Effective operators in the NCSM formalism

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Received: 12 November 2004 / Revised version: 9 January 2005 / Published online: 29 June 2005 – \odot Società Italiana di Fisica / Springer-Verlag 2005

Abstract. No-core shell model (NCSM) calculations using ab initio effective interactions are very successful in reproducing the experimental nuclear spectra. While a great deal of work has been directed toward computing effective interactions from bare nucleon-nucleon (NN) and three-nucleon forces, less progress has been made in calculating the effective operators. Thus, except for the relative kinetic energy, the proton radius, and the NN pair density, all investigations have used bare operators. We apply the Lee-Suzuki procedure to general one-body operators, investigating the importance of the approximations involved. In particular we concentrate on the limitations of the two-body cluster approximation.

PACS. 21.60.Cs Shell model – 23.20.-g Electromagnetic transitions – 23.20.Js Multipole matrix elements

A long standing problem in the phenomenological shell model was the use of effective charges which arise, in principle, from the truncation of the space. Previous perturbation theory attempts to describe phenomenological charges needed to obtain correct transition strengths have been unsuccessful [\[1\]](#page-1-0), but, on the other hand, recent investigations within the framework of the no-core shell model (NCSM) have reported some progress in explaining the large values of the effective charges [\[2\]](#page-1-1).

In the NCSM, one starts from a nucleon-nucleon (NN) interaction which describes the NN scattering data, and derives an effective interaction in a restricted model space. Three-body interactions have been shown to be important in the correct description of the energy spectra in light nuclei, but they are computationally very demanding. Therefore, in the current investigation we restricted ourselves to two-body interactions. As a result of the space truncation, one should also compute effective operators.

The Lee-Suzuki transformation [\[3\]](#page-1-2) has been used in order to accommodate the short-range two-body correlations, with the condition that the model and excluded spaces are not coupled by the Hamiltonian. Thus, the transformed Hamiltonian is given by

$$
\mathcal{H} = e^{-S} H e^S,\tag{1}
$$

with S determined so that the model space and the excluded space are decoupled, that is $P H Q = 0$, with P and Q the projectors onto the model and excluded spaces, respectively. Such a transformation ensures an energy independent effective interaction in the model space. If one determines the operator S so that the additional decoupling condition $QHP = 0$ is fulfilled, it can be shown that the effective operators determined by the transformation

$$
\mathcal{O} = e^{-S} O e^{S} \tag{2}
$$

are also energy independent [\[4,](#page-1-3)[5\]](#page-1-4). Formally, the operator S can be written by means of another operator ω as $S = \operatorname{arctanh}(\omega - \omega^{\dagger})$, where the new operator fulfills $Q\omega P = \omega$. Hence, one obtains the energy-independent effective Hamiltonian in the model space P

$$
H_{\text{eff}} = P\mathcal{H}P = \frac{P + P\omega^{\dagger}Q}{\sqrt{P + \omega^{\dagger}\omega}} H \frac{P + Q\omega P}{\sqrt{P + \omega^{\dagger}\omega}},
$$
 (3)

and, analogously, any observable can be transformed to the P space as $[4,5]$ $[4,5]$

$$
O_{\text{eff}} = POP = \frac{P + P\omega^{\dagger}Q}{\sqrt{P + \omega^{\dagger}\omega}}O\frac{P + Q\omega P}{\sqrt{P + \omega^{\dagger}\omega}}.
$$
 (4)

The operator ω can be computed simply by using the relation [\[6\]](#page-1-5)

$$
\langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{k \in \mathcal{K}} \langle \alpha_Q | k \rangle \langle \tilde{k} | \alpha_P \rangle, \tag{5}
$$

with $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ the basis states of the P and Q spaces, respectively; $|k\rangle$ denotes states from a selected set K of eigenvectors of the Hamiltonian H in the full A -body space, and $\langle \alpha_P | \tilde{k} \rangle$ is the matrix element of the inverse overlap matrix $\langle \alpha_P | k \rangle$. Therefore, an exact determination

