On Mathematical Structure of Effective Observables

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Abstract. We decompose the Hilbert space of wave functions into
two subspaces, and assign to a given observable two effective representatives
that act in the model space. The first serves to determine some of the eigen-
values of the full observable, while the second serves to determine its matrix
elements, in any basis in one of the subspaces, in terms of quantities pertaining
to the model space. We also show that if the Hamiltonian of a physical system
possesses symmetries then these symmetries continue to hold for its effective
representatives of the first type. Maximum information about the system can
be obtained in terms of two sets of effective representatives. The first set of
representatives is complete. Other observables that do not commute with all
members of the complete set have only one type of representative.

1. Introduction

Effective operators are often used in nuclear, atomic and molecular physics. The
general scheme aims to construct from the Hamiltonian of the system, acting on the
Hilbert space of wave functions, an operator that acts on a low dimensional space, so
that the eigenvalues of the latter operator are also eigenvalues of the full Hamiltonian
of the given system [1-9]. The low dimensional space, we have mentioned, is called a
model space and the operator acting on it to produce some of the eigenvalues of the
full Hamiltonian is called an effective Hamiltonian, or an effective representative of
the Hamiltonian. The latter requirement does not determine an effective representa-
tive uniquely. A general class of effective representatives was obtained by Suzuki \[6\] who also delineated forms according to the role of an arbitrary parameter, the start-
ing energy, in the iterative method of solution.\[4\], or according to their Hermiticity.
Hermitian forms have been introduced or adopted by many researchers [10-17]. A
standard non-Hermitian form \[2, 8, 18\] is relatively simple, and is commonly used for
implementing the scheme of effective representatives.
Our present work, which is concerned with the effective representation of any observable in the standard non-Hermitian scheme, has the following objectives:

1. To establish the equivalence between the decoupling condition on the transformed observable and a corresponding condition on its transformed eigenfunctions.

2. To show that the decoupling equation always has solutions and to specify the maximum number of inequivalent solutions.

3. Starting from a complete set of observables associated with the physical system, we construct a complete set of effective representatives, and prove accordingly that the symmetries of the Hamiltonian are carried over to the effective representatives.

4. Two effective representatives can be constructed associated with every observable. The first representative corresponds to the standard non-Hermitian form and gives some of the eigenvalues of the original observable. The second representative is Hermitian and has the property that the matrix elements of the original observable, in any basis of the subspace that is mapped onto the model space, can be calculated in terms of this representative and the projected basis in the model space.

2. THE MODEL SPACE

The truncated Hilbert space of square integrable functions associated with the system, denoted by $H_N$, consists of all $N$ -columns with complex entries. $H_N$ is just the unitary space of complex numbers $C^N$ through the isomorphism $\psi \in H_N \leftrightarrow \psi^t \in C^N$, where $(t)$ denotes the transpose. The standard basis in $H_N$ will be denoted by $e_i (i = 1, \ldots, N)$, so that

$$e_1=(1,0,\ldots,0)^t, \ e_2=(0,1,\ldots,0)^t, \ldots, \ e_N=(0,\ldots,0,1)^t \quad (1)$$

Let $K$ be a distinct subset of $d$ elements of the set $\{1,2,\ldots,N\}$. The subspace generated by the subset of basis elements $\{e_k : k \in K\}$ will be denoted by $\Pi_K$, and will be called a model space. The projection on $\Pi_K$ will be denoted by $P_K$, whereas $Q_K$ will denote the projection on the orthogonal complement $\Pi_K^\perp = \Pi_N \ominus \Pi_K$. It follows that $P_K + Q_K = I$, $P_KQ_K = Q_KP_K = 0$. If it is desired, one may rearrange the order of the basis elements (1) so that the vectors $e_i (i \in K)$ are placed first.

We shall assume that such reordering is done whenever it is necessary, and drop the index $K$, if no ambiguity arises. The symbol $P$ accordingly, will denote a projection on some model space $\Pi$. The reordering operation is particularly useful when we have to represent vectors and operators in matrix form.

Let $S$ be an operator in $H_N$ such that

$$S = QSP \quad (2)$$

It follows that $S^2 = 0$, and hence $e^{\pm S} = 1 \pm S$. Equation (2) implies also that
where $0_d$ is the nil $d \times d$ matrix. Consider the transformation

$$e^{-S} : H_N \rightarrow H_N, \; \psi \rightarrow \tilde{\psi} = (1 - S)\psi. \tag{4}$$

Setting $\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ where $\alpha^t \in \mathbb{C}^d$, we write

$$\tilde{\psi} \equiv \begin{pmatrix} \tilde{\alpha} \\ \tilde{\beta} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -s & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta - s\alpha \end{pmatrix} \tag{5}$$

It is apparent that the mapping $e^{-S}$ is determined by $S$ given by (3), which in turn is determined by $s : \Pi \rightarrow \Pi^\perp$.

