Nonperturbative derivation of non-Hermitian and Hermitian effective interactions and operators

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Iterative techniques of the solution of the decoupling equation are used to construct various types of effective Hamiltonians in the framework of nonorthogonal transformations. A general and numerically convenient Hermitization procedure of the non-Hermitian Hamiltonians obtained by such techniques is proposed and the definition of effective operators with the related normalization problems is reviewed. [S0556-2813(96)03808-3]

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I. INTRODUCTION

One of the central problems in many-body physics is the necessity of reducing the full space of states to some smaller dimensional model space. This reduction is obtained through the use of effective operators, acting within the model space only, which embody contributions from the complement to the model space. It is customary in nuclear physics to express the derivation of the effective operators in terms of a completely linked perturbation expansion containing both nonfolded and folded diagrams [1] for which partial resummations can be obtained by using either the Krencinglowa-Kuo (KK) technique [2] or the Lee-Suzuki (LS) method [3].

A noteworthy point is the discussion in Ref. [3] of the effective interaction theory in terms of similarity transformations which decouple the model space and the complementary space components of the Hamiltonian. Further discussion of this technique and its connections to quasidegenerate perturbation theory can be found in Ref. [4] and references quoted therein. The authors of Ref. [3], making use of a nonorthogonal transformation of the Hamiltonian, show that the decoupling requirement leads to an equation for the transformation matrix (decoupling equation), which is used to construct two resummations of the perturbative expansion for the effective Hamiltonian in the framework of the Q-box formalism of Kuo and co-workers [2,5].

It is, however, interesting in itself to examine the construction of effective operators directly in terms of the wave operator given by the decoupling equation, with no explicit reference to the perturbative expansion. We show in this paper that this is indeed possible, recovering in this way solutions equivalent to the already known KK and LS resummations, with some new observations on their convergence conditions, and suggest the possibility of constructing new types of solutions.

Since one makes use of nonorthogonal transformations of the Hamiltonian, the resulting effective operators are non-Hermitian. This is simply an artifact of the technique, with no particular physical significance, in that the resulting non-Hermitian effective Hamiltonians have by definition real eigenvalues and a nondefective system of eigenvectors. Non-Hermiticity can be, however, considered a defect, especially if one wants to compare the computed matrix element of the effective Hamiltonians with those obtained from phenomenological fits to experimental levels. In addition, the use of non-Hermitian effective interactions poses normalization problems in the definition of effective operators, which are absent for a Hermitian effective interaction [6].

A definition of a Hermitian effective interaction is therefore highly desirable and to this end some Hermitization procedure is required. The usual choice of Brandow's intermediate basis [1] has to face intrinsic difficulties inherent in the definition of the square root of a matrix. Problems of comparable complexity have to be faced also in the direct construction of a Hermitian effective interaction starting from a unitary choice of the transformation matrix [4,7].

In this paper a new Hermitization procedure is suggested based on the triangular decomposition of a symmetric positive definite matrix, which offers a simple and numerically convenient alternative to the solutions discussed in Ref. [7].

The paper is organized as follows. In Sec. II the derivation of the decoupling equation is presented. Iterative solutions for the wave operator are explicitly constructed in Sec. III. The definition of Hermitian effective interactions is given in Sec. IV, where the definition of effective operators and the related normalization problems are also discussed. Some concluding remarks are given in Sec. V.

II. FORMALISM

As usual the Hamiltonian is composed of an unperturbed, zero order part H_0 and of a residual interaction V. The eigenstates of H_0 will be written as $|t\rangle$ with eigenvalues ϵ_t. The set of these eigensolutions will be partitioned into two subsets

$$[t_1,t_2,\ldots,t_d]\cup[t_{d+1},t_{d+2},\ldots,t_n], \tag{1}$$

defining the model space $[t_1,t_2,\ldots,t_d]$ and its orthogonal complement. The projection operator on the model space is

$$P=\sum_{i=1}^{d}|t_i\rangle\langle t_i|, \tag{2}$$

and that on its orthogonal complement is

$$Q=\sum_{j=d+1}^{n}|t_j\rangle\langle t_j|. \tag{3}$$

Given any nonsingular matrix Ω, i.e., a matrix whose inverse Ω^{-1} exists, the transformed matrix

$$\mathcal{H}=\Omega^{-1}H\Omega \tag{4}$$

has the same eigenvalues of H. Therefore, if we require that Ω is such that

$$Q\mathcal{H}P=0, \tag{5}$$

the eigenvalue problem in the full space is broken into two separate eigenproblems, one in the model space (P space) and the other in its orthogonal complement (Q space).

