Approximate Treatment of Hermitian Effective Interactions and a Bound on the Error

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Abstract

The Hermitian effective interaction can be well-approximated by $(R + R\dagger)/2$ if the eigenvalues of $\omega\dagger\omega$ are small or state-independent (degenerate), where $R$ is the standard non-Hermitian effective interaction and $\omega$ maps the model-space states onto the excluded space. An error bound on this approximation is given.
Much effort has been made to calculate the shell-model effective interactions in nuclei from a realistic nucleon-nucleon interaction. In spite of a great deal of progress[1-5] in this field of physics, attention has been directed almost entirely to the well-known non-Hermitian form, which we label $R$ here. However, the empirical or phenomenological shell-model effective interactions have been assumed to be Hermitian. Therefore direct comparison between the theoretical and empirical effective interactions might cause confusion. The formal theory of constructing a Hermitian effective interaction, which we denote here by $W$, has been developed since des Cloizeaux[6] and Brandow's[1] original works. Recently an improved approach was introduced[7] and was applied to the calculation of Hermitian effective interactions, starting with modern meson-exchange nucleon-nucleon interactions, by several authors[8]. In their study it has been observed that the non-Hermiticity was rather small and $(R + R^\dagger)/2$, referred to as $W_{app}$, was a very good approximation to the exact Hermitian $W$. This raises the general question as to under what conditions the approximation $W \simeq W_{app}$ might be reliable. The origin of and bounds on the non-Hermiticity of $R$ has already been discussed by us[9]. The main purpose of this note is to derive an explicit relation with which the validity of the approximation $W \simeq W_{app}$ can be qualitatively examined. An application of our relations to a model matrix problem will be made, and we shall discuss the results.

We define two projection operators $P$ and $Q$ according to the usual definitions i.e., $P$ and $Q$ project a state onto the model space and its complement, respectively, and they satisfy $P + Q = 1$. Let $d$ be the dimension of the $P$ space. We write $d$ of the true eigenstates of $H$ to be reproduced from the
$P$-space effective interaction as\cite{10}

$$|\Phi_k\rangle \equiv (P + Q)|\Phi_k\rangle = |\phi_k\rangle + \omega |\phi_k\rangle ,$$  \hspace{1cm}  (1)

where $|\phi_k\rangle$ is the $P$-space component of $|\Phi_k\rangle$. The operator $\omega$ maps the $P$-space state $|\phi_k\rangle$ onto the $Q$ space. The operator $\omega$ is related to the usual wave operator $\Omega$ as $\omega = \Omega - P$. The operator $\omega$ is written explicitly as

$$\omega = \sum_k Q|\Phi_k\rangle \langle \tilde{\phi}_k|P .$$  \hspace{1cm}  (2)

Here $|\tilde{\phi}_k\rangle$ is the biorthogonal complement to the model space wave function $|\phi_k\rangle$, \textit{i.e.}, $\langle \tilde{\phi}_k|\phi_i\rangle = \delta_{ki}$. The Hamiltonian $H$ is divided into two parts, the unperturbed part $H_0$ and the perturbation $V$. Using $\omega$ the non-Hermitian effective interaction $R$ can be written as

$$R = PVP + PVQ\omega$$  \hspace{1cm}  (3)

which is equivalent to the usual definition of the non-Hermitian effective interaction $PV\Omega$.

The Hermitian effective interaction $W$ may be written in the $|\alpha\rangle$ basis as\cite{7, 8}

$$\langle \alpha|W|\beta\rangle = D(\alpha, \beta) \left\{ \sqrt{\mu_\alpha^2 + 1} \langle \alpha|R|\beta\rangle + \sqrt{\mu_\beta^2 + 1} \langle \alpha|R^\dagger|\beta\rangle \right\} ,$$  \hspace{1cm}  (4)

where $|\alpha\rangle$ ($|\beta\rangle$) and $\mu_\alpha$ ($\mu_\beta$) are given through the eigenvalue equation of $\omega^\dagger \omega$

$$\omega^\dagger \omega |\alpha\rangle = \mu_\alpha^2 |\alpha\rangle ,$$  \hspace{1cm}  (5)

and

$$D(\alpha, \beta) = \left\{ \sqrt{\mu_\alpha^2 + 1} + \sqrt{\mu_\beta^2 + 1} \right\}^{-1} .$$  \hspace{1cm}  (6)
From the definition of $\omega$ in Eq.(2) we easily see that the operator $\omega^\dagger \omega$ is a Hermitian operator acting in the $P$ space and it has positive or zero eigenvalues.

