is alleviated.

We think that use of similarity transformations provides a particular transparent picture of the formalism of effective and intermediate Hamiltonians. It provides a way by which a part of eigenvalue problem of H can be extracted at the same time preserving knowledge of the rest of the problem. It also allows the determination left and right eigenvectors and that can be considered as one of the advantages of the presented formalism.

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