Breaking of the one-to-one correspondence between model and target spaces in effective Hamiltonian theory: Generalized effective Hamiltonians

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A generalization of the standard effective Hamiltonian theory is presented, based on the breaking of the one-to-one correspondence between the model and the target spaces. In this way the target space can be smaller than the model space, and problems connected to the presence of intruder states can be solved. An application to the dimer of lithium is given. Moreover, it is shown how the formalism can be translated into an iterative approach, and test computations are presented.

I. INTRODUCTION

The theory of effective Hamiltonians (EH) has found applications after a long time in the fields of quantum physics and chemistry, and today it has applications in nuclear physics,[1-3] in the construction of Heisenberg Hamiltonians,[4,5] or, more generally, valence Hamiltonians,[6,7] for the diabatization of energy surfaces,[8-10] or the relativistic treatment of atoms.[11] Its objective is to reduce the full Hamiltonian H associated with a system to a smaller "effective" Hamiltonian that has eigenvalues equal to a subset of the exact eigenvalues of H. In this way the understanding of the physical content of the Hamiltonian is easier and it is also possible to use the matrix elements of the EH obtained for simple systems in order to build effective operators that can be used to study larger systems. However, we must observe that the model space (the space in which the EH is built) must not be too different from the target space (the space of eigenvectors of H whose eigenvalues are exactly reproduced by the EH); otherwise the EH is meaningless. The practical application of this formalism faces some very serious drawbacks that severely limit the use of this technique in real problems. The main inconvenience is represented by the so-called intruder states problem.[12] This problem is usually associated with the lack of convergence of the EH in particular situations, but it has been shown[13] that it is a much more serious one, and the presence of intruder states leads to strong difficulties in the construction of an EH even when the exact states are known and no need of an iterative process is concerned. Strictly connected with this problem is the fact that in the presence of intruder states the effective Hamiltonian can be strongly non-Hermitian, and this may introduce further difficulties concerning the interpretation of the obtained matrix elements and the possibility of their transferability from one system to another.

In order to overcome these difficulties a modified formulation has been recently proposed, the intermediate effective Hamiltonian (IEH) formalism[14] (see also Refs. 13 and 15 for different formulations and extensions): for a model space of dimension N, an intermediate effective Hamiltonian provides only M (with $M<N$) roots which are exact, the remaining N-M roots (called intermediate roots) being only approximations of exact ones. In this paper a different approach is considered, i.e., the breaking of the one-to-one correspondence between the model space and the target space. We assume then that to the EH $\tilde{H}$ is associated a pseudometric $\tilde{K}$, and that instead of the usual eigenvalue problem

$$\det(\tilde{H}-\lambda)=0 \tag{1a}$$

of the standard EH theory, it is the solution of the generalized eigenvalue problem

$$\det(\tilde{H}-\lambda\tilde{K})=0\ , \tag{1b}$$

which gives a set of M exact eigenvalues of H, where M is equal to or even less than N. To the best of our knowledge, this possibility was considered for the first time by Mercier, Chambaud, and Levy in their study of the low-lying states of the $(HeNe)^{2+}$ system,[16] but this approach did not receive much attention in following paper, and it has never been studied systematically as a generalization of the EH standard theory. In this paper we want to explore the possibilities of this formalism and to study its relationship with the usual one. It will be shown that this formalism is a generalization of the usual EH formalism,[17-19] to which it reduces when we put $M=N$.

To give an illustration of the reasons leading one to forsake the one-to-one correspondence between model space and target space we consider a simple ad hoc case: let the Hamiltonian H be given by the matrix

$$\begin{bmatrix} \alpha & \delta_{12} & \delta_{13} & \cdots \\ \delta_{12} & 1 & \delta_{23} & \\ \delta_{13} & \delta_{23} & 2 & \\ & & & \ddots \end{bmatrix},$$

where α is a real parameter and the δ_{ij} are (small) cou-

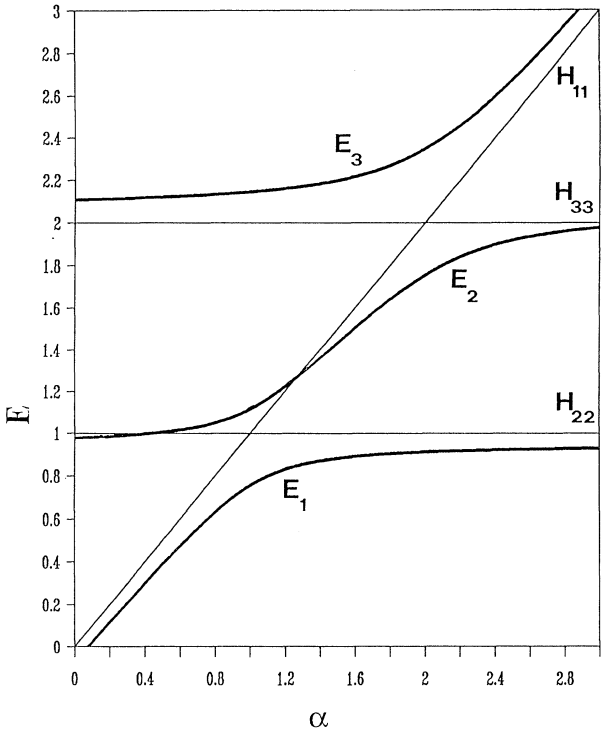

FIG. 1. Eigenvalues E_i and diagonal elements H_{ii} of the 3×3 Hamiltonian with $\delta_{ij}=0.1$ (see the text) as a function of the parameter α.

pling coefficients. (Its eigenvalues E_i and its diagonal elements H_{ii} are shown in Fig. 1 for the case $N=3$, $\delta_{ij}=0.1$.) Despite its simplicity, such a Hamiltonian can be used to visualize what happens, for instance, when an ionic bond is stretched, and we have avoided crossings between ionic and neutral configurations, as we will see in the following. If we are interested only in the lowest eigenvalue E_1 of H, we face the problem that the corresponding eigenvector $|\Psi_1\rangle$ has a large overlap with the configuration $|\Phi_1\rangle$ for $\alpha<1$, and with the configuration $|\Phi_2\rangle$ for $\alpha>1$, and we have a continuous switch between these two limit cases for intermediate values of α. If we want to keep the constraint $M=N$ of standard EH theory, we are obliged to introduce the first excited state $|\Psi_2\rangle$ (an intruder state) in the target space, but this fact leads in turn to the necessity of adding $|\Phi_3\rangle$ in the model space, in order to give a good description of the new state for every value of α. We are now obliged to introduce a new state in the target space, to keep $M=N$, and so on. We can have a complete chain of intruder states, that can arrive to involve, as in cases like this, the full space.

It is only by leaving the condition $M=N$ that we can keep such a problem inside the EH formalism: to describe the lowest state $|\Psi_1\rangle$ in the complete range of the parameter we need both $|\Phi_1\rangle$ and $|\Phi_2\rangle$. No other state can be described correctly with this model space, because of the avoided crossings occurring at $\alpha=2$. Thus we are forced to have a model space of dimension 2 to describe a target space of dimension 1.