Condition (5) is not sufficient to determine completely the matrix Ω. As an example multiplication of Ω by any block diagonal matrix leaves Eq. (5) unchanged. Supplementary conditions on Ω are therefore required, the simplest choice being, without any loss of generality,

$$P\Omega P=I_p, \quad P\Omega Q=0, \tag{6a}$$

$$Q\Omega P=\omega, \quad Q\Omega Q=I_q, \tag{6b}$$

where I_p and I_q are unit matrices in the P and Q subspaces, respectively.

With this choice the transformed matrix $\mathcal{H}$ is written

$$P\mathcal{H}P=PHP+PHQ\omega, \tag{7a}$$

$$P\mathcal{H}Q=PHQ, \tag{7b}$$

$$Q\mathcal{H}Q=QHQ-\omega PHQ, \tag{7c}$$

$$Q\mathcal{H}P=QHP+QHQ\omega-\omega PHP-\omega PHQ\omega, \tag{7d}$$

where use has been made of the fact that $\omega P=Q\omega=\omega$.

If ω is such that the decoupling condition (5) is satisfied, the d-dimensional eigenproblem for the model space effective Hamiltonian,

$$p(\omega)=P\mathcal{H}P=PHP+PHQ\omega, \tag{8}$$

gives d eigenvalues of H. The remaining $n-d$ can be obtained by a diagonalization of the Q-space effective Hamiltonian

$$q(\omega)=Q\mathcal{H}Q=QHQ-\omega PHQ. \tag{9}$$

The derivation of model space effective interactions is in this way converted to the task of identifying and enumerating the solutions of the decoupling equation

$$\omega PHQ\omega+\omega PHP-QHQ\omega-QHP=0. \tag{10}$$

This is a nonlinear matrix equation; i.e., it belongs to a class of equations for which no general solution technique is known, nor is the number of existing solutions [8]. One has therefore to resort to *ad hoc* approaches, specifically tailored to the problem at hand.

III. ITERATIVE SOLUTIONS OF THE DECOUPLING EQUATION

The construction of the solutions of the decoupling equation can be made in a rather simple way, the main point being the following proposition.

If ω_1 and ω_2 are two solutions of the decoupling equation (10)*, their difference $y=\omega_2-\omega_1$ will satisfy*

$$yPHQy+yp(\omega_1)-q(\omega_1)y=0, \tag{11}$$

where $p(\omega)$ and $q(\omega)$ are the P-space and Q-space effective Hamiltonians defined by Eqs. (8) *and* (9)*, respectively; vice versa, if ω_2 is solution of the decoupling equation* (10) *and y satisfies Eq.* (11)*, then $\omega_1=\omega_2-y$ is also solution of Eq.* (10).

This proposition can be easily proved by writing Eq. (10) for $\omega_2=\omega_1+y$ and requiring that ω_1 be a solution of Eq. (10).

Some general, but unfortunately nonconstructive considerations can be made on the solutions of the decoupling equation, based on the notion of equivalence class. Two solutions, say, ω_1 and ω_2, will be said equivalent if the resulting P-space (and obviously Q-space also) effective Hamiltonians have the same eigenvalues. This implies that the solutions of Eq. (10) fall in at most $\binom{n}{d}$ classes of equivalence. The difference $y=\omega_2-\omega_1$ must satisfy Eq. (11), which can be also written as

$$yp(\omega_2)-q(\omega_1)y=0. \tag{12}$$

Equation (12) can be satisfied by a nonzero y if and only if the set of the eigenvalues of $p(\omega_2)$ has a nonempty intersection with the set of the eigenvalues of $q(\omega_1)$ [8]. Since by hypothesis the spectra of $p(\omega_1)$ and of $p(\omega_2)$ are the same, the equivalence classes are made of a single element or a nondenumerable set of elements, depending on the presence of degeneracies in the spectrum of H.