The Hermitian form of $W$ in Eq.(4) is formally exact. However, it has been known that in some cases $W$ can be well approximated by $W_{\text{app}}[8]$. In order to measure the deviation of $W_{\text{app}}$ from the exact $W$, we introduce a quantity

$$
\Delta W = \sum_{ij} \left| \langle i|W - W_{\text{app}}|j \rangle \right| , \text{ where } W_{\text{app}} = \frac{1}{2}(R + R^\dagger) ,
$$

and $|i\rangle$, $|j\rangle$ and $|k\rangle$ are the basis states, which are the eigenstates of the unperturbed Hamiltonian $H_0$. Using a relation in the $|\alpha\rangle$ basis

$$
\frac{\mu_\alpha^2 + 1}{\sqrt{\mu_\alpha^2 + 1}} \langle \alpha|H_0 + R|\beta \rangle = \frac{\mu_\beta^2 + 1}{\sqrt{\mu_\beta^2 + 1}} \langle \alpha|H_0 + R^\dagger|\beta \rangle ,
$$

where both sides are equal to $\langle \alpha|H_0 + W|\beta \rangle[8]$, the deviation $\Delta W$ is converted to

$$
\Delta W = \frac{1}{4} \sum_{ij} \left| \sum_{\alpha\beta} C(\alpha, \beta)^2 \right. 
\times \left\{ \frac{i\langle i|\alpha\rangle \langle \beta|j \rangle}{\mu_\beta^2 + 1} \langle \alpha|H_0 + R|\beta \rangle + \frac{i\langle \beta|\alpha\rangle \langle j|i \rangle}{\mu_\alpha^2 + 1} \langle \alpha|H_0 + R^\dagger|\beta \rangle \right\} \left| ,
\right.
$$

where

$$
C(\alpha, \beta) = \sqrt{\mu_\alpha^2 + 1} - \sqrt{\mu_\beta^2 + 1} .
$$

In general, the matrix element of effective Hamiltonian $H_0 + R$ is bounded, that is,

$$
|\langle \alpha|H_0 + R|\beta \rangle| = |\langle \alpha|H|\beta \rangle + \mu_\beta \langle \alpha|V|\nu_\beta \rangle| \leq (1 + \mu_\beta) V_0 ,
$$

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where $V_0$ is the maximum value of the matrix element of $PHP$ and $PVQ$, and

$$|\nu_\beta\rangle = \mu_\beta^{-1} \omega |\beta\rangle.$$  \hspace{1cm} (12)

From Eqs.(9) and (11) and since $|\langle i|\alpha\rangle\langle\beta|j\rangle| \leq 1$, it can be proved that there exists a constant $W_0$ such that

$$\Delta W \leq W_0 Z_w,$$ \hspace{1cm} (13)

where

$$Z_w = \frac{1}{4} \sum_{\alpha\beta} C(\alpha, \beta)^2 \left\{ \frac{\mu_\alpha + 1}{\mu_\alpha^2 + 1} + \frac{\mu_\beta + 1}{\mu_\beta^2 + 1} \right\}.$$ \hspace{1cm} (14)

Here the constant $W_0$ is independent of $\mu_\alpha$ and has a bound given by $W_0 \leq d^2 V_0$ (we recall that $d$ is the dimension of the $P$ space). From Eqs.(13) and (14) we may say that the magnitude of the deviation $\Delta W$ is determined by the eigenvalues, $\mu_\alpha^2$, of $\omega^\dagger \omega$. If they are small then $C(\alpha, \beta)$ is small and therefore $Z_w$ and $\Delta W$ are also small. This may be understandable naturally because, when the $\mu_\alpha$ are small, the matrix elements $\langle\alpha|PVQ\omega|\beta\rangle$ are small and the effective interactions $R, R'$ and $W$ are almost the same. Eq.(14) gives us another criterion, namely if the $\mu_\alpha$ are state-independent, that is, the $\mu_\alpha$ are close to a constant, then $C(\alpha, \beta)$ is again small and hence so is $\Delta W$. Similar criteria govern the degree of non-Hermiticity of the non-Hermitian effective interaction $R'[9]$.  