II. GENERAL FORMALISM

We denote by H the projection of the Hamiltonian operator of the system onto a finite-dimensional space, spanned by orthonormalized basis vectors $|\Phi_i\rangle$ (they can be, for instance, Slater determinants, or spin-adapted configurations). The Schrödinger equation becomes an eigenvalue equation:

$$H|\Psi_\alpha\rangle=E_\alpha|\Psi_\alpha\rangle\ . \tag{2}$$

Usually we are interested only on a small subset of M eigenvectors, whose span L is called the *target space*. To give an approximate description of the target space we need a certain number N of vectors $|\Phi_i\rangle$, whose span L_0 is called the *model space*. Of course N cannot be less than M. Let P_0 be the orthogonal projector onto L_0, and Q_0 its orthogonal complement:

$$P_0=\sum_{n\in N}|\Phi_n\rangle\langle\Phi_n|\ , \tag{3a}$$

$$Q_0=1-P_0\ . \tag{3b}$$

We indicate by $|\overline{\Psi}_\mu\rangle$ the projection of the target vector $|\Psi_\mu\rangle$ into the model space L_0:

$$|\overline{\Psi}_\mu\rangle=P_0|\Psi_\mu\rangle,\quad \mu\in M\ . \tag{4}$$

The M vectors $|\overline{\Psi}_\mu\rangle$ (we assume they are linearly independent) span an M-dimensional subspace of L_0 that we denote by L_M, while L_I is its orthogonal complement in L_0. We indicate also by P_M and P_I the orthogonal projectors onto L_M and L_I, respectively. (In the following we indicate by M and N both the dimension of the subspaces and the set of indices of vectors generating the subspaces.)

It is convenient to introduce now the concept of biorthonormal vectors of $|\overline{\Psi}_\mu\rangle$: the vectors $\{|\overline{\Psi}_\mu^{\perp\perp}\rangle,\mu\in M\}$ are said to form the biorthonormal system of $\{|\overline{\Psi}_\mu\rangle,\mu\in M\}$ if the following two conditions are satisfied:

$$P_M|\overline{\Psi}_\mu^{\perp\perp}\rangle=|\overline{\Psi}_\mu^{\perp\perp}\rangle\ , \tag{5a}$$

$$\langle\overline{\Psi}_\mu^{\perp\perp}|\overline{\Psi}_\nu\rangle=\delta_{\mu\nu}\ . \tag{5b}$$

(It will be shown that with these assumptions the biorthonormal system exists and is unique. We notice also that by applying twice the biorthonormality transformation we obtain again the original vectors.) We define now the generalized Bloch effective Hamiltonian $\tilde{H}$, with respect to the metric $\tilde{K}$, in the following way:

$$\tilde{H}=\sum_{\mu\in M}|\overline{\Psi}_\mu\rangle E_\mu\langle\overline{\Psi}_\mu^{\perp\perp}|\ , \tag{6a}$$

$$\tilde{K}=\sum_{\mu\in M}|\overline{\Psi}_\mu\rangle\langle\overline{\Psi}_\mu^{\perp\perp}|\ . \tag{6b}$$

(Strictly speaking $\tilde{K}$ is only a pseudometric, since it is defined only on L_M, while on L_I it is zero.) It follows immediately from these definitions that the $|\overline{\Psi}_\mu\rangle$ and the

$\langle \bar{\Psi}_\mu^{\perp\perp}|$ are, respectively, the right and left eigenvectors of $\tilde{H}$ with respect to the metric $\tilde{K}$:

$$(\tilde{H}-E_\mu\tilde{K})|\bar{\Psi}_\mu\rangle=0 \ , \tag{7a}$$

$$\langle \bar{\Psi}_\mu^{\perp\perp}|(\tilde{H}-E_\mu\tilde{K})=0 \ . \tag{7b}$$

We call $\tilde{H}$ a generalized effective Hamiltonian (GEH) of Bloch type since this *generalized* eigenvalue equation becomes, in the particular case $M=N$, the eigenvalue equation defining the usual Bloch Hamiltonian.[1] In Appendix A we give a complete characterization of the class of GEH in the sense of Eq. (1b) and in Appendix B we study the relationships with the different possible choices of EH that have been given in the literature.

In order to illustrate further the characteristics of the biorthonormal system, let us introduce the two M by M Hermitian matrices $\mathcal{S}$ and $\mathcal{T}$, whose matrix elements are given by

$$\mathcal{S}_{\mu\nu}=\langle \bar{\Psi}_\mu|\bar{\Psi}_\nu\rangle \tag{8a}$$

and

$$\mathcal{T}_{\mu\nu}=(\mathcal{S}^{-1})_{\mu\nu} \ . \tag{8b}$$

We can immediately verify that

$$|\bar{\Psi}_\mu^{\perp\perp}\rangle=\sum_{\nu\in M}|\bar{\Psi}_\nu\rangle\mathcal{T}_{\nu\mu} \ . \tag{9}$$

The metric is then given by

$$\tilde{K}=\sum_{\mu,\nu\in M}|\bar{\Psi}_\mu\rangle\mathcal{T}_{\mu\nu}\langle\bar{\Psi}_\nu| \ , \tag{10a}$$

from which we deduce that the metric is (as it might be) an Hermitian operator. Since it projects onto L_M, it is *the* orthogonal projector onto L_M. The effective Hamiltonian is given by

$$\tilde{H}=\sum_{\mu,\nu\in M}|\bar{\Psi}_\mu\rangle E_\mu\mathcal{T}_{\mu\nu}\langle\bar{\Psi}_\nu| \ , \tag{10b}$$

and it is in general not Hermitian. In order to understand better this important point, we compute the quantity

$$\tilde{H}^{+}-\tilde{H}=\sum_{\mu,\nu\in M}|\bar{\Psi}_\mu\rangle(E_\mu-E_\nu)\mathcal{T}_{\mu\nu}\langle\bar{\Psi}_\nu| \ , \tag{11}$$

from which is clear that a *sufficient* condition to have Hermiticity is one of the following: (a) the target space is exactly degenerate; (b) the $|\bar{\Psi}_\mu\rangle$ form an orthogonal system, hence $\mathcal{S}$ (and then $\mathcal{T}$) are diagonal matrices.