Through an obvious isomorphism we may overlook $\Pi$ as being a subspace of $H_N$ and consider it as a space on its own right. Hence, and whenever it is convenient, we may set $P\psi = \alpha$, $P\tilde{\psi} = \tilde{\alpha}$, and thus consider $P\psi, P\tilde{\psi}$ as $d$-vectors instead of being $N$-vectors with vanishing components in $\Pi^\perp$. A similar statement is applicable to $\Pi^\perp$ and to the vectors $Q\psi, Q\tilde{\psi}$, and hence we may set $Q\psi = \beta$, $Q\tilde{\psi} = \tilde{\beta}$. It is evident from (5) that if $\alpha = 0$ then $\psi = \tilde{\psi}$, and hence every point in the invariant subspace \{\begin{pmatrix} 0 \\ \beta^t \end{pmatrix} : \beta^t \in \mathbb{C}^{N-d} \} is a fixed point of the transformation $e^{-S}$.

Let $\Psi = \{\psi_i \in H_N : i = 1, \ldots, d\}$ be a linearly independent set of vectors. Hence there exists at least one subspace $\Pi_K$ in which the set of projections of these vectors is linearly independent. This last statement is equivalent to say that the rank of the matrix $[<e_j | \psi_i>]$, $(i = 1, \ldots, d; j = 1, \ldots, N)$ is $d$. The symbol $<|>$ designates the inner product.

We shall choose the matrix $S$ such that

(i) $Q\tilde{\psi}_i = 0 \quad (i = 1, \ldots, d)$

(ii) The set of vectors $P\Psi = \{P\psi_i : i = 1, \ldots, d\}$, where $P$ is the projection corresponding to $\{1, 2, \ldots, d\}$, is linearly independent.

Requirement (ii) can always be satisfied through reordering the basis if necessary. By (3), requirement (i) implies $s\alpha_i - \beta_i = 0 (i = 1, \ldots, d)$, or

$$sP\psi_i - Q\psi_i = 0 \quad (i = 1, \ldots, d) \tag{6}$$

We write (3) collectively as a matrix equation $s[P\Psi] - [Q\Psi] = 0$, in which $[P\Psi] = [P\psi_1; \ldots; P\psi_d]$, $[Q\Psi] = [Q\psi_1; \ldots; Q\psi_d]$. As its columns are linearly independent the matrix $[P\Psi]$ is invertible, and hence

$$s = [Q\Psi][P\Psi]^{-1} \tag{7}$$
Therefore requirements (i) and (ii) yield equation (7). It is easy to see that equation (7), which embodies in it that the matrix \([P\Psi]\) is invertible, is fact equivalent to conditions (i) and (ii).

With \(s\) so chosen, the matrix \(S\) given by (3) has the property: \(e^{-S}\) projects every vector of the \(d\)-dimensional space \(\text{Lin}\Psi\), generated by the set of vectors \(\Psi = \{\psi_1, \ldots, \psi_d\}\), onto the model space \(\text{Lin}\{\alpha_1, \ldots, \alpha_d\} \equiv \Pi\). This follows immediately from requirement (i) and linearity of \(e^{-S}\). In other words, an arbitrary vector \((\alpha s 0)^t\in\text{Lin}\Psi\) is mapped by \(e^{-S}\) to \((\alpha 0)^t\in\Pi\). The operator \(e^{-S}\) is not a projection operator as implied by the mathematical definition of a projection operator. The word "project" however is used here in a geometrical sense to describe an operation in which every vector of a certain subspace (visualized as hyperplane) is mapped to a vector that has the same first \(d\) components, whereas its remaining components are zeros (visualized as a vector in a coordinate hyperplane). Also if \(\phi \notin \text{Lin}\Psi\), then its image \(\tilde{\phi}\) is not in the model space. The proof of the last fact relies on the regularity of \(e^{-S}\), which implies that the image of the independent set \(\{\psi_1, \ldots, \psi_d, \phi\}\) namely \(\{\alpha_1, \ldots, \alpha_d, \tilde{\phi}\}\) is linearly independent, and hence \(\phi \notin \text{Lin}\{\alpha_1, \ldots, \alpha_d\} = \Pi\). The vector \(\tilde{\phi}\) therefore has at least one non-vanishing component outside the space \(\Pi\).