As has been discussed in Ref.[9], a set of states

$$|\zeta_\alpha\rangle = \frac{|\alpha\rangle + \mu_\alpha |\nu_\alpha\rangle}{\sqrt{\mu_\alpha^2 + 1}}, (\alpha = 1, 2, ..., d)$$ \hspace{1cm} (15)

span a $d$-dimensional orthogonal subspace, denoted by $S$, where $|\alpha\rangle$ are the eigenstates of $\omega^\dagger \omega$ and $|\nu_\alpha\rangle$ are the $Q$-space states defined in Eq.(11). One
can prove that the space $S$ is an invariant subspace with respect to $H$. In other words, the diagonalization of $H$ within $S$ yields $d$ true eigenstates $|\Phi_k\rangle$ of $H$ in Eq.(1). Since $|\Phi_k\rangle$ can be expressed in terms of only $|\zeta_\alpha\rangle$, the ratio $\mu_\alpha$ of mixing of $|\nu_\alpha\rangle$ into $|\alpha\rangle$ is preserved in any true eigenstate of $H$. The validity of the approximation $W \simeq W_{app}$ is related to the state dependence of the mixing ratio $\mu_\alpha$ between the $P$- and $Q$-space states. If the $Q$-space states mix into the $P$-space states with a constant mixing ratio, the approximation $W \simeq W_{app}$ can be acceptable.

For a simple illustration of the analysis of the approximation $W \simeq W_{app}$ we consider a model problem with an exactly solvable Hamiltonian. The model Hamiltonian we shall use is $H = H_0 + V$, where the unperturbed part is $H_0 = \text{diag}(1, 1, 3, 9)$ and the perturbation is $V = [V_{ij}]$ given by

$$V = \begin{pmatrix}
0 & 5x & -5x & 5x \\
5x & 25x & 5x & -8x \\
-5x & 5x & -5x & x \\
5x & -8x & x & -5x
\end{pmatrix},$$

where $x$ is a parameter that we shall vary. This Hamiltonian was introduced originally by Hoffmann et al.[11], but the matrix elements $V_{13} = V_{31}$ and $V_{24} = V_{42}$ are changed from their original values of zero. The Hamiltonian $H$ has already been applied to the study of non-Hermiticity in the effective interaction by the authors[9].

We shall take the lowest two eigenstates of $H_0$ to be our model space ($P$ space). In principle, provided the true eigenstates have non-zero components in the $P$ space, any set of the true eigenvalues of $H$ can be reproduced from the $P$ space effective Hamiltonian, i.e., $H_0 + R$ with the non-Hermitian
effective interaction $R$ or $H_0 + W$ with the Hermitian form $W$. However, in
the present study we discuss only the effective interactions which reproduce
the true eigenstates with the largest $P$-space overlaps, because our main aim
is not to show the variety of effective interactions but to clarify the validity
of the approximation $W \simeq W_{\text{app}}$.

The effective interaction $R$ reproducing the largest $P$-space overlaps can
be calculated according to the iteration scheme of Krenciglowa and Kuo[12],
which corresponds to the resummation of folded diagrams[13] to infinite or-
der. In the next step by applying Eq.(4), we obtain the Hermitian effective
interaction $W$. In Eq.(4) $W$ is given in the $|\alpha\rangle$ basis, but it will be easy to
rewrite it in terms of the $|\hat{\gamma}\rangle$ basis states which are eigenfunctions of $H_0$. Then
$\Delta W$ can be computed exactly and compared with the bound of Eqs.(13) and
(14).

The exact solution for the eigenstates of $H$ shows that for small $x$ the
states with largest $P$-space overlaps are the first and second lowest states.
As $x$ increases, the largest $P$-space overlap states change to the eigenstates
with the first and third lowest eigenvalues for $0.0689 < x < 0.2655$, while for
$x > 0.2655$ they are the first and fourth eigenvalues. In Table 1 the exact
eigenvalues $E_k$ to be reproduced are shown for six values of $x$ together with
the $P$-space overlaps $I_k$ defined by

$$I_k = \frac{\sum_{i=1}^{2} \langle \hat{\gamma} | \Phi_k \rangle^2}{\langle \Phi_k | \Phi_k \rangle},$$

