Effective shell-model hamiltonians from realistic nucleon-nucleon potentials within a perturbative approach

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Abstract

This paper discusses the derivation of an effective shell-model hamiltonian starting from a realistic nucleon-nucleon potential by way of perturbation theory. More precisely, we present the state of the art of this approach when the starting point is the perturbative expansion of the $\hat{Q}$-box vertex function. Questions arising from diagrammatics, intermediate-states and order-by-order convergences, and their dependence on the chosen nucleon-nucleon potential, are discussed in detail, and the results of numerical applications for the $p$-shell model space starting from chiral next-to-next-to-next-to-leading order potentials are shown. Moreover, an alternative graphical method to derive the effective hamiltonian, based on the $\hat{Z}$-box vertex function recently introduced by Suzuki et al., is applied to the case of a non-degenerate $(0+2)$ $\hbar \omega$ model space. Finally, our shell-model results are compared with the exact ones obtained from no-core shell-model calculations.

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1. Introduction

The shell model is the basic theoretical tool for the microscopic description of nuclear structure. As is well known, this model is based on the hypothesis that, as a first approximation, each nucleon inside the nucleus moves independently from the others, in a spherically symmetric mean field. The nucleons then arrange themselves into groups of levels, the "shells", well separated from each other.

The shell model reduces the complex nuclear many-body problem to a very simplified one, where only a few active nucleons (valence nucleons) interact in a truncated model space spanned by a single major shell above an inert core.

This scheme does not take into account neither the degrees of freedom of the core nucleons nor the excitations of the valence nucleons into the shells above the model space. Actually, the physical observables must be calculated within an effective theory, namely the shell-model hamiltonian has to take into account all the degrees of freedom that are not considered explicitly.

The derivation of the effective shell-model hamiltonian may follow two paths. The first and very successful one is phenomenological, where the one- and two-body components of the hamiltonian - the single-particle (SP) energies and the residual interaction - contain free parameters that are fixed to reproduce a set of experimental data. This can be done either using an analytical expression for the residual interaction with adjustable parameters, or treating the hamiltonian matrix elements directly as free parameters (see [1, 2]).

The alternative approach to the derivation of the effective shell-model hamiltonian is the microscopic one, where one starts from a realistic nucleon-nucleon ($NN$) potential, and possibly a three-nucleon one ($3N$), and derive the effective hamiltonian in the framework of the many-body theory. This means that when diagonalizing the shell-model hamiltonian in the model space, its eigenvalues belong to the set of eigenvalues of the full nuclear hamiltonian, defined in the whole Hilbert space.

The most successful way to derive a realistic effective shell-model hamiltonian is rooted in the energy-independent linked-diagram perturbation theory [3], which has been widely employed in shell-model calculations during the last forty years (see review papers [4, 5]). The core of this approach is the perturbative expansion of a vertex function, the so-called $\hat{Q}$-box, as a collection of irreducible valence-linked Goldstone diagrams. The $\hat{Q}$-box is then
employed to solve non-linear matrix equations to derive the desired effective hamiltonian, which can be done by way of iterative techniques \[6\]. In all applications the Lee-Suzuki and Krenciglowa-Kuo iterative methods have been commonly employed, both of them based on the calculation of the derivatives of the \(\hat{Q}\)-box with respect to the energy.

Recently, Suzuki and coworkers \[7\] have introduced an alternative way to derive the shell-model effective hamiltonian, which is a graphical method based on the introduction of another vertex function, the so-called \(\hat{Z}\)-box, whose main advantages are that only the first derivative of the \(\hat{Q}\)-box is needed, and that it can be easily extended to the case of a non-degenerate model space.

In such a scenario, one should keep in mind that in modern nuclear structure calculations it has been evidenced the role of \(3N\) forces, in particular for light nuclei with \(A \leq 12\) \[8, 9, 10\]. Within the framework of the shell-model effective hamiltonian theory, the inclusion of \(3N\) forces yields an effective hamiltonian that consists of one- and two-body components, including also core-polarization effects arising from the \(3N\) force, and an effective three-body interaction that should be explicitly considered in the calculations. The derivation of such a hamiltonian, even if not requiring any refinement of the theory, is a very hard task, and up to the present a shell-model effective hamiltonian derived treating on equal footing both \(NN\) and \(3N\) forces has never been calculated. In this connection it is worth to cite the work by Otsuka et al. \[11\], where only first-order contributions of the normal-ordered two-body parts of \(3N\) forces are taken explicitly into account. On these grounds, we confine our study, without any loss of generality, to effective shell-model hamiltonians derived starting from purely two-body realistic potentials.