We are, however, interested in constructing explicitly a certain number of solutions of the decoupling equation, using specific iterative techniques. In this way some considerations on the convergence conditions are necessary and alternative inversion techniques can be explored for the computation of effective interactions. Furthermore, the preceding argument on the number of solutions in a given equivalence class shows that, aside from quite exceptional circumstances, one can resort to different techniques to construct the same solution of the decoupling equation, a significant advantage in the presence of divergences in the iterative procedures.

The general technique used to construct iterative solutions is the following. Suppose that ω satisfies the decoupling equation (10) and define

$$\begin{aligned}\omega&=x_0+y_1,\\ y_1&=x_1+y_2,\\ &\cdots,\\ y_{n-1}&=x_{n-1}+y_n,\end{aligned} \tag{13}$$

where x_0 is some suitably chosen starting point for the iteration and the x_n satisfy a recurrence relation $x_n=g(x_{n-1})$. Successive substitutions of Eq. (13) in the decoupling equation give a chain of equations for $y_1,\ldots,y_n$. At the $(n+1)$th step one obtains

$$y_{n+1}PHQy_{n+1}+y_{n+1}p(x_0+x_1+\cdots+x_n) - q(x_0+x_1+\cdots+x_n)y_{n+1}+x_nf(x_0,x_1,\ldots,x_n) = 0, \quad (14)$$

where the form of the function f depends on the recurrence relation that has been chosen.

Then, if $x_n\to 0$, defining

$$\sigma=\sum_{i=0}^{\infty} x_i$$

and $y=y_\infty$, one has

$$\omega=\sigma+y,$$

where y satisfies

$$yPHQy+yp(\sigma)-q(\sigma)y=0,$$

which coincides with Eq. (11), so that by the preceding proposition σ is a solution of the decoupling equation.

A. LS-type solutions

We call the class of solutions presented in this section LS-type solutions essentially because of the similarity, and strict equivalence in one case, of the recurrence relations from which they originate to that used in Ref. [3] to construct the LS resummation technique.

The x's are given successively by

$$x_0=\frac{-1}{QHQ}QHP,$$

$$x_1=\frac{1}{q(x_0)}x_0p(x_0),$$

$$x_2=\frac{1}{q(x_0+x_1)}x_1p(x_0+x_1), \quad (15)$$

$$\cdots,$$

$$x_n=\frac{1}{q(x_0+x_1+\cdots+x_{n-1})}x_{n-1}p(x_0+x_1+\cdots+x_{n-1}),$$

and the function f in Eq. (14) is

$$f(x_0,x_1,\ldots,x_n)=p(x_0+x_1+\cdots+x_n). \quad (16)$$

In any matrix norm [9] $\|\cdot\|\equiv\|\cdot\|_p$, we have, from the definitions (15),

$$\|x_n\|\leqslant\|x_{n-1}\|\frac{\|p(\sigma_{n-1})\|}{|\lambda_{qm}|}, \quad (17)$$

where

$$\sigma_{n-1}=x_0+x_1+\cdots+x_{n-1}$$

and λ_{qm} is the eigenvalue of $q(\sigma_{n-1})$ of minimum absolute value. Moreover, again in any matrix norm, $\|p(\sigma_{n-1})\|$ is greater than the absolute value of any of the eigenvalues of $p(\sigma_{n-1})$. Therefore the condition $x_n\to 0$ implies, through inequality (17),

$$|\lambda_{pM}|<|\lambda_{qm}|, \quad (18)$$

where λ_{pM} is the eigenvalue of $p(\sigma_{n-1})$ of maximum absolute value, giving as a necessary condition for the convergence that the eigenvalues of $p(\sigma)$ be the d eigenvalues of H of smallest absolute value. Obviously a suitably chosen shift of the eigenvalues, i.e., subtracting from H a multiple of the identity, cI_n, will make the procedure convergent to the set of d eigenvalues nearest to the chosen constant c. It is worth noting that no hypothesis of a degenerate model space is necessary in the preceding proof.

