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General theory of effective Hamiltonians

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All effective Hamiltonians fulfilling three very general conditions are derived. It is shown that they all stem both from a transformation operator implicitly defined by a nonlinear equation, and an arbitrary "diagonal" and nonsingular operator. The canonical case is discussed, as well as the particular restrictions that lead to the previous schemes of Bloch, des Cloizeaux, and Jørgensen.

I. INTRODUCTION

No one can deny the fundamental role played by effective Hamiltonians in the quantum theory of matter. To name some of the more important cases: Nuclear shell, atomic shell, Foldy-Wouthuysen, Born-Oppenheimer, crystal and ligand field, Pariser-Parr-Pople, Bardeen-Cooper-Schrieffer, Hubbard, Anderson, Heisenberg, Ising as well as all other spin Hamiltonians used in the theory of magnetism, are nothing but examples of suitably defined effective Hamiltonians.

Mathematical (symmetry) or physical arguments are often used in order to reduce the number of terms appearing in model Hamiltonians, so that comparison with experiments may be possible. But in the end a full understanding of the problem requires tracing back the origin of each term in the model Hamiltonian by assimilating it with a well-defined effective Hamiltonian, difficult as this last step may be.

Several reviews have been made of the subject[1,2,3] wherein abundant references may be found, but somehow the problem does not seem to have been studied in its full generality. In a previous work[4] it was discussed how one may derive all effective Hamiltonians H_s which satisfy three very general conditions [see Eqs. (6)–(8) below]. It was shown there that H_S is not uniquely determined due to the arbitrariness in the election of a diagonal [in the sense of Eq. (16)] and nonsingular operator $\langle S\rangle$. In what follows we discuss how to solve in detail the different cases as well as the connections with the more usual schemes and, in a superficial way, with perturbation theory. It turns out that there are two cases from which all others may be derived: the unit-diagonal case, which turns out to be the generalization of Bloch's approach,[5] and the canonical-symmetric case which is the generalization of des Cloizeaux's[6] and Soliverez's[7] approach. All other effective Hamiltonians may be related to some of these two cases.

II. THE GENERAL EQUATIONS

We consider the discrete eigenvalue problem

$$H|\alpha\rangle = E_\alpha|\alpha\rangle, \quad \langle\alpha|\beta\rangle = \delta_{\alpha\beta} \quad (\alpha,\beta = 1,2,\ldots,n), \tag{1}$$

of a given Hermitian Hamiltonian H, within the vectorial space Ω spanned by a finite subset of eigenvectors of a soluble part H_0. That is, if

$$H = H_0 + V, \tag{2}$$

$$H_0|\alpha\rangle_0 = e_\alpha|\alpha\rangle_0, \quad {}_0\langle\alpha|\beta\rangle_0 = \delta_{\alpha\beta}, \tag{3}$$

where the eigenvalues e_α and the eigenvectors $|\alpha\rangle_0$ are known, then Ω is spanned by the subset $\{|\alpha\rangle_0\}$, where $\alpha = 1,2,\ldots,n$.

The spectral decomposition of H_0 is

$$H_0 = \sum_e eP_e, \tag{4}$$

where P_e is the projector over the manifold Ω_e spanned by the eigenvectors $|\alpha\rangle_0 = |e,j\rangle$ $(j = 1,2,\ldots,g_e)$ with g_e-degenerate eigenvalue e. That is,

$$P_e = \sum_j |e,j\rangle\langle e,j|, \quad P_eP_{e'} = \delta_{ee'}P_e. \tag{5}$$

The advantage of using projectors is that the formulation is then independent of the specific election of the degenerate subset $\{|e,j\rangle\}$, thus making the bookkeeping easier and the notation simpler.

Experience shows that a judicious choice for the effective Hamiltonians H_S associated both with H and H_0 fulfills the following conditions.