The operator \(e^{-S}\), with \(s\) given by (6), as projects the subspace \(\text{Lin}\Psi\) orthogonally on \(\Pi\), is thus determined solely by \(\text{Lin}\Psi\) and \(\Pi\), and is independent of the particular choice of a set of \(d\) independent vectors in \(\text{Lin}\Psi\). Indeed if \(\Psi' = \{\psi'_1, \ldots, \psi'_d\}\) is another set of independent vectors in \(\text{Lin}\Psi\), then

\[
\psi'_i = \sum_{j=1}^{d} c_{ji} \psi_j \quad (i = 1, \ldots, d)
\]  

where \(c_{ji}\) are constants. Denoting the matrix whose elements are \(c_{ji}(i, j = 1, \ldots, d)\) by \(C\), and the matrices whose columns are \(\psi_i\) and \(\psi'_i\) by \([\Psi]\) and \([\Psi']\) respectively, we write the last relation as \([\Psi'] = [\Psi]C\). Equivalently we have \([P\Psi'] = [P\Psi]C\) and \([Q\Psi'] = [Q\Psi]C\). Substituting from these equations for \([P\Psi]\) and \([Q\Psi]\) in (7) we get

\[
s = [Q\Psi'][P\Psi]^{-1},
\]

which proves our assertion.

We finally note that as \(e^{-S}\) is invertible, the inverse image of every vector \(\alpha \in \Pi\), which also is identifiable with \((\alpha s 0)^t\), is retrievable as \((\alpha s 0)^t\).

3. Lee and Suzuki Transformation

Let \(O\) be a Hermitian \(N \times N\) matrix, with an independent set of eigenvectors \(\{\psi_i : i = 1, \ldots, N\}\), and consider the eigenequation

\[
O \psi_i = E_i \psi_i \quad (i = 1, \ldots, N)
\]
Applying the Lee and Suzuki similarity transformation \([5]\) to the matrix \(O\) and to the truncated space \(H_N\), we obtain

\[
\tilde{O} \tilde{\psi}_i = E_i \tilde{\psi}_i \quad (i = 1, \ldots, N),
\]

(10)

where we have used tilde to designate transformed quantities so that

\[
\tilde{O} = e^{-S} O e^S, \quad \tilde{\psi} = e^{-S} \psi.
\]

(11)

Our work will be distinguished from that of Lee and Suzuki through our identification of additional freedom in the choice of \(S\). Multiplying both sides of (10) by \(P\) and injecting \(I = P + Q\) conveniently in the right hand side we get

\[
P \tilde{O} P \tilde{\psi}_i + P \tilde{O} Q \tilde{\psi}_i = E_i P \tilde{\psi}_i \quad (i = 1, \ldots, N).
\]

(12)

In a similar way we get

\[
Q \tilde{O} P \tilde{\psi}_i + Q \tilde{O} Q \tilde{\psi}_i = E_i Q \tilde{\psi}_i \quad (i = 1, \ldots, N).
\]

(13)

We shall choose the transformation (11) such that there exists a subset \(J \subset \{1, \ldots, N\}\) with \(\text{card } J = d\), for which (i) the set of vectors \(\{P \tilde{\psi}_i : i \in J\}\) is linearly independent, and (ii) \(Q \tilde{\psi}_i = 0 (i \in J)\). Such a choice, as we have seen in the previous section, is certainly possible.

Proposition 1: Let \(J \subset \{1, \ldots, N\}\) be such that the set \(\{P \tilde{\psi}_i : i \in J\}\) is linearly independent. The following assertions concerning the Lee and Suzuki transformation are equivalent:

A1. \(Q \tilde{\psi}_i = 0 (i \in J)\)

A2. \(s_J = [\Psi_J][P \Psi_J]^{-1}\)

A3. (i) the decoupling equation \(Q \tilde{O} P = 0\) holds, and

(ii) \(P \tilde{\psi}_i (i \in J)\) are eigenvectors of \(P \tilde{O} P\).

Proof. We have seen in section 2 that the assertions A1 and A2 are equivalent (this expression of \(s_J\) was first given by Navratil and Barrett \([10]\) ). To prove that assertion A1 implies A3, we set \(Q \tilde{\psi}_i = 0 (i \in J)\) in (12) and (13) to find that \(P \tilde{\psi}_i (i \in J)\) are eigenvectors of \(P \tilde{O} P\), and \(Q \tilde{O} \tilde{\psi}_i = 0 (i \in J)\). Due to the linear independence of \(P \tilde{\psi}_i (i \in J)\), the later \(d\) equations imply that \(Q \tilde{O} P = 0\). Conversely, if \(\alpha_k (i = 1, \ldots, d)\) are linearly independent eigenvectors of \(P \tilde{O} P\) then the \(N\)-vectors \((\alpha_k) (k = 1, \ldots, d)\) are eigenvectors of \(\tilde{O}\). It follows that the inverse image of these vectors \(\{e^S(\alpha_k) : k = 1, \ldots, d\}\) coincides with a subset \(\Psi_J = \{\tilde{\psi}_i : i \in J\}\) of eigenvectors of \(O\). The subset \(\Psi_J\) clearly fulfills assertion 1. Hence A1 is equivalent to A3.
4. The Effective Form

When the transformed operator $\tilde{O}$ is such that $Q_K \tilde{O} P_K = 0$, for some subset $K \subset \{1, \ldots, N\}$, with $\text{card } K = d$, we refer to the operator $O_{\text{eff}} \equiv P_K \tilde{O} P_K$ as an effective representative of the operator $O$ corresponding to the model space $\Pi_K$, and to the form taken by $\tilde{O}$ as an effective form. When $\tilde{O}$ is in an effective form corresponding to the model space $\Pi$, the matrix elements $(O_{\text{eff}})_{ij}$ are all zero except those for which $i, j \leq d$, and consequently we make the identification $O_{\text{eff}} : \Pi \rightarrow \Pi$, in which $O_{\text{eff}}$ is considered a $d \times d$ matrix. In a similar way we treat $Q \tilde{O} Q$ as an $(N - d) \times (N - d)$ matrix.