The iterative solution defined by the definitions (15) is easily shown to be equivalent to the LS vertex renormalization solution [3]. In fact we have

$$\sigma_n=\sigma_{n-1}+\frac{1}{q(\sigma_{n-1})}x_{n-1}p(\sigma_{n-1}) \quad (19)$$

or

$$\sigma_n=\frac{1}{q(\sigma_{n-1})}[x_{n-1}p(\sigma_{n-1})+q(\sigma_{n-1})\sigma_{n-1}], \quad (20)$$

so that, using the definitions of p and q, we obtain the recurrence relation

$$\sigma_n=\frac{1}{q(\sigma_{n-1})}[x_{n-1}PHP+q(\sigma_{n-2})\sigma_{n-1}]. \quad (21)$$

Equation (21) can finally be iterated giving

$$\sigma_n=\frac{1}{q(\sigma_{n-1})}[\sigma_{n-1}PHP-QHP], \quad (22)$$

which is equivalent to the iterative relation from which the LS solution is derived in Ref. [3].

A noteworthy point is that the solution defined by iteration (15) is not the only existing solution of this type. In fact making use of the iteration defined by

$$x_0=QHP\frac{1}{PHP},$$

$$\cdots, \quad (23)$$

$$x_n=q(\sigma_{n-1})x_{n-1}\frac{1}{p(\sigma_{n-1})},$$

we obtain at the $(n+1)$th step an equation for y_{n+1} of the type (14).

We have now, from Eq. (23),

$$\|x_n\|\leqslant\|x_{n-1}\|\frac{\|q(\sigma_{n-1})\|}{|\lambda_{p_m}|}, \quad (24)$$

where λ_{p_m} is the eigenvalue of $p(\sigma_{n-1})$ of minimum absolute value.

The convergence condition $x_n\to 0$ then implies

$$|\lambda_{qM}|<|\lambda_{pm}|, \tag{25}$$

where λ_{qM} is the eigenvalue of $q(\sigma_{n-1})$ of maximum absolute value, giving as a necessary condition that the iteration (23) define a P-space effective Hamiltonian whose eigenvalues are the d eigenvalues of H of greatest absolute value.

Clearly both Eqs. (15) and (23) offer a practicable way for computing effective Hamiltonians through matrix inversion techniques, aside from the quite exceptional case of an accidental degeneracy in the eigenvalues of H. Which one should be used in realistic calculations is merely a matter of convenience and balance of contrasting computing requirements. As an example, while both iterations can be made convergent to the set of d lowest eigenvalues of H, iteration (23) tends to be slower in convergence, since it usually requires a greater shift in the eigenvalues; on the other hand, since the dimensions of the model space are much smaller then that of the Q space, by far less numerical work is required in the inversion of the $p(\sigma_{n-1})$ matrices as compared to the inversion of the $q(\sigma_{n-1})$ matrices implied in solution (15).

The iteration schemes discussed until now can give, through the eigenvalue-shifting technique, only sets of d consecutive eigenvalues of H, supposed ordered in nondecreasing order. These procedures can, however, be generalized in a way essentially similar to that presented in Ref. [10].

Given any matrix A, with elements a_{mn}, let us define $(A)_i$ as a matrix of the same dimensions of A, whose elements are $a_{mn}\delta_{ni}$, i.e., a matrix whose only nonzero column is the ith, which coincides with the ith column of A. Clearly,

$$A=\sum_i (A)_i . \tag{26}$$

If M is any d-dimensional diagonal matrix, $M=\mathrm{diag}(m_1, \ldots, m_d)$, one has

$$\omega(M)_i = m_i(\omega)_i . \tag{27}$$

The decoupling equation (10), making use of Eq. (26), can be decomposed as

$$\omega PHQ(\omega)_i+\omega(PHP-M)_i-(QHQ-m_iI_q)(\omega)_i -(QHP)_i=0 \quad (i=1,\ldots,d). \tag{28}$$