(a) H and H_S have the same set of eigenvalues, that is, if

$$H|\alpha\rangle = E_\alpha|\alpha\rangle,$$

then

$$H_S|\alpha\rangle_S = E_\alpha|\alpha\rangle_S. \tag{6}$$

(b) There is a one-to-one correspondence between the eigenvectors of H and H_S,

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$$|\alpha\rangle = S|\alpha\rangle_S, \quad |\alpha\rangle_S = S^{-1}|\alpha\rangle , \tag{7}$$

where S is the nonsingular transformation operator called by some authors the wave operator.

(c) H_S has no matrix elements connecting eigenvectors belonging to different eigenvalues of H_0,

$$P_e H_S P_{e'} = \delta_{ee'} P_e H_S P_e . \tag{8}$$

As there are in the literature several examples of non-Hermitian effective Hamiltonians,[5,1] S is not necessarily unitary. It is sometimes convenient, though not required in our treatment, to impose the adiabatic condition

$$\lim_{V \to 0} H_S = H . \tag{9}$$

It should be noticed that, because of condition (c), each $|\alpha\rangle_S$ belongs to a single manifold Ω_e. Therefore the eigenvalue problem of H_S can be solved separately within each manifold Ω_e. The eigenvectors $|\alpha\rangle_S$ are the effective eigenvectors or good zeroth-order eigenvectors, and are not necessarily orthogonal unless H_S is Hermitian. The remainder V in Eq. (2) is not required to be small except when one takes a perturbative approach. The latter is not always the case because sometimes either one can find an exact solution, or one wishes to generate effective Hamiltonians with disposable parameters to be adjusted from experiment. The latter is, for instance, the case of the spin Hamiltonians used in the theory of magnetism, the former being unfortunately a very rare event.

From Eqs. (6) and (7) it follows that if $\{|\alpha\rangle_S\}$ is a complete set of basis vectors, then

$$H_S = S^{-1} H S . \tag{10}$$

There is an infinite number of effective Hamiltonians that satisfy Eqs. (6) and (7). Assume that

$$S = AB , \tag{11}$$

where A and B are nonsingular operators. From Eqs. (6), (7), (10), and (11) it then follows that

$$H_A = A^{-1} H A = B H_S B^{-1}, \quad B|\alpha\rangle_S = |\alpha\rangle_A , \tag{12}$$

$$H_A |\alpha\rangle_A = E_\alpha |\alpha\rangle_A, \quad |\alpha\rangle = A|\alpha\rangle_A , \tag{13}$$

thus showing that H_A is as good an effective Hamiltonian as H_S. One of our goals is to fully characterize the family of transformation operators that fulfill the given conditions.

It turns out that it is convenient to write

$$H_S = H_0 + W_S . \tag{14}$$

The operator W_S is often called the level-shift operator because

$$W_S |\alpha\rangle_S = (E_\alpha - e_\alpha)|\alpha\rangle_S = \Delta E_\alpha |\alpha\rangle_S , \tag{15}$$

as it is easily seen from Eqs. (6), (14), and (3).

It is now convenient to define the diagonal part $\langle A\rangle$ of an operator A with respect to H_0 by[8,9]

$$\langle A\rangle = \sum_e P_e A P_e . \tag{16}$$

Then A is said to be diagonal if $A = \langle A\rangle$. It follows from Eqs. (4), (8), and (14) that H_0, H_S, and W_S are diagonal:

$$H_0 = \langle H_0\rangle, \quad H_S = \langle H_S\rangle, \quad W_S = \langle W_S\rangle . \tag{17}$$