While, given H, we cannot act on (a), condition (b) can be approximately satisfied if we choose a model space that gives a good description of the target space (in the sense that $\langle\Psi_\mu|Q_0|\Psi_\mu\rangle\ll 1$ for every $\mu\in M$). Thus a "good" model space will always give a quasi-Hermitian effective Hamiltonian, and this is why people dislike strongly non-Hermitian EH. But we must notice that the contrary is false, since we can have Hermitian EH associated with poor model spaces. In fact, we have that a good model space implies a matrix $\mathcal{S}$ not only almost diagonal, but near to the identity: since

$$\delta_{\mu\nu}=\langle\Psi_\mu|\Psi_\nu\rangle=\langle\Psi_\mu|P_0|\Psi_\nu\rangle+\langle\Psi_\mu|Q_0|\Psi_\nu\rangle \ ,$$

we have

$$|\delta_{\mu\nu}-\mathcal{S}_{\mu\nu}|^2=|\langle\Psi_\mu|Q_0|\Psi_\nu\rangle|^2\le\|Q_0\Psi_\mu\|\,\|Q_0\Psi_\nu\| \ . \tag{12}$$

A second way to obtain the biorthonormal vectors is via the operators (defined in L_M) S and T, defined as

$$S=\sum_{\mu\in M}|\bar{\Psi}_\mu\rangle\langle\bar{\Psi}_\mu| \tag{13a}$$

and

$$T=S^{-1} \ , \tag{13b}$$

where the inverse is taken in L_M and not in L_0, since otherwise it would not be defined. S and T are related to the biorthonormal vectors by the equations

$$|\bar{\Psi}_\mu^{\perp\perp}\rangle=T|\bar{\Psi}_\mu\rangle \ , \tag{14a}$$

$$|\bar{\Psi}_\mu\rangle=S|\bar{\Psi}_\mu^{\perp\perp}\rangle \ , \tag{14b}$$

as can be immediately verified. We notice also that $S^{-1/2}$ and $\mathcal{S}^{-1/2}$ (i.e., $T^{1/2}$ and $\mathcal{T}^{1/2}$) transform the projected vectors $|\bar{\Psi}_\mu\rangle$ into the symmetrically orthonormalized vectors (according to Löwdin) $|\bar{\Psi}_\mu^{\perp}\rangle$:

$$|\bar{\Psi}_\mu^{\perp}\rangle=\sum_{\nu\in M}|\bar{\Psi}_\nu\rangle(\mathcal{T}^{1/2})_{\nu\mu} \ , \tag{15a}$$

$$|\bar{\Psi}_\mu^{\perp}\rangle=T^{1/2}|\bar{\Psi}_\mu\rangle \ , \tag{15b}$$

and also

$$|\bar{\Psi}_\mu^{\perp}\rangle=\sum_{\nu\in M}|\bar{\Psi}_\nu^{\perp\perp}\rangle(\mathcal{S}^{1/2})_{\nu\mu} \ , \tag{15c}$$

$$|\bar{\Psi}_\mu^{\perp}\rangle=S^{1/2}|\bar{\Psi}_\mu^{\perp\perp}\rangle \ . \tag{15d}$$

In Fig. 2 an example of all these vectors is shown, together with some of the relations occurring among them.

III. NUMERICAL APPLICATIONS

To illustrate the proposed formalism we considered the low-lying states of the lithium dimer at different internuclear distances. We used a valence $2s2p$ basis set on each Li atom, plus pseudopotentials[20] to describe the inner $1s$ electrons, as fully specified in Ref. 13. We have then only two electrons explicitly treated, and the self-consistent-field (SCF) computation gives an occupied molecular orbital of σ_g symmetry, while the first excited orbital is a σ_μ one. (In the following when we refer to the σ_g or σ_u orbitals we mean the lowest SCF orbitals of these sym-

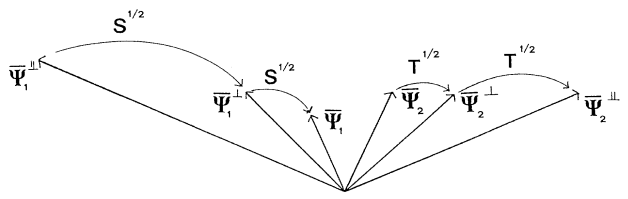

FIG. 2. Projected eigenvectors $|\bar{\Psi}_\mu\rangle$, their biorthonormals $|\bar{\Psi}_\mu^{\perp\perp}\rangle$ and corresponding symmetrically orthonormalized vectors $|\bar{\Psi}_\mu^{\perp}\rangle$ in a case with $M=2$. Some of the relations between these vectors are shown in the figure.

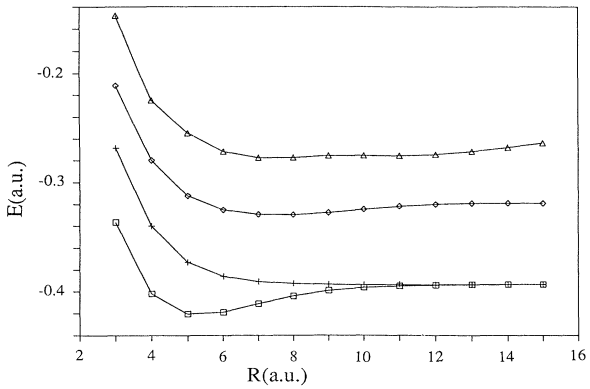

FIG. 3. Energy of the three lowest $^1\Sigma_g$ states and of the lowest $^3\Sigma_u$ state as a function of the internuclear distance R: (□) $^1\Sigma_g$, (+) $^2\Sigma_u$, (◇) $^1\Sigma_g'$, (△) $^1\Sigma_g''$.

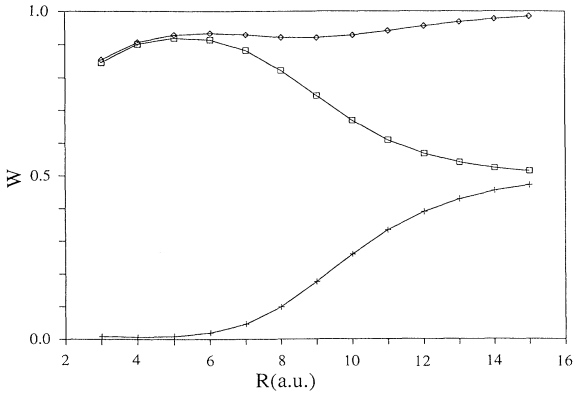

FIG. 4. Weight W of the ground state $^1\Sigma_g$ in three different model spaces as a function of the internuclear separation R: (□) $\langle {}^1\Sigma_g|\sigma_g\bar{\sigma}_g\rangle^2$, (+) $\langle {}^1\Sigma_g|\sigma_u\bar{\sigma}_u\rangle^2$, (◇) $\langle {}^1\Sigma_g|\sigma_g\bar{\sigma}_g\rangle^2 + \langle {}^1\Sigma_g|\sigma_u\bar{\sigma}_u\rangle^2$.

metries.) Notice that, contrary to the previously quoted paper, we did not localize the molecular orbitals, since we wanted to use symmetry in order to simplify the effective Hamiltonian structure. A second reason for avoiding localization is connected with the possibility of a perturbative treatment, since the diagonal of H is usually greater in the canonical SCF basis than in a localized basis. In Fig. 3 we reported the energy curves of the three lowest $^1\Sigma_g$ states and of the lowest $^3\Sigma_u$ state, which is the first excited one, regardless of symmetry.