The set of equations (28) can then be solved using any of the preceding iteration schemes; if to be definite we use iteration (15), we have, for the ith equation and with obvious meaning of the symbols,

$$(x_n)_i=\frac{1}{q(\sigma_{n-1})-m_iI_q}x_{n-1}(p(\sigma_{n-1})-M)_i , \tag{29}$$

and the corresponding convergence condition gives, using Gershgorin bounds on the eigenvalues [11],

$$|\lambda_{p_i}-m_i|\leq|\lambda_{q_m}-m_i| \quad \forall i,m, \tag{30}$$

which shows that convergence implies that the eigenvalues of $p(\sigma)$ be the d eigenvalues of H nearest to the numbers m_i. Of course, if the matrix M is a multiple of I_p—i.e., all the m_i are equal—the preceding results are recovered.

Two points deserve further discussion, being relevant in practical applications. The first one is that both Eqs. (10) and (14) are invariant with respect to the choice of the numbers m_i, which therefore may be changed at any step of the iteration; as a consequence, if we take them at the nth step as the eigenvalues of $p(\sigma_{n-2})$, the convergence of the iteration can be made faster.

To illustrate the second point, let us note that the arguments leading to Eqs. (28) and (29) can also be made using a row decomposition, i.e., defining matrices ${}_j(A)$ whose only nonzero row is the jth, which coincides with the jth row of A. Then, if M is an $(n-d)$-dimensional diagonal matrix, $M=\mathrm{diag}(\alpha_1, \ldots, \alpha_{n-d})$, the decoupling equation is decomposed as

$${}_j(\omega)PHQ\omega+{}_j(\omega)[PHP-\alpha_jI_p]-{}_j(QHQ-M)\omega -{}_j(QHP)=0 \quad (j=1,\ldots,n-d), \tag{31}$$

where use has been made of ${}_j(M)\omega={}_j(\omega)\alpha_j$.

Using iteration (23) to solve the set of equations (31) gives as convergence condition that the eigenvalues of the P-space effective Hamiltonian, λ_{p_i}, are those eigenvalues of H for which the differences $|\lambda_{p_i}-\alpha_j|, \forall j$ are maxima. Then, if we take as α_j the eigenvalues of QHQ, the eigenvalues of the effective P-space Hamiltonian will have maximum distance from the QHQ eigenvalues, i.e., are those whose full space eigenvectors have greatest P-space components. This means that the solution just discussed corresponds to the one obtained by the Q-box resummation of Krencinglowa and Kuo [2].

B. KK-type solutions

Although the technique discussed in the preceding paragraph allows one in principle to obtain any desired solution, we discuss here, for the sake of completeness, other iteration schemes more closely related to the standard form of the KK technique.

Let us consider a first example of this kind of iteration. In this case the x's are solution of the linear equations

$$\begin{aligned} &x_0PHP-QHQx_0-QHP=0,\\ &x_1p(x_0)-QHQx_1+x_0PHQx_0=0,\\ &\ldots,\\ &x_np(\sigma_{n-1})-QHQx_n+\sigma_{n-1}PHQx_{n-1}=0, \end{aligned} \tag{32}$$

and y_{n+1} satisfies the equation

$$y_{n+1}PHQy_{n+1}+y_{n+1}p(\sigma_n)-q(\sigma_n)y_{n+1}+\sigma_nPHQx_n=0. \tag{33}$$

This kind of iteration has already been discussed in Ref. [3] where it is used to obtain the KK resummation of the perturbative series. We reformulate it in our formalism just to show explicitly the existence of different iteration schemes which converge to the same effective Hamiltonians.

This point can be of great practical relevance, since the convergence rates of the alternative schemes can be very different.