Upon multiplication with S by the left, and taking due account of Eqs. (14) and (2), Eq. (10) becomes

$$[H_0, S] = S W_S - V S . \tag{18}$$

We now have to solve Eq. (18) for S and W_S. It should first be noticed that no information is contained there about $\langle S\rangle$. This comes about, because for an arbitrary operator A, it always happens that

$$[H_0, \langle A\rangle] = 0 . \tag{19}$$

On the other hand, it may be easily verified that the nondiagonal part $A - \langle A\rangle$ is fully determined from $[H_0, A]$, being given by[8]

$$A = \langle A\rangle + h_0([H_0, A]) , \tag{20}$$

where h_0 is the superoperator

$$h_0(A) = \sum_{e \neq e'} \sum \frac{P_e A P_{e'}}{e - e'} . \tag{21}$$

Equation (20) is the generalization to operators of the well-known vector identity

$$\vec{a} = \vec{h}(\vec{h} \cdot \vec{a}) - \vec{h} \times (\vec{h} \times \vec{a}) ,$$

where $\vec{h}$ is an arbitrary unit vector. The operator H_0 plays the role of $\vec{h}$, and the superoperators $\langle\,\rangle$, $[H_0, \,]$ and h_0 play the role of the dyadic operators $\vec{h}\vec{h}$, $\vec{h}\times$, $\vec{h}\times$. From this analogy it seems reasonable to call $h_0([H_0, A])$ the normal part of A (with respect to H_0). From Eqs. (18) and (20) it follows that

$$S = \langle S\rangle + h_0(S W_S - V S) . \tag{22}$$

Taking the diagonal part in Eq. (18) we obtain for the level-shift operator the condition

$$\langle S\rangle W_S = \langle V S\rangle , \tag{23}$$

where use has been made of Eq. (19) and of the properties,

$$\langle A\langle B\rangle\rangle = \langle A\rangle\langle B\rangle, \quad H_0\langle A\rangle = \langle A\rangle H_0 . \tag{24}$$

Equations (22) and (23) implicitly define S as a function of H_0, V, and $\langle S\rangle$. The indetermination in the election of S discussed in connection with Eqs. (11)—(13) is now seen to reduce to the in-

determination in the election of $\langle S\rangle$. From Eq. (23) it is evident that W_S is not fully defined if $\langle S\rangle$ is singular. Therefore it is necessary that $\langle S\rangle^{-1}$ exists, and Eq. (23) then gives

$$W_S = \langle S\rangle^{-1}\langle VS\rangle . \tag{25}$$

The operator $\langle S\rangle$ has a very simple physical meaning that we now discuss. If $|\alpha\rangle_S$ is an effective eigenvector belonging to Ω_e, from Eqs. (7) and (16) it may be shown that

$$P_e|\alpha\rangle = \langle S\rangle|\alpha\rangle_S . \tag{26}$$

From its nonsingular character it is thus seen that $\langle S\rangle$ connects in a one-to-one correspondence the eigenvectors of H_S with the projections of the eigenvectors of H.

If R is the particular transformation operator such that

$$\langle R\rangle = 1 , \tag{27}$$

it is seen from Eq. (26) that

$$|\alpha\rangle_R = P_e|\alpha\rangle , \quad |\alpha\rangle_S = \langle S\rangle^{-1}|\alpha\rangle_R . \tag{28}$$

From Eqs. (7), (13), (28), and (11) we obtain

$$S = R\langle S\rangle , \tag{29}$$

while from Eqs. (12), (14), and (24)

$$W_S = \langle S\rangle^{-1} W_R \langle S\rangle . \tag{30}$$

The problem is thus reduced to the study of the unit-diagonal operator R, and its corresponding level-shift operator W_R. From them one may obtain all the operators S and W_S through the use of Eqs. (29) and (30), by making an up to now arbitrary choice of the nonsingular operator $\langle S\rangle$. Equation (29) shows that all transformation operators have the remarkable property that $S\langle S\rangle^{-1}$ is independent of S (see the discussion below).

III. THE UNIT-DIAGONAL CASE

We will now discuss the determination of R and W_R. From Eqs. (22), (27), and (23) one easily obtains

$$R = 1 + h_0(R\langle VR\rangle - VR) , \tag{31}$$

$$W_R = \langle VR\rangle . \tag{32}$$

Equation (31) determines R as an implicit function of H_0 and V. The projected version of this equation was first found by Bloch[5] using an approach completely different from our own. His operators $\mathfrak{U}$ and $\mathcal{A}$ correspond to our RP_e and $W_R P_e$, respectively.