The aim of the present work is to try to assess the state of the art of the derivation of the realistic shell-model effective hamiltonian from the perturbative expansion of the \(Q\)-box. In particular, we shall discuss in detail the behavior of the perturbative series, with respect to both the dimension of the space of the intermediate states and the order-by-order convergence.

In this context, we will show the results of shell-model calculations for \(p\)-shell nuclei starting from realistic \(NN\) potentials based on the chiral perturbation theory at next-to-next-to-next-to-leading order (\(N^3\)LO) \[12, 13, 14\]. Moreover, we shall present results of calculations within the \((0 + 2) \hbar \omega\ psd\) model space, using an effective hamiltonian derived by the graphical \(\hat{Z}\)-box method.
The paper is organized as follows. In Section 2 we give an outline of the derivation of the shell-model effective hamiltonian within a perturbative approach. Section 3 is devoted to the discussion of the problematics concerning the diagrammatics and convergence of the $Q$-box perturbative expansion. This is done showing our results for the $p$-shell nuclei, using both 0 and $(0 + 2)$ $\hbar\omega$ model spaces. In Section 4 we compare shell-model results obtained starting from the $N^3$LO potential [12, 13] with the exact ones provided by the \textit{ab initio} no-core shell model [15, 10]. A summary and concluding remarks are given in Section 5.

2. The shell-model effective hamiltonian

In this section, we describe the formalism of the shell-model effective hamiltonian theory.

Let us consider the Schrödinger equation for the $A$-nucleon system in the whole Hilbert space:

$$ H |\Psi_\nu\rangle = E_\nu |\Psi_\nu\rangle. \tag{1} $$

As mentioned in the Introduction, in the frame of the shell-model approach an auxiliary one-body potential $U$ is introduced to break up the nuclear hamiltonian as the sum of an unperturbed one-body term $H_0$, which describes the independent motion of the nucleons, and the interaction hamiltonian $H_1$.

We then write $H = H_0 + H_1$ with $H_0 = \sum_{i=1}^A h_{0i} = \sum_{i=1}^A (T_i + U_i)$ and $H_1 = \sum_{i<j} (V_{ij}^{NN} - U_i)$.

In the shell model, the nucleus is schematized as an inert core plus $n$ interacting valence nucleons moving in the mean field $H_0$. The SP potential $U$ generates an energy spectrum organized in shells. The large energy difference between shells enables to define the core as the $A-n$ nucleons that fill completely the lowest shells. The SP states accessible to the $n$ valence nucleons are then the lowest in energy above the closed core.

Now, it is possible to define a reduced Hilbert space, the model space, in terms of a finite subset of $d$ eigenvectors of $H_0$

$$ |\Phi_i\rangle = [a_1^\dagger \ldots a_n^\dagger] |c\rangle, \tag{2} $$

where $|c\rangle$ represents the inert core, the subscripts 1, 2, ..., $n$ denote the SP valence states and $i$ stands for all the other quantum numbers that specify the state.
More explicitly, we define the projection operators $P$ and $Q = 1 - P$, which project from the complete Hilbert space onto the model space and its complementary space, respectively. They satisfy the properties $P^2 = P$, $Q^2 = Q$, and $PQ = QP = 0$. In terms of eigenvectors of $H_0$, $P$ is defined as

$$P = \sum_{i=1}^{d} |\Phi_i\rangle\langle\Phi_i| .$$ (3)

Our aim is to reduce the eigenvalue problem of Eq. (1) to the model-space eigenvalue problem

$$H_{\text{eff}}P|\Psi_\alpha\rangle = E_\alpha P|\Psi_\alpha\rangle ,$$ (4)

where $\alpha = 1, \ldots, d$ and $H_{\text{eff}}$ is defined only in the model space. In other words, we are looking for a new hamiltonian $\mathcal{H}$ that has the same eigenvalues of the $A$-nucleon system hamiltonian $H$, and satisfies the decoupling equation between the model space $P$ and its complement $Q$:

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

so that the desired effective hamiltonian is $H_{\text{eff}} = P\mathcal{H}P$.