Suppose we want to obtain an EH that describes the ground molecular state, of $^1\Sigma_g$ symmetry. This state is of almost pure $\sigma_g\bar{\sigma}_g$ character at short and intermediate internuclear distances, while it becomes a mixing of equal parts of $\sigma_g\bar{\sigma}_g$ and $\sigma_u\bar{\sigma}_u$ at very long distances, where both configurations are needed in order to give the correct ground-state dissociation Li(2s)+Li(2s) (see Fig. 4). The model space L_0 must contain then these two configurations. Within this Σ_g space we can construct only $^1\Sigma_g$ type states, so, if we want to keep the constraint $M=N$, we must add to the target space a second state of this symmetry. This is a problematic task, since the two obvious candidates, the first and second excited $^1\Sigma_g$ states, are poorly described by our model space (see Fig. 5). Moreover, while it is the first state which has a dominant weight at short and long distances, it is the other which is more important at intermediate distances. Thus, if we decide to use at each distance the weight on the model space as a criterion of choice, we have problems of discontinuity of the effective Hamiltonian.

It could be countered that perhaps a rotation at short distance within the set of the σ_u molecular orbitals could lead to a better model space, but this solution (besides the drawback that it should necessarily be a distance-dependent rotation) would be by no means a general one: If we would like to have also a Σ_u effective Hamiltonian to describe the first $^3\Sigma_u$ state, we would be obliged to keep the SCF orbitals, since this state has a large component on the $\sigma_g\bar{\sigma}_u$ and $\sigma_u\bar{\sigma}_g$ configurations at any distance (see Fig. 5).

Thus the solution is to build a generalized effective Hamiltonian that describes the $^1\Sigma_g$ ground state, using $\sigma_g\bar{\sigma}_g$ and $\sigma_u\bar{\sigma}_u$ as model space. In Table I we reported, for four different values of the internuclear distance R, the Bloch GEH associated with this $^1\Sigma_g$ state, together

TABLE I. Effective operator of $^1\Sigma_g$ symmetry at different values of the internuclear distance R. The two basis configurations are $\sigma_g\bar{\sigma}_g$ and $\sigma_u\bar{\sigma}_u$. (a) Generalized effective Hamiltonian for the ground state. (b) Pseudometric corresponding to case (a). (c) Bloch effective Hamiltonian for the ground and first excited states. (d) Bloch effective Hamiltonian for the ground and second excited states.

R	(a)		(b)		(c)		(d)	
3.0	−0.333 08	0.033 29	0.990 11	−0.098 95	−0.340 38	−0.039 76	−0.322 83	0.135 85
	0.033 29	−0.003 33	−0.098 95	0.009 89	0.012 92	−0.207 17	0.017 48	−0.161 52
5.0	−0.416 18	0.041 49	0.990 16	−0.098 72	−0.419 72	0.006 06	−0.419 08	0.012 44
	0.041 49	−0.004 14	−0.098 72	0.009 84	0.010 72	−0.312 81	0.016 38	−0.256 08
9.0	−0.322 73	0.156 75	0.809 11	−0.393 00	−0.383 62	0.031 38	−0.381 58	0.035 58
	0.156 75	−0.076 14	−0.393 00	0.190 89	0.027 26	−0.342 74	0.051 52	−0.292 80
15.0	−0.205 14	0.196 35	0.521 87	−0.499 52	−0.355 33	0.039 43	−0.331 30	0.064 54
	0.196 35	−0.187 94	−0.499 52	0.478 13	0.034 74	−0.356 78	0.064 56	−0.325 64

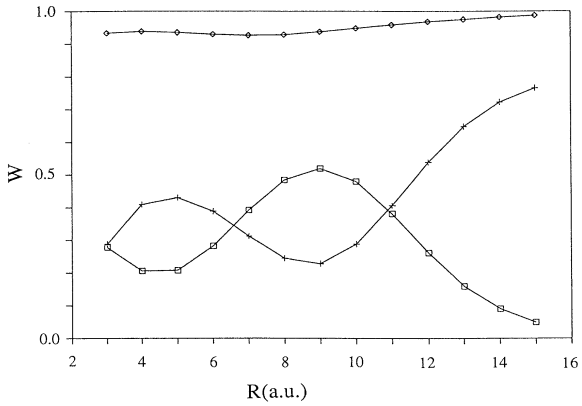

FIG. 5. Weight W of the two lowest excited states $^1\Sigma_g$ and of the lowest $^3\Sigma_u$ on two different model spaces as a function of the internuclear separation R: (+) $\langle {}^1\Sigma_g' | \sigma_g \bar{\sigma}_g \rangle^2 + \langle {}^1\Sigma_g' | \sigma_u \bar{\sigma}_u \rangle^2$, (□) $\langle {}^1\Sigma_g'' | \sigma_g \bar{\sigma}_g \rangle^2 + \langle {}^1\Sigma_g'' | \sigma_u \bar{\sigma}_u \rangle^2$, (◇) $\langle {}^3\Sigma_u | \sigma_g \bar{\sigma}_u \rangle^2 + \langle {}^3\Sigma_u | \sigma_u \bar{\sigma}_g \rangle^2$.

with the corresponding metric. We reported also the standard Bloch effective Hamiltonians including, besides the ground state, the first or the second $^1\Sigma_g$ excited states, respectively. We notice that at short internuclear distance both Bloch effective Hamiltonians are strongly non-Hermitian, a phenomenon related, as we have seen, to the nonorthogonality of the target vectors projected onto the model space.

IV. PERTURBATIVE DEVELOPMENTS

The dimension of the Hamiltonian matrix H is often extremely large, and it is useful therefore to have iterative algorithms able to compute $\tilde{H}$ without solving the complete eigenvalue problem. For this purpose the *wave operator* Ω is introduced, given by

$$\Omega = \sum_{\mu \in M} |\Psi_\mu\rangle \langle \bar{\Psi}_\mu^{\perp\perp}| \ . \tag{16}$$

Ω is a nonorthogonal projector, since $\Omega^2 = \Omega$ but $\Omega^+ \neq \Omega$. It verifies the relations

$$P_0 \Omega = P_M \Omega = P_M \ , \tag{17a}$$

$$\Omega P_0 = \Omega P_M = \Omega \ . \tag{17b}$$

The effective Hamiltonian can be easily computed once Ω is known:

$$\tilde{H} = P_0 H \Omega = P_M H \Omega \ . \tag{18}$$

Moreover, we have the relation

$$H\Omega = \Omega \tilde{H} \tag{19}$$

that is a multidimensional analog of an eigenvector equation, with Ω corresponding to the eigenvector, and $\tilde{H}$ to the eigenvalue. From Eqs. (18) and (19) we obtain the fundamental relation

$$H\Omega = \Omega H \Omega \ , \tag{20}$$

which can be used to compute Ω by means of an iterative expansion. However, it is not the purpose of this article to present a systematic study of the various iterative and perturbative procedures employed to solve Eq. (20) (see, for instance, Ref. 21 for a discussion of the standard case $M = N$); we have simply implemented a straightforward iterative scheme and we want to show that the relaxation of the usual constraint $M = N$ leads to a substantial improvement of the convergence in critical cases.