In a few cases, it is possible to solve R explicitly,[7] but more often a perturbative approach is used. In the last case one makes successive replacements of the second member Eq. (31) into the argument of h_0, and collects terms of the same degree in an order parameter λ. It is then seen that writing H_R to order λ^m is equivalent to eliminating to that order the nondiagonal part of V in Eq. (10). It was from such a point of view that Van Vleck[10-12] first introduced the idea of an effective Hamiltonian.

The problem of the class of remainders V such that Eq. (31) defines a nonsingular operator R (or a linearly independent set of eigenvectors $|\alpha\rangle_R$) is to our knowledge still unsolved. In what follows we shall always assume the existence of R^{-1}.

From Eq. (32) it is easily seen that W_R is not Hermitian. Therefore its eigenvectors $|\alpha\rangle_R$,

$$W_R|\alpha\rangle_R = \Delta E_\alpha |\alpha\rangle_R , \tag{33}$$

are not orthogonal and, as may be seen from Eq. (28), not even normalized. It then follows that, in general,

$${}_R\langle\alpha|\beta\rangle_R = (\underline{g}_R)_{\alpha\beta} , \tag{34}$$

where $\underline{g}_R$ is the metric matrix of the basis set $\{|\alpha\rangle_R\}$. The eigenvalue equation (33) determines $|\alpha\rangle_R$ up to an as yet indeterminate coefficient c_α. In order to fix its value we have to use the orthonormality of the eigenvectors $|\alpha\rangle$, that is,

$$|\alpha\rangle = R|\alpha\rangle_R , \quad \langle\alpha|\beta\rangle = {}_R\langle\alpha|R^\dagger R|\beta\rangle_R = \delta_{\alpha\beta} . \tag{35}$$

This indirect method can be made explicit in the following fashion. From the eigenvalue equation for W_R we first determine a set $\{|\alpha\rangle_i\}$ of initial eigenvectors where we make some arbitrary but explicit choice of normalization, the metric matrix $\underline{g}_i$ being given by

$$(\underline{g}_i)_{\alpha\beta} = {}_i\langle\alpha|\beta\rangle_i . \tag{36}$$

The eigenvector $|\alpha\rangle_R$ is then related to $|\alpha\rangle_i$ by

$$|\alpha\rangle_R = c_\alpha |\alpha\rangle_i , \tag{37}$$

where all c_α may be taken to be real and positive. In order to make use of Eq. (35) it is convenient to use the matrix representation of R in the basis $\{|\alpha\rangle_i\}$,

$$(\underline{R}_i)_{\alpha\beta} = {}_i\langle\alpha|R|\beta\rangle_i , \tag{38}$$

and also to define the matrix $\underline{C}$ with elements

$$C_{\alpha\beta} = \delta_{\alpha\beta} c_\alpha , \quad \underline{C}^\dagger = \underline{C} . \tag{39}$$

As may be easily verified, the unit operator can be written as

$$1 = \sum_{\alpha'}\sum_{\beta'} |\alpha'\rangle_i (\underline{g}_i)^{-1}_{\alpha'\beta'} {}_i\langle\beta'| . \tag{40}$$

Inserting (40) into Eq. (35) and using Eqs. (37) and (39) we obtain

$$\underline{C} = (\underline{R}_i^\dagger \cdot \underline{g}_i^{-1} \cdot \underline{R}_i)^{-1/2} . \tag{41}$$

The square root of matrix $\underline{R}_i^\dagger \cdot \underline{g}_i^{-1} \cdot \underline{R}_i$ always exists as long as $|\alpha\rangle_i$ (that is, $|\alpha\rangle_R$) is a complete set of linearly independent vectors. In that case $\underline{g}_i$ is an Hermitian positive definite matrix, and $\underline{g}_i^{-1/2}$ exists. Then Eq. (41) may be rewritten as

$$\underline{C} = [(\underline{g}_i^{-1/2} \cdot \underline{R}_i)^\dagger \cdot \underline{g}_i^{-1/2} \underline{R}_i]^{-1/2} , \tag{42}$$

where it is now seen that the argument is also a positive definite matrix as long as R is nonsingular. Therefore, it is now known how to normalize the $|\alpha\rangle_R$'s which are thus completely determined.