Using the definition of the Q-space effective interaction $q(\sigma)$, we have, from Eq. (32),

$$x_n p(\sigma_{n-1}) - QHQx_n = [q(\sigma_{n-1}) - QHQ]x_{n-1}. \quad (34)$$

Let $\eta_{\alpha,n-1}$ and μ_q be the eigenvalues of $p(\sigma_{n-1})$ and QHQ, respectively, and $|\phi_{\alpha,n-1}\rangle$ and $|\xi_q\rangle$ their corresponding eigenvectors. Then Eq. (33) gives

$$(\eta_{\alpha,n-1} - \mu_q)\langle \xi_q | x_n | \phi_{\alpha,n-1}\rangle = \langle \xi_q | [q(\sigma_{n-1}) - \mu_q] x_{n-1} | \phi_{\alpha,n-1}\rangle. \quad (35)$$

The eigenvectors $\langle \xi_q|$ can be expanded in terms of the left eigenvectors of $q(\sigma_{n-1})$,

$$\langle \psi_{\beta,n-1} | q(\sigma_{n-1}) = \lambda_{\beta,n-1} \langle \psi_{\beta,n-1}|, \quad (36)$$

so that

$$\langle \xi_q | [q(\sigma_{n-1}) - \mu_q] x_n | \phi_{\alpha,n-1}\rangle \leqslant \Delta_{q,n-1} \langle \xi_q | x_{n-1} | \phi_{\alpha,n-1}\rangle, \quad (37)$$

where

$$\Delta_{q,n-1} = \max_\beta (\lambda_{\beta,n-1} - \mu_q). \quad (38)$$

Finally, from the convergence condition and Eq. (35) it follows that

$$\Delta_{q,n-1} < \eta_{\alpha,n-1} - \mu_q \quad \forall \alpha, q, \quad (39)$$

which means that iteration (32) gives an effective Hamiltonian whose eigenvalues have maximum distance from the QHQ eigenvalues.

Also in this case iteration (32) is not the only existing solution of this type. In fact, it can be shown, using techniques similar to Eqs. (35)–(39), that the iteration defined by the first of Eqs. (32) and

$$x_n PHP - q(\sigma_{n-1}) x_n + x_{n-1} PHQ \sigma_{n-1} = 0 \quad (40)$$

converges to a solution of the decoupling equation which defines a P-space effective Hamiltonian whose eigenvalues are the d eigenvalues of H nearest to the PHP eigenvalues.

IV. CONSTRUCTION OF HERMITIAN EFFECTIVE INTERACTIONS AND OPERATORS

The effective Hamiltonians obtained from the solutions of the decoupling equation are obviously non-Hermitian. This is in principle not a problem since very efficient techniques of solution of nonsymmetric eigenproblems are known and coded in mathematical libraries.

The construction of Hermitian effective interactions is, however, a problem not only interesting in itself but also of practical relevance, since many shell model computer codes make use of the symmetry of the Hamiltonian matrix. The relation between Hermitian and non-Hermitian forms of the effective interaction has already been discussed in Ref. [7], where an explicit, rather complex expansion for the Hermitian effective interaction has been given. The present use of nonperturbative techniques, however, makes this construction very simple. The essential point has already been made in [12], where the quasi-Hermitian character of the effective interaction has been evidenced, but the Hermitization procedure suggested is in our context unnecessarily complicated. A much simpler construction can be obtained in the following way. From the definition (4) of the transformed Hamiltonian one has

$$\Omega \mathcal{H} = H \Omega \quad (41)$$

or, making use of the symmetry of H,

$$\Omega^\dagger \Omega \mathcal{H} = \mathcal{H}^\dagger \Omega^\dagger \Omega, \quad (42)$$

whose P-space part can be written as

$$T p(\omega) = p^\dagger(\omega) T. \quad (43)$$

The matrix

$$T = I_p + \omega^\dagger \omega \quad (44)$$

is manifestly symmetric and positive definite; it therefore admits the Cholesky decomposition [11]

$$T = L L^T, \quad (45)$$

where L is a lower triangular matrix and L^T is its transpose. Rewriting Eq. (43) as

$$L L^T p(\omega) = p^\dagger(\omega) L L^T, \quad (46)$$

multiplying by L^{-1} on the left and by $(L^T)^{-1} = (L^{-1})^T$ on the right, gives

$$L^{-1} p^\dagger(\omega) L = L^T p(\omega) (L^{-1})^T = [L^{-1} p^\dagger(\omega) L]^T. \quad (47)$$

Equation (47) shows that $L^T p(\omega) (L^{-1})^T$ is a Hermitian matrix which has the same eigenvalues of $p(\omega)$, since L is nonsingular; i.e., it is the required Hermitian form of the effective interaction. The present procedure of Hermitization is numerically much more convenient with respect to the solutions suggested in Refs. [7,13], which require the construction of eigenvalues and eigenvectors of $\omega^\dagger \omega$.