For this purpose, let us split the total Hamiltonian H into its diagonal and off-diagonal parts (in the basis of the configurations $|\Phi_n\rangle$):

$$H = H_0 + V \ , \tag{21a}$$

where

$$H_0 = \mathrm{diag}(H) \ , \tag{21b}$$

i.e., its elements are given by the scalar products $\langle \Phi_n | H | \Phi_n \rangle$. If we introduce Eq. (21a) into Eq. (20) we obtain

$$\Omega H_0 \Omega - H_0 \Omega = V\Omega - \Omega V \Omega \ .$$

The term $\Omega H_0 \Omega$ can be transformed into

$$\Omega H_0 \Omega = \Omega P_0 H_0 \Omega = \Omega H_0 P_0 \Omega = \Omega H_0 P_M = \Omega H_0 - \Omega H_0 P_I ,$$

so that we can write finally

$$[\Omega, H_0] = V\Omega - \Omega V \Omega + \Omega H_0 P_I \ . \tag{22}$$

By multiplication by P_0 and Q_0 on the left we obtain, respectively,

$$P_I H_0 P_M + P_0 (V\Omega - \Omega V \Omega) = 0 \tag{23a}$$

and

$$-Q_0 [\Omega, H_0] + Q_0 (V\Omega - \Omega V \Omega + \Omega H_0 P_I) = 0 \ . \tag{23b}$$

If we introduce the *Liouvillian superoperator* $[*, H_0]$ (see, for instance, Ref. 22) Eq. (23b) can be rewritten as

$$-Q_0 [*, H_0](\Omega) + Q_0 (V\Omega - \Omega V \Omega + \Omega H_0 P_I) = 0 \ . \tag{23c}$$

(The Liouvillian is also indicated by $\mathcal{L}_{H_0}$. However, we prefer the notation $[*, H_0]$, which we think more transparent. In Appendix C a brief account of the properties of this superoperator is given and the problems connected with the definition of its inverse are also discussed.)

Equation (23c) is suitable for an iterative solution, by isolating the part containing H_0 and linear in the unknown Ω: if we denote by $\Omega^{[n]}$ the approximant to Ω at the nth iteration, we obtain

$$Q_0 \Omega^{[n+1]} = Q_0 [*, H_0]^{-1} (V\Omega^{[n]} - \Omega^{[n]} V \Omega^{[n]} + \Omega^{[n]} H_0 P_I^{[n]}) \ . \tag{24a}$$

Equation (23a) is more difficult to solve, since the part containing H_0 is nonlinear in the *unknown* operator P_M. We are able, however, to obtain an approximant of P_M at every iteration by diagonalizing the correspondent approximated GEH:

$$P_M^{[n+1]}=\sum_{\mu\in M}|\bar{\Psi}_\mu^{[n+1]}\rangle\langle\bar{\Psi}_\mu^{[n+1]}|\ , \tag{24b}$$

where the vectors $|\bar{\Psi}_\mu^{[n+1]}\rangle$ are the eigenvectors of $\tilde{H}^{[n+1]}$, which is given by

$$\tilde{H}^{[n+1]}=P_0H\Omega^{[n]}\ . \tag{25}$$

However, Eq. (18) is not the only possible definition of $\tilde{H}$ since we can add to it any operator defined on L_I on the right without affecting the eigenvectors $|\bar{\Psi}_\mu\rangle$. Therefore we can also choose, for instance, the expression

$$\tilde{H}'=P_0HP_0+P_0HQ_0\Omega=\tilde{H}+P_0HP_I\ . \tag{26}$$

While both Eqs. (18) and (26) have the vectors $|\bar{\Psi}_\mu\rangle$ as eigenvectors, they give different approximations of these vectors during the iterative process, and the second one is more convenient: it gives as approximate EH the expression

$$\tilde{H}^{[n+1]}=P_0HP_0+P_0HQ_0\Omega^{[n]} \tag{27}$$

instead of Eq. (25), and has the advantage of being independent of P_M at each iteration, and is therefore preferable with respect to Eq. (25) since it is more stable during the iterative process. In this case the whole algorithm can be summarized as follows.

(1) Compute a guess $|\bar{\Psi}_\mu^{[0]}\rangle$ by diagonalizing P_0HP_0 (or guess from input).
(2) $\Omega^{[0]}=\sum_{\mu\in M}|\Psi_\mu^{[0]}\rangle\langle\bar{\Psi}_\mu^{[0]\perp\perp}|$.
(3) $\tilde{H}^{[n]}=P_0HP_0+P_0HQ_0\Omega^{[n-1]}$.
(4) Solve the eigenvalue problem $\tilde{H}^{[n]}|\bar{\Psi}_\mu^{[n]}\rangle=E_\mu^{[n]}|\bar{\Psi}_\mu^{[n]}\rangle$, $\mu\in N$.
(5) Select the M vectors $|\bar{\Psi}_\mu^{[n]}\rangle$ which are more similar to the guess $|\bar{\Psi}_\mu^{[0]}\rangle$.
(6) $P_M^{[n]}=\sum_{\mu\in M}|\bar{\Psi}_\mu^{[n]}\rangle\langle\bar{\Psi}_\mu^{[n]_{\perp\perp}}|$.
(7) $X^{[n]}=Q_0X^{[n]}P_0$

$$=Q_0[*,H_0]^{-1}(V\Omega^{[n-1]}-\Omega^{[n-1]}V\Omega^{[n-1]}+\Omega^{[n-1]}H_0P_I^{[n-1]}).$$

(8) $Q_0\Omega^{[n]}=Q_0X^{[n]}P_M^{[n]}$.
(9) Go to (3).

Notice that step (8) has been introduced since we want Ω to remain a projector at each iteration.

A classical convergence test of the various perturbative or iterative schemes is given by the solution of the Mathieu equation.[23] This equation can be written as

$$-\left[\frac{d^2}{d\theta^2}+s\cos^2\theta\right]\psi(\theta)=E\psi(\theta) \tag{28}$$

and we seek the periodical solutions of period 2π. If we introduce the basis set

$$\phi_0^+=(2\pi)^{-1/2}\ , \tag{29a}$$

$$\phi_n^+=\pi^{-1/2}\cos(n\theta),\quad n=1,2,\ldots \tag{29b}$$

$$\phi_n^-=\pi^{-1/2}\sin(n\theta),\quad n=1,2,\ldots \tag{29c}$$

Eq. (28) becomes an eigenvalue equation (with infinite matrix). The functions $\phi_{2n}^+,\phi_{2n+1}^+,\phi_{2n+1}^-,\phi_{2n+2}^-$, $n=0,1,2,\ldots$, form four uncoupled subspaces, and we can then solve Eq. (28) separately in each subspace. Considering the kinetic part as the unperturbed Hamiltonian and the potential as the perturbation, the matrix elements of H_0 and V relative to the first subspace are (we make the substitution $\phi_{2n}^+\rightarrow|n\rangle$, $n=0,1,2,\ldots$)