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Fig. 1. $B(E2)$ in ¹²C using effective interaction derived from AV8' potential [\[7\]](#page-1-6). Results as a function of the dimension of the Q-space included (circles) are compared with the bare operator (square) and the experimental value (diamond).

of the operator ω necessary to obtain the effective operators requires the exact solution of the A-body problem, which is the final goal. For practical applications, we approximate the operator ω , by solving eq. [\(5\)](#page-0-0) for a cluster of $a < A$ particles. For further details, we refer the reader to previous publications, e.g., [\[6\]](#page-1-5) and references therein. In the present paper, we restrict the investigation to the two-body cluster, that is $a = 2$. Since, in this case, the transformation ω is a two-body operator, we write the one-body operators in a two-body form, introducing a dependence upon the number of particles.

In this paper, we obtain corrections to electromagnetic multipoles, and the results for a selected quadrupole transition strength are shown in fig. [1.](#page-1-7) We point out that, because non-scalar operators can connect different channels with good angular momentum, the procedure to obtain effective operators is more involved than for the Hamiltonian. Therefore, for general one and two-body operators, one has to restrict the number of states from the Q-space included in the calculation [\[8\]](#page-1-8), checking the convergence of the many-body matrix elements with the number of states included. In fig. [1](#page-1-7) we show how the renormalization of the E2 operator varies with the number of states in the Q-space included in the calculation. The $B(E2)$ remains almost constant, with negligible contributions from the states in the Q-space. This is somehow surprising, as the quadrupole operator connects the model space with the excluded space, and the renormalization was expected to improve the B value obtained with the bare operator. The same result is obtained for the M1 operator, but this result is easier to understand as this operator is defined completely in the model space. Generally, our calculations in large model spaces have shown that the theoretical M1 strengths are often in reasonable accord with the experimental values. The quadrupole transitions involving collective states, however, are usually underestimated, even in the largest model spaces.

The two-body cluster approximation is the main difference between our present approach and a previous NCSM calculation that reported effective charges for ⁶Li in agreement with the phenomenological charges usually employed in shell model calculations. Thus, in ref. [\[2\]](#page-1-1), the authors have performed a Lee-Suzuki transformation which includes up to six-body correlations, by transforming the Hamiltonian from an initial $6\hbar\Omega$ space to a $0\hbar\Omega$ model space, equivalent to a core calculation which fixes four particles in the 0s shell. The electromagnetic operators which they calculated reproduced the transition strengths obtained with bare operators in $6\hbar\Omega$, which were considered to be the correct values. This suggests that the higher-order clusters are important for renormalization of electromagnetic operators.

By using a Gaussian operator of variable range, we can show that the renormalization, obtained at the two-body cluster level [\[6\]](#page-1-5), depends strongly upon the range of the operator [\[9\]](#page-1-9). Thus, for short-range operators, such as the relative kinetic energy, the renormalization is strong, while for long-range operators, it is very weak. The quadrupole operator is infinite range and therefore very weakly renormalized at the two-body cluster level.

In summary, we have implemented the Lee-Suzuki procedure for the renormalization of general one- and twobody operators, at the two-body cluster level. The renormalization is much more involved than for the Hamiltonian, so that we include in the renormalization states from the excluded space one shell at a time, observing the convergence of matrix elements. We have shown that the renormalization fails to improve the transition strengths obtained with bare operators, and we conclude that this is due to the two-body cluster approximation, which renormalizes short-range correlations. The electromagnetic multipoles, however, are infinite range and, thus, are very weakly renormalized. Work on renormalizing form factors is underway where we expect greater success, especially at higher momentum transfers.

I.S. and B.R.B. acknowledge partial support by NFS grants PHY0070858 and PHY0244389. The work was performed in part under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. P.N. received support from LDRD contract 04-ERD-058. J.P.V. acknowledges partial support by USDOE grant No. DE-FG-02-87ER-40371.

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