We elaborate here on the effective form and develop a more explicit framework. We write the eigenequation (9) as

$$
\begin{pmatrix}
  a & b \\
  b & f
\end{pmatrix} \begin{pmatrix}
  \alpha_i \\
  \beta_i
\end{pmatrix} = E_i \begin{pmatrix}
  \alpha_i \\
  \beta_i
\end{pmatrix} \quad (i = 1, \ldots, N) \tag{14}
$$

where the matrix $O$ has been partitioned to submatrices corresponding to $\Pi$ and $\Pi^\perp$, with $a$ is a $d \times d$ matrix. By (11) the last equation is transformed to

$$
\begin{pmatrix}
  a + bs & b \\
  -s(a + bs) + b^+ & f - sb
\end{pmatrix} \begin{pmatrix}
  \alpha_i \\
  \beta_i - s\alpha_i
\end{pmatrix} = E_i \begin{pmatrix}
  \alpha_i \\
  \beta_i - s\alpha_i
\end{pmatrix} \quad (i = 1, \ldots, N) \tag{15}
$$

The later equation is equivalent to (12) and (13) together. It is easy to check that every $s_J$, given as in proposition 1, puts $\tilde{O}$ into an effective form corresponding to some model space $\Pi$. In other words, every $s_J$ is a solution to the decoupling equation

$$
Q \tilde{O} P \equiv -s(a + bs) + b^+ + fs = 0. \quad (16)
$$

To demonstrate the converse we assume that the later equation is satisfied by some $s$, and hence the action of $Q \tilde{O} P$ on any vector in $\Pi$ is zero. In particular this action is zero for all vectors $\alpha_i$ such that $\psi_i = \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix}, (i = 1, \ldots, N)$ are eigenvectors of $O$, and hence

$$
-s(a + bs)\alpha_i + b^+ \alpha_i + f s \alpha_i = 0 \quad (i = 1, \ldots, N) \tag{17}
$$

Making use of (14) we reduce the last equation to the eigenequation

$$
(f - sb)(s\alpha_i - \beta_i) = E_i(s\alpha_i - \beta_i) \quad (i = 1, \ldots, N) \tag{18}
$$

which is the same as embodied in equation (15) but now extended to all $i$. However, not all vectors $s\alpha_i - \beta_i$ can be eigenvectors of $(f - sb)$ because the later operator has only $N - d$ eigenvectors. It follows that there exists a subset $J$ consisting of $d$ elements of $\{1, \ldots, N\}$ such that $s\alpha_i - \beta_i = 0 (i \in J)$, which implies that $s = s_J$, as given in proposition 1.
We list here the following comments on the effective form assuming from now on
that \( \tilde{O} \) is in such a form. i.e. the transformation (10) is such that
\( \tilde{Q}\tilde{O}P = 0 \).

1. If \( \tilde{O} \) is the effective form corresponding to the model space \( \Pi \) then the right
hand-side of the secular (characteristic) equation \( \det(\tilde{O} - EI_N) = 0 \) can be factorized
to a product of two polynomials; one of which is of degree \( d \) in \( E \)
\[
\det(\tilde{O}_{\text{eff}} - EI_d) . \det(\tilde{Q}\tilde{O}Q - EI_{N-d}) = 0.
\]
(19)
The eigenvalues of \( O \) is the set of zeros of these two polynomials. In practical problems
the secular equation of \( \tilde{O}_{\text{eff}} \) can be solved numerically as it is of low degree in \( E \),
whereas that of \( \tilde{Q}\tilde{O}Q \) is of high degree in \( E \) and it is often hopeless to approach
it for direct solution. One may apply the method of effective form described in the
previous section afresh to the operator \( \tilde{Q}\tilde{O}Q \). Or alternatively one may pick up a
new set of eigenvectors, say \( \Psi' \), determine \( s_j \), and consequently a new effective form.
Alternatively the matrix \( s_j \) could be determined by iterative methods [4, 11, 7].