$$\langle n|H_0|n\rangle=E_0^{(n)}=4n^2 \tag{30}$$

and

$$\langle n|V|n\rangle=s\ , \tag{31a}$$

$$\langle 0|V|1\rangle=\langle 1|V|0\rangle=\frac{s}{\sqrt{8}}\ , \tag{31b}$$

$$\langle n|V|n+1\rangle=\langle n+1|V|n\rangle=\frac{s}{4}\ . \tag{31c}$$

We have applied the proposed iterative scheme to this Hamiltonian, for different values of the parameter s (chosen equal to 2.0, 4.0, 8.0, and 16.0), and the results at different orders of iteration are reported in Table II. We report for comparison the results given by Bloch[1] and by Gadea,[24] when available, i.e., for $s=2.0$ and 4.0. In fact, the two values $s=8.0$ and 16.0 are beyond the radius of convergence of these expansions, as well as the method here proposed if $N=1$. But enlarging the dimension of L_0, we see that convergence is achieved, and it becomes much faster with the growth of N. We notice also that, for $s=2.0$ and 4.0 the method proposed by Gadea is better than ours with $N=1$, as is expected, since at the nth iteration the former involves contribution up to $2n-1$ V terms instead of n V terms. It should be possible to use this technique in connection with the GEH formalism, in order to join the advantages of the two methods.

V. CONCLUSIONS

We have shown that in the presence of intruder states it can be convenient to leave the constraint $M=N$ in effective Hamiltonian theory, and to introduce a generalized effective Hamiltonian together with the corresponding pseudometric. This approach can be compared to the recently proposed intermediate Hamiltonian formalism,[14] and its generalizations.[15] In one case we have an EH with a number of eigenvalues smaller than its dimension, in the other case the EH has only a certain number of exact eigenvalues, while the others are only approximated. (In a certain sense, a GEH can be seen as a particular case of IEH, where the N-M approximated eigenvalues are all set equal to zero.)

The advantages of the formalism here proposed consist essentially of two main facts.

(a) The IEH is defined starting from an ordinary EH with a model space isomorphic with its main target space (the space of states of H which are exactly reproduced by the IEH), so we can have the same problems of choice of the model space, as in the standard theory. (But it is possible to define an IEH starting from a GEH, and preliminary results show that this choice gives better results than the usual one.)

(b) The IEH can depend strongly on the partition of H into H_0 and V (and this even at infinite order in the perturbative expansion) and this introduces a nonuniqueness of the whole formalism that can be rather disturbing.

On the other side, in the GEH any information about the so-called intermediate spectrum (the N-M approximated eigenvalues of H in the IEH theory) is lost, and this fact can pose problems if we want to transfer the matrix elements obtained in simple cases to larger systems, since we do not use part of the information that could be

TABLE II. Approximated values of the ground-state eigenvalue of the Mathieu equation for different values of the parameter s. We reported the results for different dimensions of the model space, as specified at the top of each column. When available, we reported also the corresponding results obtained with the methods of Bloch (Ref. 1), indicated by (B), and Gadea (Ref. 24), indicated by (G). We indicate by the ellipses the iteration from which all the following ones are equal to the exact value (up to the considered precision). (a) $s=2.0$, $E=0.878\,234$; (b) $s=4.0$, $E=1.544\,861$; (c) $s=8.0$, $E=2.486\,043$; (d) $s=16.0$, $E=3.719\,481$.

(a)	$N=1$	$N=2$	(B)	(G)
1	1.000 000	0.878 680	1.000 000	1.000 000
2	0.875 000	0.878 229	0.875 000	0.878 788
3	0.878 906	0.878 236	0.875 000	0.878 318
4	0.878 178	0.878 234	0.878 418	0.878 235
5	0.878 241	⋮	0.878 418	
6	0.878 234		0.878 221	
7	0.878 235		0.878 221	
8	0.878 234		0.878 235	
	⋮			
(b)	$N=1$	$N=2$	(B)	(G)
1	2.000 000	1.550 510	2.000 000	2.000 000
2	1.500 000	1.544 600	1.500 000	1.555 5
3	1.562 500	1.544 953	1.500 000	1.548 8
4	1.540 039	1.544 852	1.554 7	1.545 2
5	1.546 269	1.544 863	1.554 7	
6	1.544 458	1.544 861	1.542 1	
7	1.544 978	⋮	1.542 1	
8	1.544 827		1.545 7	
9	1.544 871		1.545 7	
10	1.544 859			
(c)	$N=1$	$N=2$	$N=3$	$N=4$
1	4.000 000	2.535 898	2.486 354	2.486 044
2	2.000 000	2.479 346	2.486 023	2.486 043
3	3.000 000	2.488 970	2.486 047	⋮
4	2.125 000	2.485 261	2.486 043	
5	2.824 219	2.486 292	⋮	
6	2.233 969	2.485 969		
7	2.714 100	2.486 066		
8	2.309 484	2.486 036		
9	2.642 024	2.486 045		
10	2.362 313	2.486 042		
(d)	$N=1$	$N=2$	$N=3$	$N=4$
1	8.000 000	4.000 000	3.725 169	3.719 515
2	0.000 000	3.629 630	3.718 621	3.719 478
3	16.000 000	3.780 712	3.719 809	3.719 482
4	14.000 000	3.684 128	3.719 391	3.719 481
5	10.000 000	3.740 783	3.719 509	⋮
6	2.819 444	3.706 750	3.719 473	
7	7.455 488	3.727 116	3.719 484	
8	−1.411 359	3.714 908	3.719 480	
9	22.071 319	3.722 222	3.719 481	
10	47.148 954	3.717 839	⋮	

embedded in the EH. In any case the behavior with respect to transferability of all these different possible extensions of EH is still to be investigated.

Also to be investigated is the behavior of a GEH with respect to the problem of size consistency: while the Bloch perturbative approach can be shown to be size consistent (at least with a suitable choice of H_0 and by keeping separate the different orders in the expansion of Ω), we can suspect that the diagonalization of the approximate generalized effective Hamiltonian during the iterative process destroys this important property. At the moment it is not clear whether it is possible to implement an efficient iterative process able to conserve size consistency at any order.