(16)

where $|\Phi_k\rangle$ is the true eigenstates of $H$. The approximate Hermitian effective
interaction $W_{\text{app}}$ and the exact one $W_{\text{exact}}(=W)$, as well as the deviation $\Delta W$
of $W_{\text{app}}$ from $W_{\text{exact}}$, are presented. The quantity $\delta E$ represents a measure
of the deviation of the eigenvalues $E_k^{app}$ of $H_0 + W_{app}$ from the exact values $E_k$, which is defined by

$$\delta E = \sum_{k=1}^2 |E_k^{app} - E_k| .$$

(17)

The values of $\mu^2_\alpha$, the eigenvalues of $\omega^\dagger \omega$ in Eq.(5), are also presented.

For $x$ of 0.04 the overlap of the true eigenstates with the model space is close to 1 and the matrix elements of $W_{app}$ are identical to $W_{exact}$ to the accuracy quoted. Correspondingly $\Delta W$ is very small, as is $\delta E$. As $x$ increases, the overlaps $I_k$ become smaller and conversely the deviation $\Delta W$ starts to grow. However, at $x$ of 0.22 the deviation $\Delta W$, as well as $\delta E$, is reduced drastically, although the overlaps $I_k$ are not so large. At this value of $x$ we see that the eigenvalues $\mu_\alpha$ are almost the same. Therefore we may say that if the $\mu_\alpha$ are nearly degenerate, $\Delta W$ becomes small and the approximation $W \simeq W_{app}$ is justified. This fact is an expected result of the theoretical prediction for $\Delta W$ in Eqs.(13)–(14). For the larger values of $x$ in Table 1 we notice that, even though we reproduce the eigenstates with the largest $P$-space overlap, the deviation $\Delta W$ and the error in the approximate eigenvalues $\delta E$ become quite sizeable. Our discussion indicates that this is due to one of the $\mu_\alpha$ being large and the other small.

In order to see that $\Delta W$ is bounded by $W_0Z_w$, as shown in Eq.(13), we show $\Delta W$ and $W_0Z_w$ as functions of $x$ in Fig.1. We here take $W_0$ to be 0.6 + 15x which is 3/20 of $d^2V_0$. In Fig.1 there appear two “level-crossing” points, i.e., $x = 0.0689$ and $x = 0.2655$. At these points the second eigenstate with the predominant $P$-space component moves from the second lowest state to the third and subsequently from the third to the fourth. The curves are
discontinuous at these “level-crossing” points. Fig.1 shows clearly that $\Delta W$ never exceeds $W_0 Z_w$, that is, $\Delta W$ is bounded by $W_0 Z_w$. Since $W_0$ is a constant when $x$ is fixed, the validity of the approximation $W \simeq W_{app}$ is governed by $Z_w$ which is a function of $\mu_\alpha$. The characteristics of the function $Z_w$ are that if all $\mu_\alpha$ are small, $Z_w$ becomes small, and if the $\mu_\alpha$ are state independent, i.e., close to a constant, $Z_w$ can also be small. If $\mu_\alpha$ are large and have strong state dependence, $Z_w$ becomes large and the approximation $W \simeq W_{app}$ will be poor. This situation is quite similar to the case of the degree of non-Hermiticity in the effective interaction $R$ as has been discussed in Ref.[9]. In general, we may say that if the degree of non-Hermiticity is small, the approximation $W \simeq W_{app}$ will be good.

In summary, the accuracy of approximating the Hermitian effective interaction $W$ by $W_{app} = (R + R^\dagger)/2$ with the usual non-Hermitian effective interaction $R$ is best judged by the eigenvalues $\mu^2$ of $\omega^\dagger \omega$, where $\omega$ is the operator which maps the model-space states onto the excluded space. Both the theoretical prediction and a model calculation show that if the eigenvalues $\mu^2$ are small or state-independent, the approximation is justified. Our study shows that the accuracy of the approximation $W \simeq W_{app}$ cannot be judged merely by the magnitude of the $Q$-space overlaps in the true eigenstates to be reproduced.

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References


Figure Caption

Figure 1. Comparison of $\Delta W$ (solid line), the deviation of the approximate and the exact Hermitian effective interactions, with the upper bound $W_0Z_w$ as a function of the strength parameter $x$. 