2. If \( P\psi_i \) is an eigenvector of \( \tilde{O}_{\text{eff}} \) corresponding to \( E_i \) then by (12)
\( \tilde{Q}\tilde{O}\tilde{Q}\psi_i = 0 \) which implies that the \((N - d)\) vector \( \tilde{Q}\psi_i \) is complex orthogonal to the rows of
\( d \times (N - d) \) matrix \( \tilde{P}\tilde{O}Q \), and the vector \( \tilde{Q}\psi_i \) is not necessarily zero. Therefore, if
\( \alpha \) is an eigenvector of \( \tilde{O}_{\text{eff}} \) then, though \( \begin{pmatrix} \alpha_0 \\ \gamma \end{pmatrix} \) is an eigenvector of \( \tilde{O} \) belonging to the
eigenvalue \( E_i \), there may exist another eigenvector \( \begin{pmatrix} \alpha_0 \\ \gamma \end{pmatrix} \) of \( \tilde{O} \) that belongs to the same
eigenvalue \( E_i \). In the latter case \( b\gamma = 0 \) and \( \gamma \) is an eigenvector of \( \tilde{Q}\tilde{O}Q \) belonging
to the eigenvalue \( E_i \). It is clear that \( \begin{pmatrix} 0 \\ \gamma \end{pmatrix} \) is an eigenvector of \( \tilde{O} \) that belongs to the
eigenvalue \( E_i \). We summarize the latter observations by the following proposition

**Proposition 2.** Let \( \phi \) be an eigenvector of \( \tilde{O} \) belonging to the eigenvalue \( E \).

(i) If \( Q\phi \neq 0 \) then \( E \) is an eigenvalue of \( \tilde{O}_{\text{eff}} \) to which the eigenvector \( P\phi \) belongs.
(ii) If \( Q\phi \neq 0 \) then \( Q\phi \) is an eigenvector of \( \tilde{Q}\tilde{O}Q \) belonging to the eigenvalue \( E \).
If in addition, \( P\phi \neq 0 \), then \( P\phi \) is not an eigenvector of \( \tilde{O}_{\text{eff}} \) unless \( bQ\phi = 0 \). In the
latter case \( E \) is a common eigenvalue of \( \tilde{O}_{\text{eff}} \) and \( \tilde{Q}\tilde{O}Q \) to which the independent
eigenvectors \( \begin{pmatrix} P\phi_0 \\ 0 \end{pmatrix} \) and \( \begin{pmatrix} 0 \\ Q\phi \end{pmatrix} \) belong. In the latter case the spectra of \( \tilde{O}_{\text{eff}} \) and \( \tilde{Q}\tilde{O}Q \)
intersect.

(iii) \( P\phi \) is an eigenvector of \( \tilde{O}_{\text{eff}} \) does not necessitate that \( Q\phi = 0 \). However if the
spectra of \( \tilde{O}_{\text{eff}} \) and \( \tilde{Q}\tilde{O}Q \) do not intersect in \( E \), then \( Q\phi = 0 \) \( \Leftrightarrow \) \( P\phi \) is an eigenvector
of \( \tilde{O}_{\text{eff}} \) belonging to the eigenvalue \( E \).

3. If the matrix \( [P\Psi_f] \) is singular for some choice of model space, say \( \Pi \), then
we have to replace it by another \( \Pi' \) such that the matrix \( [P'\Psi_f] \) is invertible. There
certainly exists such a new choice of model space, otherwise the set \( \Psi_f \) would be
linearly dependent.

We demonstrate here that for a given set of eigenvectors \( \Psi_f \), two legimate choices
of model spaces lead to two effective representatives which are related by a similarity
transformation. Let \( \Pi \) and \( \Pi' \) be two legimate choices and denote the projections on
the corresponding model spaces by $P$ and $P'$ respectively. This leads to two distinct $s$, say $s$ and $s'$, and hence to two distinct effective representatives $O_{\text{eff}} = P\tilde{O}P$ and $O'_{\text{eff}} = P'\tilde{O}'P'$. If \{$E_i : i \in J$\} is the set of eigenvalues to which $\Psi_J$ belong, then

$$O_{\text{eff}}[P\Psi_J] = [P\Psi_J]\Lambda_J, \quad O'_{\text{eff}}[P'\Psi_J] = [P'\Psi_J]\Lambda_J$$

(20)

where $\Lambda_J$ is a diagonal matrix with diagonal elements ($E_i : i \in J$). From (20) we deduce that

$$O_{\text{eff}} = [P\Psi_J][P'\Psi_J]^{-1}O'_{\text{eff}}[P'\Psi_J][P\Psi_J]^{-1}$$

(21)

which proves our claim.

Each independent set of eigenvectors $\Psi_J$ provide at least one model space $\Pi_K$. The number of possible choices of $\Pi_K$ is not less than one and not greater than \(\binom{N}{d}\), which is of course the number of independent sets of projections \{\(P_K\Psi_J : \text{card}K = d, \ K \subset \{1, ..., N\}\)\}. All such choices lead of course to the same set of eigenvalues $\Lambda_J$.