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APPENDIX A

In this appendix we want to establish the most general form that can be assumed by a generalized effective Hamiltonian, and to see how this is connected to the Bloch particular formalism. Before starting, we need to establish some simple properties of the biorthonormal system that follow directly from its definition, and that we give without demonstration. Suppose $|Y_\mu\rangle$ are any set of linearly independent vectors in L_0, spanning an M-dimensional subspace L; we indicate by P the orthogonal projector onto L. Let A be an operator defined in L and invertible therein. [Since A is defined only on L, we indicate by A^{-1} the generalized inverse of A, i.e., the operator $P(\alpha\bar{P}+PAP)^{-1}P$, where $\bar{P}$ is the complement of P in L_0: $\bar{P}=P_0-P$, and α is any nonzero real number. We notice that with such a definition A^{-1} does not depend on α.] Then the following relations hold:

$$P=\sum_{\mu\in M}|Y_\mu\rangle\langle Y_\mu^{\perp\perp}| \ , \tag{A1a}$$

$$|AY_\mu\rangle^{\perp\perp}=A^{-1+}|Y_\mu^{\perp\perp}\rangle \ , \tag{A1b}$$

$$A|Y_\mu\rangle=a_\mu|Y_\mu\rangle \Longleftrightarrow \langle Y_\mu^{\perp\perp}|A=\langle Y_\mu^{\perp\perp}|a_\mu \ . \tag{A1c}$$

(We indicate by $|AY_\mu\rangle^{\perp\perp}$ the biorthogonal of $A|Y_\mu\rangle$ in the subspace L.)

We are able now to introduce the formalism of generalized effective Hamiltonians: we call a generalized effective Hamiltonian any operator $\tilde{H}$ defined on the model space for which the generalized eigenvalue problem (with respect to a metric $\tilde{K}$) gives as generalized eigenvalues the eigenvalues of the target space. (We recall that, in the general case $M<N$, strictly speaking $\tilde{K}$ is only a pseudometric, i.e., a non-negative Hermitian matrix that has also N-M zero eigenvalues.) More precisely, let $\tilde{H}$ be an operator defined on the model space L_0, and let $\{E_\mu,\mu\in M\}$ be a set of eigenvalues of the full Hamiltonian H. We say $\tilde{H}$ is a generalized effective Hamiltonian with respect to the Hermitian pseudometric $\tilde{K}$ if there exist vectors $|\Xi_\mu\rangle$ that verify the generalized eigenvector equation

$$(\tilde{H}-E_\mu\tilde{K})|\Xi_\mu\rangle=0 \ . \tag{A2a}$$

This implies the existence of vectors $|\Sigma_\mu\rangle$ such that

$$\langle\Sigma_\mu^{\perp\perp}|(\tilde{H}-E_\mu\tilde{K})=0 \ , \tag{A2b}$$

where the relation between the vectors $|\Xi_\mu\rangle$ and $|\Sigma_\mu\rangle$ will be now elucidated.

We indicate now by L the range of $\tilde{K}$, and by P the orthogonal projector onto L; L will be obviously of dimension M, if all the E_μ are nonzero. Since $\tilde{K}$ is Hermitian, it can be expressed as $\tilde{K}=P\tilde{K}P$. Moreover, $\tilde{K}$ is invertible on L. From Eqs. (A2) we see that also $\tilde{H}$ is restricted to the subspace L: $\tilde{H}=P\tilde{H}P$, so it is not restrictive to work in this subspace. Eqs. (A2) imply

$$(\tilde{K}^{-1/2}\tilde{H}\tilde{K}^{-1/2}-E_\mu)\tilde{K}^{1/2}|\Xi_\mu\rangle=0 \ , \tag{A3a}$$

$$\langle\Sigma_\mu^{\perp\perp}|\tilde{K}^{1/2}(\tilde{K}^{-1/2}\tilde{H}\tilde{K}^{-1/2}-E_\mu)=0 \ . \tag{A3b}$$

Thus, from Eq. (A1c), the vectors $|\tilde{K}^{1/2}\Xi_\mu\rangle$ are the biorthonormals (in L) of the vectors $|\tilde{K}^{1/2}\Sigma_\mu^{\perp\perp}\rangle$:

$$|\tilde{K}^{1/2}\Xi_\mu\rangle=|\tilde{K}^{1/2}\Sigma_\mu^{\perp\perp}\rangle^{\perp\perp}=\tilde{K}^{-1/2}|\Sigma_\mu\rangle \ , \tag{A4}$$

where we made use of Eq. (A1b) in order to obtain the second equality. We come then to the conclusion that

$$|\Sigma_\mu\rangle=\tilde{K}|\Xi_\mu\rangle \ , \tag{A5}$$

which shows the relation between the right and left eigenvectors of $\tilde{H}$ with metric $\tilde{K}$.

The projector P can be written as [see Eq. (A1a)]:

$$P=\sum_{\mu\in M}|\tilde{K}^{-1/2}\Sigma_\mu\rangle\langle\Sigma_\mu\tilde{K}^{-1/2}|^{\perp\perp} \ . \tag{A6}$$

Using Eq. (A4) we obtain

$$P=\sum_{\mu\in M}|\tilde{K}^{-1/2}\Sigma_\mu\rangle\langle\Xi_\mu\tilde{K}^{1/2}|^{\perp\perp} \ , \tag{A7}$$

which in turn gives

$$\tilde{K}=|\Sigma_\mu\rangle\langle\Xi_\mu^{\perp\perp}| \ . \tag{A8}$$

We can express also $\tilde{H}$ in a similar way: from Eq. (A3a) we obtain

$$\tilde{K}^{-1/2}\tilde{H}\tilde{K}^{-1/2}=\sum_{\mu\in M}|\tilde{K}^{1/2}\Xi_\mu\rangle E_\mu\langle\tilde{K}^{1/2}\Xi_\mu|^{\perp\perp} \ , \tag{A9}$$

from which

$$\tilde{H}=\sum_{\mu\in M}|\Sigma_\mu\rangle E_\mu\langle\Xi_\mu^{\perp\perp}| \ . \tag{A10}$$

But the converse is also true: given any operator U that transforms the projected eigenvectors $|\bar{\Psi}_\mu\rangle$ into a new set $|\tilde{\Psi}_\mu\rangle$ and any pseudometric $\tilde{K}$ defined on L we pose

$$|\Xi_\mu\rangle=\tilde{K}^{-1/2}|\tilde{\Psi}_\mu\rangle \tag{A11a}$$

and

$$|\Sigma_\mu\rangle = \tilde{K}^{1/2}|\tilde{\Psi}_\mu\rangle \ . \tag{A11b}$$

We *define* now the effective Hamiltonian as in Eq. (A10), and it is easy to verify that it satisfies Eqs. (A2). (Strictly speaking the operator U must be such that the $|\tilde{\Psi}_\mu\rangle$ are linearly independent.)

This gives a complete characterization of generalized effective Hamiltonians as defined by Eqs. (A2): given $\tilde{K}$ and U (only the *PUP* part of U need be considered) we can express the GEH as

$$\tilde{H} = \tilde{K}^{1/2} U \tilde{H}_{\text{Bloch}} U^{-1} \tilde{K}^{1/2} \ , \tag{A12a}$$

and the metric as

$$\tilde{K} = \tilde{K}^{1/2} U \tilde{K}_{\text{Bloch}} U^{-1} \tilde{K}^{1/2} \ . \tag{A12b}$$

APPENDIX B

Most of the effected Hamiltonians presented in the literature can be derived from the formalism presented in Appendix A by putting $M = N$ (hence $P_M = P_0$) and

$$\tilde{K} = S^k \tag{B1a}$$

and

$$U = S^u \ , \tag{B1b}$$

where k and u are real parameters. Let us examine some values of these parameters that lead to important forms of EH.