The main advantage in using a Hermitian form of the effective Hamiltonian is, however, related to the construction of effective operators in the chosen model space. The problem with non-Hermitian Hamiltonians, as thoroughly discussed in Refs. [6,14], is connected to the fact that left and right eigenvectors can be independently normalized. This is not the case with Hermitian effective Hamiltonians; on the contrary we will show that one has only to compute matrix elements of a suitably defined operator between normalized P-space eigenstates.

Let $[\lambda_\alpha]$ $(\alpha = 1, \ldots, d)$ be the set of eigenvalues of the full Hamiltonian H reproduced by the P-space effective Hamiltonians p, non-Hermitian, and p_e, the Hermitian transform defined by Eq. (47). Let $|\Psi_\alpha\rangle$, $|\phi_\alpha\rangle$, and $|\chi_\alpha\rangle$ be their corresponding eigenvectors, respectively.

By definition, these eigenvectors are connected by the transformations

$$|\Psi_\alpha\rangle = \Omega |\phi_\alpha\rangle = (I_p + \omega) |\phi_\alpha\rangle, \quad (48a)$$

$$|\phi_\alpha\rangle=(L^T)^{-1}|\chi_\alpha\rangle. \tag{48b}$$

If $\hat{O}$ is any operator defined in the full space, we have, using normalized full space eigenvectors $\langle\Psi_\alpha|\Psi_\alpha\rangle = 1$, $\forall\alpha$,

$$\langle\Psi_\alpha|\hat{O}|\Psi_\beta\rangle=\langle\phi_\alpha|(I_p+\omega^\dagger)\hat{O}(I_p+\omega)|\phi_\beta\rangle$$

$$=\langle\chi_\alpha|L^{-1}(I_p+\omega^\dagger)\hat{O}(I_p+\omega)(L^T)^{-1}|\chi_\beta\rangle. \tag{49}$$

Normalization problems are in this case absent; in fact we have

$$\langle\Psi_\alpha|\Psi_\alpha\rangle=\langle\phi_\alpha|(I_p+\omega^\dagger\omega)|\phi_\alpha\rangle=\langle\phi_\alpha|LL^T|\phi_\alpha\rangle=\langle\chi_\alpha|\chi_\alpha\rangle, \tag{50}$$

and the correct procedure requires only the calculation of matrix elements of the effective operator

$$\hat{O}_{\text{eff}}=L^{-1}(I_p+\omega^\dagger)\hat{O}(I_p+\omega)(L^T)^{-1} \tag{51}$$

between normalized P-space eigenvectors.

V. CONCLUDING REMARKS

We have presented in this paper matrix inversion techniques which offer a viable alternative to the well-established perturbative construction of the shell model effective interaction.

A number of iterative schemes have been explicitly constructed which converge to any desired subset of the eigenvalues of the Hamiltonian matrix in the full space of states.

The main advantage of the present techniques relies on the fact that the direct solution of the decoupling equation allows the construction of the wave operator ω. It is precisely its knowledge that makes very simple the construction of the Hermitian transform of the Hamiltonian and of effective operators.

It is worth noting the rather strict connection of the nonperturbative techniques of the construction of effective interactions shown in this paper to other well-known ones, in particular to the large matrix diagonalization technique pioneered by Lo Iudice *et al.* [15]. This point, together with a diagrammatic analysis of the solutions presented in this paper, is currently under study.

While being aware of the difficulties intrinsic to these nonperturbative approaches, especially the presence of some unlinked terms due to space truncation effects [16,17], one should not underestimate the possibility, offered by the present techniques, to obtain a well-converged solution. Convergence problems have been very often underestimated, a common practice being rough evaluations or qualitative order of magnitude arguments, in contrast to the strict control on convergence offered by the methods discussed here.

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