The new hamiltonian $\mathcal{H}$ can be obtained by way of a similarity transformation defined in the whole Hilbert space:

$$\mathcal{H} = X^{-1}HX .$$ (6)

There is of course an infinite class of transformation operators $X$ that satisfy the decoupling equation (5). Suzuki and Lee [6] considered an operator $X$ defined as $X = e^{\omega}$. Without loss of generality, they chose $\omega$ so as to satisfy the following properties:

$$\omega = Q\omega P ,$$ (7)

$$P\omega P = Q\omega Q = P\omega Q = 0 .$$ (8)

Eq. (7) implies that

$$\omega^2 = \omega^3 = \ldots = 0 .$$ (9)

The above equation enables to write $X = 1 + \omega$, and consequently it can be obtained
\[ H_{\text{eff}} = PHP = PHP + PHQ\omega . \] (10)

The operator \( \omega \) may be obtained by solving the decoupling equation (5), which may be rewritten in the following form

\[ QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0 . \] (11)

The above matrix equation is non-linear and can be easily solved, once the hamiltonian \( H \) is explicitly known in the whole Hilbert space. However, this is not an easy task for nuclei with mass \( A > 2 \), and has been recently done only for light nuclei within the framework of ab-initio approaches [16].

The standard approach to solve Eq. (11) in a shell-model calculation is to introduce a vertex function, the \( \hat{Q} \)-box, that can be then expressed as a perturbative expansion.

Let us consider our model space, which we assume to be degenerate:

\[ PHP = \epsilon_0 P . \] (12)

Then, taking into account the decoupling equation (5), the effective hamiltonian \( H_{1\text{eff}} = H_{\text{eff}} - PHP \) can be written in terms of \( \omega \)

\[ H_{1\text{eff}} = PHP - PHP = PHP + PHQ\omega . \] (13)

We now employ the above identity, the decoupling equation (11), and the properties of \( H_0 \) and \( H_1 \), to obtain a recursive equation for the effective hamiltonian \( H_{1\text{eff}} \).

First, since \( H_0 \) is diagonal, we can write the following identity:

\[ QHP = QH_1P + QH_0P = QH_1P . \] (14)

The decoupling equation (11) can then be rewritten in the following form:

\[ QH_1P + QHQ\omega - \omega(\epsilon_0P + H_{1\text{eff}}) = 0 . \] (15)

Using this form of the decoupling equation, we can write the following identity for the operator \( \omega \):

\[ \omega = Q\frac{1}{\epsilon_0 - QHQ}QH_1P - Q\frac{1}{\epsilon_0 - QHQ}\omega H_{1\text{eff}} . \] (16)
Finally, inserting Eq. (16) into the identity (13) that defines $H^{\text{eff}}_1$, we obtain a recursive equation:

$$H^{\text{eff}}_1(\omega) = PH_1 P + PH_1 Q \frac{1}{\epsilon_0 - QHQ} QH_1 P - PH_1 Q \frac{1}{\epsilon_0 - QHQ} \omega H^{\text{eff}}_1(\omega).$$

(17)

We define the vertex function $\hat{Q}$-box by the following identity:

$$\hat{Q}(\epsilon) = PH_1 P + PH_1 Q \frac{1}{\epsilon - QHQ} QH_1 P,$$

(18)

so that the recursive equation (17) can be expressed as

$$H^{\text{eff}}_1(\omega) = \hat{Q}(\epsilon_0) - PH_1 Q \frac{1}{\epsilon_0 - QHQ} \omega H^{\text{eff}}_1(\omega).$$

(19)

Suzuki and Lee [6] suggested two possible iterative techniques to solve Eq. (19), both of them based on the calculation of $\hat{Q}$-box derivatives. In the next subsections, we shall briefly describe these two methods, which have become known as the Krenciglowa-Kuo (KK) and the Lee-Suzuki (LS) techniques.