If the eigenvalues of $O$ are non-degenerate then different choices of $\Psi_J$ out of the set of $N$ independent eigenvectors $\Psi_J$, result in effective representatives with different spectra. The total choices of inequivalent effective representations corresponding to $O$ is \(\binom{N}{d}\); and within each of these there are a maximum number of \(\binom{N}{d}\) equivalent representatives.

The above-identified freedoms are new and extend the work of Lee and Suzuki.

5. Spectral Representation of $O_{\text{eff}}$

Let $O_{\text{eff}}$ be an effective representative of the operator $O$ in the model space $\Pi$, and let \{\(E_i : i \in J\)\} be the spectrum of $O_{\text{eff}}$, to which the vectors $P\Psi_i (i \in J)$ belong, so that $O_{\text{eff}}P\psi_i = E_i P\psi_i (i \in J)$. Since each $P\psi_i$ lies in the model space we have

$$P\psi_i = \sum_{\mu=1}^{d} c_{i\mu} e_\mu \quad (i \in J)$$

(22)

$$<P\psi_i | P\psi_j> = \sum_{\mu=1}^{d} c_{i\mu}^* c_{j\mu} \equiv \gamma_{ij} \quad (i, j \in J)$$

(23)

The matrix $\gamma$ is clearly Hermitian, and determines the overlap the eigenvector of $O_{\text{eff}}$ one with respect to another. Let

$$\chi = \sum_{j \in J} b_j P\psi_j$$

(24)

be an arbitrary vector in the model space, then

$$<P\psi_i | \chi> = \sum_{j \in J} \gamma_{ij} b_j \quad (i \in J)$$

(25)
Hence
\[ \sum_{i \in J} \gamma_{ki}^{-1} < P \psi_i | \chi > = b_k \quad (k \in J) \]  
(26)

where \( \gamma^{-1} \) is the inverse of the matrix \( \gamma \). It is clear that \( \gamma^{-1} \) always exists since \( P \psi_i (i \in J) \) are linearly independent. Applying \( O_{\text{eff}} \) to \( \chi \) where \( b_k \) are given by (26) we get
\[ O_{\text{eff}} | \chi > = \sum_{i, k \in J} \gamma_{ki}^{-1} < P \psi_i | \chi > E_k P \psi_k \]
(27)

This yields
\[ O_{\text{eff}} = \sum_{i, k \in J} E_i \gamma_{ik}^{-1} | P \psi_i > < P \psi_k | \]

which expresses \( O_{\text{eff}} \) in terms of quantities pertaining to the model space.

6. A Complete Set of Effective Representatives

Let \( O_1 \equiv H \) be the Hamiltonian of a physical system and \( O^2, ..., O^c \) be a set of observables pertaining to the system so that the set of observables \( \Gamma = \{O^1, O^2, ..., O^c\} \) is complete. It follows from the latter assumption that
\[ [O^\rho, O^\sigma] = 0 \quad (\rho, \sigma = 1, ..., c) \]
(28)

The energy eigenvectors \( \{e_i : i = 1, 2, ..., \} \) of any suitably chosen simple Hamiltonian could be taken as a basis for the Hilbert space of wave functions of the physical system. For example, these could be the eigenstates of the simple harmonic oscillator, when considering the bound states of the nucleus. Observables pertaining to the system are represented by Hermitian matrices in terms of this basis. Unless the matrices representing observables are given by recurrence formulae, we have to be content with finite matrix approximations, which imply truncating the infinite basis \( \{e_i\}_1^\infty \) at some sufficiently large term \( N \). The space generated by the truncated basis \( [e_1, ..., e_N] \equiv H_N \) will hopefully contain good approximations of all states of interest to the problem we consider.

It must be noted that, whenever the eigenvalue problem is to be solved numerically, which is usually the case in physically interesting problems, truncation is an inevitable task. We note that truncating an infinite basis by a finite one with a sufficiently large number of basis elements is justified by the fact that the sequence \( (e_N) \) tends weakly to zero as \( N \) tends to infinity. This means that for every wave function \( \psi \in H \) the sequence of numbers \( (e_N | \psi >) \) tends to zero as \( N \) tends to infinity \[19, 20\]. Alternatively, an upper cutoff, \( N \), can be safely applied without seriously changing the low-lying properties.
It is noted that all the algebra carried out in the previous section, or to be carried out in the forthcoming discussion, is valid for infinite matrices as much as it is valid for finite ones, and hence we may replace \( N \) by \( \infty \) without affecting the validity of these results.