Once the $|\alpha\rangle_R$'s are known, the metric matrix $\underline{g}_R$ can be written in terms of $\underline{R}_R$ using Eq. (41) with $\underline{C} = \underline{1}$,

$$\underline{R}_R^\dagger \cdot \underline{g}_R^{-1} \cdot \underline{R}_R = \underline{1} ,$$

that is,

$$\underline{g}_R = \underline{R}_R \cdot \underline{R}_R^\dagger . \tag{43}$$

It is now explicitly seen how the completeness and linear independence of the basis $\{|\alpha\rangle_R\}$ are equivalent to the non singular nature of R.

In order to fully establish the connections between our approach and that of Kato[13-15] and Bloch[5] one should work in terms of biorthonormal bases. For that purpose we introduce the new basis $\{|\bar{\alpha}\rangle_R\}$ defined by

$${}_R\langle \alpha | \bar{\beta} \rangle_R = {}_R\langle \bar{\alpha} | \beta \rangle_R = \delta_{\alpha\beta} . \tag{44}$$

For the benefit of the readers not familiar with the concept of biorthonormal bases, we should mention that they are very often found in the physics literature disguised under names such as reciprocal bases (crystallography), bras and kets (quantum mechanics), or covariant and contravariant bases vectors (electromagnetism). They are the natural concepts whenever one is dealing with a nonorthogonal basis.

We will now prove that the $|\bar{\alpha}\rangle_R$'s are nothing but the properly normalized eigenvectors of $W_R^\dagger$,

$$W_R^\dagger |\bar{\alpha}\rangle_R = \Delta E_\alpha |\bar{\alpha}\rangle_R , \tag{45}$$

where

$$W_R^\dagger = \langle VR \rangle^\dagger = \langle R^\dagger V \rangle , \tag{46}$$

$$|\alpha\rangle = (R^\dagger)^{-1} |\bar{\alpha}\rangle_R . \tag{47}$$

In order to do so we have to find first the connections between $R^\dagger$, R^{-1}, and R.

We start discussing the equation defining $R^\dagger$. Taking the Hermitian adjoint of Eqs. (31) and (32) we find

$$R^\dagger = 1 + h_0(R^\dagger V - \langle R^\dagger V \rangle R^\dagger) , \tag{48}$$

and Eq. (46).

Next we consider the equation defining R^{-1}. Upon multiplication of Eq. (10) by the right with S^{-1}, and making use of Eqs. (14) and (2) it follows for $S = R$,

$$[H_0, R^{-1}] = R^{-1} V - W_R R^{-1} . \tag{49}$$

From Eq. (20) we obtain

$$R^{-1} = \langle R^{-1} \rangle + h_0(R^{-1} V - W_R R^{-1}) , \tag{50}$$

and taking the diagonal part in Eq. (49),

$$W_R \langle R^{-1} \rangle = \langle R^{-1} V \rangle . \tag{51}$$

Notice that, in general, $\langle R^{-1} \rangle \neq \langle R \rangle^{-1} = 1$. Writing

$$R^{-1} = \langle R^{-1} \rangle T , \tag{52}$$

where, for the time being, we assume the existence of $\langle R^{-1} \rangle^{-1}$, replacing into Eqs. (50) and (51), T is found to satisfy the equation

$$T = 1 + h_0(TV - \langle TV \rangle T) , \tag{53}$$

while

$$W_R = \langle R^{-1} \rangle \langle TV \rangle \langle R^{-1} \rangle^{-1} . \tag{54}$$