(a) $k = 0$, $u = 0$, Bloch.[1] We obtain

$$\tilde{H}_{\text{Bloch}} = \sum_{\mu \in M} |\overline{\Psi}_\mu\rangle E_\mu \langle \overline{\Psi}_\mu^{\perp\perp}| \ . \tag{B2}$$

(b) $k = 0$, $u = -\frac{1}{2}$, des Cloizeaux,[2] Van Vleck.[25] We obtain

$$\begin{aligned} \tilde{H}_{\text{des Cloizeaux}} &= S^{-1/2} H_{\text{Bloch}} S^{1/2} \\ &= \sum_{\mu \in M} |\overline{\Psi}_\mu^{\perp}\rangle E_\mu \langle \overline{\Psi}_\mu^{\perp}| \ . \end{aligned} \tag{B3}$$

(c) $k = 0$, $u = 1$, Ôkubo.[11] We obtain

$$\tilde{H}_{\hat{\text{O}}\text{kubo}} = S^{-1} \tilde{H}_{\text{Bloch}} S = \sum_{\mu \in M} |\overline{\Psi}_\mu^{\perp\perp}\rangle E_\mu \langle \overline{\Psi}_\mu| \ . \tag{B4}$$

(d) $k = 1$, $u = 0$, Kato.[26] We obtain

$$\tilde{H}_{\text{Kato}} = S \tilde{H}_{\text{Bloch}} = \sum_{\mu \in M} |\overline{\Psi}_\mu\rangle E_\mu \langle \overline{\Psi}_\mu| \ . \tag{B5}$$

In cases (a)–(c) we have $\tilde{K} = P_0$, and this is the most common choice. This is not the case, however, for the EH proposed by Kato, which has the particularity of being Hermitian and that its eigenvectors are the projections onto the model space of the exact eigenvalue of H (but we need a metric different from the identity). This formalism is also useful if we want to analyze the various Hermitian effective Hamiltonians different from the standard des Cloizeaux form (see, for instance, Ref. 27): if U is the matrix of any transformation that orthogonalizes the $|\overline{\Psi}_\mu\rangle$, then the EH which is generated is Hermitian, regardless of the choice of $\tilde{K}$.

APPENDIX C

We recall here a few properties of the Liouvillian superoperator and of its inverse. A more complete discussion can be found in Ref. 22. A linear *superoperator* is a linear operator function that acts on normal operators (matrices) in the same way that a normal operator acts on vectors. It can be defined in an abstract way, or by giving its components on a basis of operators. For this we need a scalar product in the linear space of operators, which is given by

$$\langle A|B\rangle \equiv \text{Tr}(A^+ B) \ . \tag{C1}$$

Usually as the operator basis we choose the elementary operators

$$P_{ij} = |\Phi_i\rangle\langle\Phi_j| \ , \tag{C2}$$

which are sometimes called shift operators since they transform $|\Phi_j\rangle$ into $|\Phi_i\rangle$.

If A is any fixed linear operator defined on the linear space L, we define the *Liouvillian superoperator* associated with A as the (linear) superoperator $\mathcal{L}_A$ which transforms any operator X into its commutator with A:

$$\mathcal{L}_A(X) \equiv [X, A] \ . \tag{C3a}$$

With a less compact but more transparent notation, the Liouvillian will be also indicated by the expression $[*, A]$ [and this is the notation employed in Eqs. (23) and (24)]:

$$[*, A](X) \equiv [X, A] \ . \tag{C3b}$$

Let us compute now the components of the Liouvillian on the basis of elementary operators. It is convenient to choose A to be diagonal (if it is not, we can always transform the vector basis so that it is), since in this case the Liouvillian is also diagonal in the operator basis P_{ij}. Its components are

$$(\mathcal{L}_A)_{ij,ij} \equiv \langle P_{ij}|\mathcal{L}_A|P_{ij}\rangle = A_{jj} - A_{ii} \ . \tag{C4}$$

From this it appears evident that $\mathcal{L}_A$ is a *singular* operator, with a zero eigenvalue associated with every P_{ij} which has A_{ii} equal to A_{jj} (and hence at least $\mathcal{L}_A$ has a zero eigenvalue associated with every P_{ii}). So strictly speaking the Liouvillian is not invertible, but we can compute a *generalized inverse* by restricting both B and X to the orthogonal complement of the null space of $\mathcal{L}_A$ (in an analogous way to what has been done in Appendix A for singular operators). In this case the equation

$$\mathcal{L}_A(X) = B \tag{C5}$$

admits a unique solution that will be indicated as

$$X = \mathcal{L}_A^{-1}(B) \ . \tag{C6}$$

In particular, if A is diagonal Eq. (C5) has components

$$X_{ij}=\frac{B_{ij}}{A_{jj}-A_{ii}} \ . \tag{C7}$$

As a final remark, we notice that neither $\mathcal{L}_A$ nor $\mathcal{L}_A^{-1}$ are multiplicative superoperators, i.e., there does not exist in general a linear operator $\tilde{A}$ such that

$$\mathcal{L}_A(X)=\tilde{A}X \tag{C8a}$$

or

$$\mathcal{L}_A^{-1}(X)=\tilde{A}X \ . \tag{C8b}$$

This implies that, in general,

$$\mathcal{L}_A(X)Y\neq\mathcal{L}_A(XY) \tag{C9a}$$

and

$$\mathcal{L}_A^{-1}(X)Y\neq\mathcal{L}_A^{-1}(XY) \tag{C9b}$$

and this is the reason why we must indicate explicitly with brackets on which operator $\mathcal{L}_A$ acts.

Let us consider now, in particular, Eq. (24a): in this case $A=H_0$ is diagonal and the equation has the form

$$\mathcal{L}_{H_0}(Q_0\Omega P_0)=B \ , \tag{C10a}$$

where B is given by

$$B=Q_0(V\Omega-\Omega V\Omega+\Omega H_0P_I) \tag{C10b}$$

(so $B=Q_0BP_0$ and, if the outer space is not degenerated with the model space, B belongs to the orthogonal complement to the null space of $\mathcal{L}_A$). In this case the solution of Eq. (C10a) is given by

$$Q_0\Omega P_0=Q_0\mathcal{L}_{H_0}^{-1}(B) \tag{C11a}$$

or, in components,

$$(Q_0\Omega P_0)_{ij}=\frac{B_{ij}}{(H_0)_{jj}-(H_0)_{ii}} \ . \tag{C11b}$$

We notice that since the inverse of the Liouvillian is not a multiplicative operator, by multiplying Eq. (C11a) on the right by P_M (this can always be done since $\Omega P_0P_M=\Omega P_M=\Omega$) we do not eliminate the term ΩH_0P_I, contained in B.

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