The Hermitian commuting set of matrices \( \Gamma \) is complete, and there exists accordingly a complete set of simultaneous eigenfunctions \( \psi_i \) of the observables \( O^\sigma \) such that

\[
O^\sigma \psi_i = E_i^\sigma \psi_i \quad (i = 1, \ldots, N; \sigma = 1, \ldots, c)
\]

where \( E_i^\sigma \) are the eigenvalues of the observable \( O^\sigma \) to which the eigenvector \( \psi_i \) belongs. The eigenvectors given by (29) are preserved when the similarity transformation (11) is applied to the Hilbert space of wave functions \( H_N \) and to the operators acting on \( H_N \), and hence

\[
\tilde{O}^\sigma \tilde{\psi}_i = E_i^\sigma \tilde{\psi}_i \quad (i = 1, \ldots, N; \sigma = 1, \ldots, c)
\]

Assume that the eigenvectors \( \tilde{\psi}_1, \ldots, \tilde{\psi}_d \) are such that the set \( \{ P\tilde{\psi}_1, \ldots, P\tilde{\psi}_d \} \) is linearly independent, and take

\[
s = [Q\tilde{\psi}_1 \ldots Q\tilde{\psi}_d][P\tilde{\psi}_1 \ldots P\tilde{\psi}_d]^{-1}
\]

The matrix \( s \) is the same for observables forming the complete set \( \Gamma \), for it is constructed of the same subset of the simultaneous eigenvectors of \( \tilde{O}^\sigma (\sigma = 1, \ldots, c) \). The resulting transformed observables \( \tilde{O}^\sigma \), have the same effective form, and hence have \( P\tilde{\psi}_i (i = 1, \ldots, d) \) as a common subset of eigenvectors \( \{ \psi_i : i = 1, \ldots, N \} \). Define a set of effective representatives

\[
O^\sigma_{\text{eff}} = P\tilde{O}^\sigma P \quad (\sigma = 1, \ldots, c)
\]

and hence

\[
O^\sigma_{\text{eff}} P\tilde{\psi}_i = E_i^\sigma P\tilde{\psi}_i \quad (i = 1, \ldots, d; \sigma = 1, \ldots, c)
\]

It follows, and since the set \( \{ P\psi_i : i = 1, \ldots, d \} \) is complete in the model space \( \Pi \), that

\[
[O^\rho_{\text{eff}}, O^\sigma_{\text{eff}}] = 0 \quad (\sigma, \rho = 1, \ldots, c)
\]

The effective Hamiltonian \( H_{\text{eff}} \equiv O^1_{\text{eff}} \) and the effective representatives \( O^\sigma_{\text{eff}} (\sigma = 2, \ldots, c) \) we have constructed have the virtue that the symmetries exhibited by the original Hamiltonian \( H \) are carried over to \( H_{\text{eff}} \) with the effective representatives \( O^\sigma_{\text{eff}} (\sigma = 2, \ldots, c) \) playing the role of generators of symmetry for \( H_{\text{eff}} \).
The matrices (32) are obviously non-Hermitian and, consequently, the expectation value of an effective representative in a state $P\psi$ in the model space is generally a complex number. An exception to this fact is that when $P\psi$ is an eigenvector $P\psi_i$ of $O_{eff}$. In this case

$$<O_{eff}>_{P\psi_i} = <P\psi_i | O_{eff} | P\psi_i> / \| P\psi_i \|^2 = E_i$$

(35)

7. A Second Type of Effective Representative.

The role of an effective operator seems limited to producing some of the eigenvalues of the original observable. However, we may enhance the scheme of "effectiveness" and make a further step as follows: The matrix $S$ which is determined by iterative methods [4, 7, 17] and utilized to construct the effective representative $O_{eff}$ can also be utilized to construct an effective representative of a second type $O_{eff}^\prime$ that satisfy the property

$$<\psi | O | \phi> = <P\psi | O_{eff}^\prime | P\phi>$$

(36)

for all $\psi, \phi \in Lin\{\psi_1,...,\psi_d\}$. Using (11) and the definition of the adjoint operator, we have

$$\langle \psi | O | \phi \rangle = \left< e^{-S}\bar{\psi} | O | e^{-S}\bar{\phi} \right> = \left< \bar{\psi} | e^{-S^*}O e^{-S} | \bar{\phi} \right>$$

$$= \left< P\bar{\psi} | e^{-S^*}O e^{-S} | P\bar{\phi} \right> = \left< P\psi | Pe^{-S^*}O e^{-S} | P\phi \right>$$

(37)

The requirement (36) is fulfilled on taking

$$O_{eff}^\prime = Pe^{-S^*}O e^{-S}$$

(38)

In particular $<\psi_i | O | \psi_j> = <\alpha_i | O_{eff}^\prime | \alpha_j>$. We therefore associate with every observable $O^\sigma \in \Gamma$ two effective representatives. The first, $O_{eff}$, serves to determine some of the eigenvalues of $O^\sigma$ and the projection of the corresponding eigenvectors on the model space; the second $O_{eff}^\prime$ has the important property: the matrix elements of the original operator $O^\sigma$ with respect to any basis in the space $Lin\{\psi_1,...,\psi_d\}$ is given in terms of $O_{eff}^\prime$ and the projected basis in the model space. It is evident that the last matrix can be calculated easily since $O_{eff}^\prime$ is known whenever $S$ is known, and since the basis elements of the model space have finite components. We mention that the matrix $< P\psi_i | O_{eff}^\prime | P\psi_j >$ is not the matrix of $O_{eff}$ since $\{P\psi_i\}_{i=1}^d$ is not orthogonal. In particular, and if $\psi \in Lin\Psi$ then

$$< O >_{\psi} = < P\psi | O_{eff}^\prime | P\psi > = \| P\psi \|^2 < O_{eff}^\prime >_{P\psi}$$