Comparing Eqs. (53) and (48) we see that T and $R^\dagger$ satisfy the same equation. It therefore follows that $T = R^\dagger$ and

$$R^{-1} = \langle R^{-1} \rangle R^\dagger , \quad \langle R^{-1} \rangle = (R^\dagger R)^{-1} , \tag{55}$$

$$W_R = (R^\dagger R)^{-1} \langle R^\dagger V \rangle (R^\dagger R) , \tag{56}$$

where it is seen that $\langle R^{-1} \rangle$ is a positive definite operator whenever R is nonsingular. From Eqs. (33), (46), and (56) we obtain

$$W_R^\dagger R^\dagger R |\alpha\rangle_R = \Delta E_\alpha R^\dagger R |\alpha\rangle_R , \tag{57}$$

thus showing $\{R^\dagger R |\alpha\rangle_R\}$ to be the eigenvectors of $W_R^\dagger$. Finally, taking into account Eqs. (35) and (1) it is easily seen that

$${}_R\langle \alpha | R^\dagger R | \beta \rangle_R = \langle \alpha | \beta \rangle = \delta_{\alpha\beta} , \tag{58}$$

thus proving

$$|\bar{\alpha}\rangle_R = R^\dagger R |\alpha\rangle_R \tag{59}$$

to be the vector biorthornormal to $|\alpha\rangle_R$. Equation (35) leads immediately to Eq. (47) thus proving all our previous equations.

Equation (59) may be used to transform any expression written in terms of biorthonormal bases so that it contains only $|\alpha\rangle_R$ and R. Thus Bloch's operators[5] A, B, $\mathcal{P}$, and P may be written as

$$A = W_R (R^\dagger R)^{-1} P_e , \quad B = P_e (R^\dagger R)^{-1} P_e ,$$

$$\mathcal{P} = R P_e (R^\dagger R)^{-1} P_e , \quad P = R P_e (R^\dagger R)^{-1} P_e R^\dagger . \tag{60}$$

Kato's[13-15] approach is based upon a perturbative expansion of P, which obviously turns out to be more cumbersome than that of R. The importance of his work is that he gives criteria for the convergence of the perturbation series.

At first sight it might seem curious that a non-Hermitian operator like W_R should have real eigenvalues. A little reflection shows that this is nothing but a trivial consequence of Eqs. (33), (45), and (44).

IV. THE CANONICAL FORMULATION

One may raise at least two objections to the use of non-Hermitian effective Hamiltonians. The first is mainly of a practical nature: non-Hermitian operators are clumsy because of the nonorthogonality of its eigenvectors. The second is a more fundamental one: While in an exact formulation the eigenvalues of W_S are always real, this does not necessarily hold for the approximate effective Hamiltonians obtained from perturbation theory. Therefore, if a not too high price is to be paid, one should always prefer to deal with Hermitian effective Hamiltonians.

For this purpose it is best to start discussing the orthonormalization of set $\{|\alpha\rangle_R\}$. There is an infinite number of transformations yielding an orthonormal set of basis vectors $\{|\alpha\rangle_U\}$, all of which are obtained when varying the unitary operator U in the following equation:

$$|\alpha\rangle_U = U(R^\dagger R)^{1/2}|\alpha\rangle_R , \tag{61}$$

where

$$U^\dagger = U^{-1} , \tag{62}$$

$$_U\langle\alpha|\beta\rangle_U = {}_R\langle\alpha|R^\dagger R|\beta\rangle_R = \delta_{\alpha\beta} . \tag{63}$$

According to Eq. (28) the $|\alpha\rangle_U$'s are permissible effective eigenvectors if

$$\langle S\rangle = (R^\dagger R)^{-1/2}U^{-1} .$$

As Eq. (55) shows that $R^\dagger R$ is a diagonal operator, therefore U should also be diagonal,

$$U = \langle U\rangle , \tag{64}$$

thus giving

$$\langle S\rangle = (R^\dagger R)^{-1/2}\langle U\rangle^{-1} , \tag{65}$$

where

$$\langle U\rangle^{-1} = \langle U\rangle^\dagger . \tag{66}$$

The corresponding effective Hamiltonians [Eq. (30)] are

$$W_S = \langle U\rangle(R^\dagger R)^{1/2}W_R(R^\dagger R)^{-1/2}\langle U\rangle^{-1} , \tag{67}$$

which from Eqs. (56) and (46) may be easily verified to be Hermitian,

$$W_S^\dagger = W_S . \tag{68}$$

The transformation operator

$$S = R\langle S\rangle = R(R^\dagger R)^{-1/2}\langle U\rangle^{-1} , \tag{69}$$

where

$$\langle U\rangle^{-1} = \langle U\rangle^\dagger ,$$

then turns out to be unitary,

$$S^{-1} = S^\dagger . \tag{70}$$

Equations (66) and (69) therefore define the more general canonical transformations leading to Hermitian effective Hamiltonians.

An evident choice is

$$\langle U\rangle = 1 , \tag{71}$$

which corresponds to Löwdin's symmetric orthonormalization[16] of the $|\alpha\rangle_R$'s. This was the implicit election made by des Cloizeaux[6] and the present author[7] in order to obtain Hermitian effective Hamiltonians. From Eq. (65) this choice is equivalent to the condition

$$\langle S\rangle = \langle S\rangle^\dagger . \tag{72}$$

Other possible unitary schemes have been discussed by Klein[1] and Jørgensen[2] but we will not deal with them here. For all nonperturbative schemes it is easy to establish the connections with our general approach. This is not so for those schemes which are essentially perturbative in nature, as that of Van Vleck,[10-12] because then the choice for $\langle S\rangle$ is not explicitly made and it is not easy to unravel it. Nevertheless, Jørgensen[2] has discussed how to transform both Van Vleck's and Prima's[8,9] methods so that they both satisfy Eq. (72). We give below the relationship between some of Jørgensen's operators and our own, thus showing them to be redundant:

$$G = P_e W_S P_e , \quad u = SP_e , \quad p = P_e\langle S\rangle P_e ,$$

$$t = P_e S^{-1} , \quad \tau = P_e R^{-1} . \tag{73}$$

It is remarkable that Jørgensen was able to find most of our results in spite of the complications introduced by his constraining to a projected formulation.

V. CONCLUSIONS

It has been shown that under the very general conditions [Eqs. (6)—(8)] there are an infinity of effective Hamiltonians equivalent to the original one. All of them are obtained from the transformation operator R defined by Eq. (31) and an arbitrary nonsingular diagonal operator $\langle S\rangle$. All

operators appearing in the effective Hamiltonian schemes devised by different authors may be written as functions of R, $\langle S\rangle$, and the projection operators P_e. All canonical formulations reduce to some specific choice of the unitary diagonal operator $\langle U\rangle$ in Eq. (69). Perturbation theory follows from an iterative solution of Eq. (31), and the corresponding expansions for the related operators. No study was made of the class of remainders V, Eq. (2), such that Eq. (31) defines a nonsingular operator R, which remains an open problem. There does not seem to be much room for relaxing the conditions [Eqs. (6)—(8)], so it is expected that the effective Hamiltonians here defined are the most general ones.

In referring to the relative merits of the different choices for $\langle S\rangle$, I do not feel that any general prescription can be given. Numerical considerations might make preferable the unit-diagonal scheme $\langle S\rangle = 1$, where the number of operations involved in any calculation are reduced to a minimum. If Hermitian effective Hamiltonians are required, in certain cases an Hermitian $\langle S\rangle$ may be convenient, corresponding to a symmetric orthonormalization of the $|\alpha\rangle_R$'s, but in other cases a canonical orthonormalization[16] might be more suitable. This can be so because, while the symmetric basis is highly localized being of the Wannier type, the canonical basis is strongly delocalized, being of the Bloch type.[16]

No detailed discussion has been made of the different perturbative schemes. This is a field where there seems to be ample room for improvement, particularly in what refers to the partial summation of terms in many-body systems. This field might perhaps profit from the more explicit expressions here given for the freedom in the choice of effective Hamiltonians.

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