Expressed in words, the expectation value of the observable $O$ in the state $\psi \in Lin\Psi$ is equal to the expectation value of its representative of the second type in the projection of the given state on the model space times the square norm of this projection.
For observables $O$ that do not commute with all elements of the complete set $\Gamma$ we can define only one effective representative, that is the effective representative of the second type $O_{eff}$. This serves to give a portion of the transition matrix of $O$, namely that which corresponds to a basis of $Lin\Psi$.

A systematic study of the system is achieved by decomposing the space $H_N$ into linear subspaces $Lin\Psi_{J_r}$ $(r = 1, 2, ..., a)$, with $J_r \cap J_s = \emptyset$ if $(r \neq s)$, so that

$$H_N = Lin\Psi_{J_1} \oplus ... \oplus Lin\Psi_{J_a} \quad (39)$$

Now in each subspace $Lin\Psi_{J_r}$ we assign to every observable $O$ in a complete set of observables an effective representative of the first type $O_{eff}$ and an effective observable of the second type $O_{reff}$. These effective representatives, of first or second type, differ from one subspace to another as does $s_J$. If representatives of the first type are all obtained, all eigenvalues of the full observable $O$ become known. Also if $\chi, \chi' \in Lin\Psi_{J_r}$ then we have

$$<\chi | O | \chi'> = < P_r \chi | O_{reff} | P_r \chi'>$$

where $P_r$ denotes the projection on the model space corresponding to the subspace $Lin\Psi_{J_r}$. Although similar relations are valid for every two vectors in the same subspace, one can not express $<\chi | O | \chi'>$ in terms of representatives of second type when $\chi$ and $\chi'$ belong to different subspaces, and consequently when they are arbitrary vectors in $H_N$.

8. Towards Practical Applications

Following the traditional lines of thinking for many-body problems, we suggest that $S$ is developed for small sub-systems and used as an approximation for the full $S$. For example two and three body problems may be solved with high precision using current numerical techniques [16, 17]. A set of solutions $P\psi_i (i = 1, ..., d)$ is selected, $S$ is evaluated and the resulting $H_{eff}$ is then used in many body problems within the appropriately restricted model space. Detailed tests will be needed for specific Hamiltonians to determine the efficacy of this approach and the utility of the various freedoms we have identified within the present work.

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References

[1] Barrett B R and Kirson M, Adv. Nucl. Phys. 6(1973) 219

[2] Brandow B H, Rev. Mod. Phys. 39 (1967) 771
[3] Ellis P J and Osnes E, Rev. Mod. Phys. 49 (1977) 777
[4] Kuo T T S, Ann. Rev. Nucl. Sci. 24 (1974) 101
[5] Lee S Y and Suzuki K, Phys. Lett. B91(1980) 173
[6] Suzuki K and Lee S Y, Prog. Theor. Phys. 64 (1980) 2091; Suzuki K, Progress Theor. Phys. 68 (1982) 246
[7] Zheng D C, Vary J P and Barrett B R, Nucl. Phys. A560 (1993) 211
[8] Fields T J, Vary J P and Gupta K S, Mod. Phys. Lett. A11 (1996) 2233
[9] Suzuki K and Okamoto R, Prog. Theor. Phys. 71 (1984) 1221
[10] Brandow B H, Lecture Notes in Physics (Springer-Verlag, 1975) Vol. 40
[11] Des Cloizeaux J, Nucl. Phys. 20 (1960) 321
[12] Klien D J and Chem. Phys. 61 (1974) 786
[13] Poves A and Zuker A, Phys. Rep. 71 (1981) 141
[14] Shavitt I and Redmon L T, J. Chem. 73 (1981) 141
[15] Westhaus P, Int. J. Quantum Chem. 20 (1981) 1243
[16] Navratil P and Barrett B R, Phys. Lett. B 369(1996) 193-200.
[17] Vary J P, Effective Hamiltonian Method for the Nuclear Shell Model and Quantum Field Theory. Lectures presented at the International Summer School "Structure and Stability of Nucleons and Nuclear Systems" Preda\l, Romania, 1998. To be published in the Proceedings by World Scientific, Singapore.
[18] Suzuki K, Okamoto R and Kumagai H , Nucl. Phys. A580 (1994)
[19] Fano G, Mathematical Methods of Quantum Mechanics (McGraw Hill, 1967).
[20] Prugovecki E, Quantum Mechanics in Hilbert Space (Academic Press, 1971)