2.1. The Krenciglowa-Kuo iterative technique

This iterative approach originates from the observation that Eq. (19), coupled with the recursive expression for the operator $\omega$, Eq. (16), leads to the iterative equation:

$$H^{\text{eff}}_1(\omega_n) = \sum_{m=0}^{\infty} \left[-PH_1 Q \left(\frac{-1}{\epsilon_0 - QHQ}\right)^{m+1} QH_1 P \right] \left[H^{\text{eff}}_1(\omega_{n-1})\right]^m.$$

(20)

It should be noted that the quantity inside the square brackets in Eq. (20), which from now on we write as $\hat{Q}_m(\epsilon_0)$, is equal to:

$$\hat{Q}_m(\epsilon_0) = -PH_1 Q \left(\frac{-1}{\epsilon_0 - QHQ}\right)^{m+1} QH_1 P = \frac{1}{m!} \left[\frac{d^m \hat{Q}(\eta)}{d\eta^m}\right]_{\eta=\epsilon_0}.$$

(21)

This identity allows to rewrite Eq. (20) in the final form:
\[
H_{\text{eff}}^{1}(\omega_n) = \sum_{m=0}^{\infty} \frac{1}{m!} \left[ \frac{d^m \hat{Q}(\eta)}{d\eta^m} \right]_{\eta=\epsilon_0} \left[ H_{\text{eff}}^{1}(\omega_{n-1}) \right]^m = \sum_{m=0}^{\infty} \hat{Q}_m(\epsilon_0) \left[ H_{\text{eff}}^{1}(\omega_{n-1}) \right]^m.
\]

(22)

The above approach is known as the Krenciglowa-Kuo iterative method, since, if we make the assumption \(H_{\text{eff}}^{1}(\omega_0) = \hat{Q}(\epsilon_0)\), Eq. (22) can be rewritten as

\[
H_{\text{eff}} = \sum_{i=0}^{\infty} F_i ,
\]

(23)

where

\[
\begin{align*}
F_0 &= \hat{Q}(\epsilon_0) \\
F_1 &= \hat{Q}_1(\epsilon_0)\hat{Q}(\epsilon_0) \\
F_2 &= \hat{Q}_2(\epsilon_0)\hat{Q}(\epsilon_0)\hat{Q}(\epsilon_0) + \hat{Q}_1(\epsilon_0)\hat{Q}_1(\epsilon_0)\hat{Q}(\epsilon_0) \\
&\quad \ldots
\end{align*}
\]

(24)

This is the well-known folded-diagram expansion of the effective hamiltonian as introduced by Kuo and Krenciglowa in [17], where the following operatorial identity has been demonstrated:

\[
\hat{Q}_1\hat{Q} = -\hat{Q} \int \hat{Q} ,
\]

(25)

the integral sign representing the so-called folding operation [18].

### 2.2. The Lee-Suzuki iterative technique

Suzuki and Lee [6] suggested another iterative technique, which can be introduced by rearranging Eq. (19) so as to have an explicit expression of the effective hamiltonian \(H_{\text{eff}}^{1}\) in terms of the operators \(\omega\) and \(\hat{Q}\):

\[
H_{\text{eff}}^{1}(\omega) = \left( 1 + P\hat{H}_1Q \frac{1}{\epsilon_0 - QHQ^{\omega}} \right)^{-1} \hat{Q}(\epsilon_0) .
\]

(26)

The above equation can be rewritten in an iterative form:
$$H_{1}^{\text{eff}}(\omega_{n}) = \left(1 + PH_{1}Q\frac{1}{\epsilon_{0} - QHQ}\omega_{n-1}\right)^{-1}\hat{Q}(\epsilon_{0}) \quad (27)$$

and similarly for the recursive equation (28):

$$\omega_{n} = Q\frac{1}{\epsilon_{0} - QHQ}QH_{1}P - Q\frac{1}{\epsilon_{0} - QHQ}\omega_{n-1}H_{1}^{\text{eff}}(\omega_{n}) \quad (28)$$

The iterative procedure can start from the choice $\omega_{0} = 0$, so we can write:

$$H_{1}^{\text{eff}}(\omega_{1}) = \hat{Q}(\epsilon_{0})$$

$$\omega_{1} = Q\frac{1}{\epsilon_{0} - QHQ}QH_{1}P$$

By doing some algebra, it is possible to demonstrate:

$$\hat{Q}_{1}(\epsilon_{0}) = -PH_{1}Q\frac{1}{\epsilon_{0} - QHQ}Q\frac{1}{\epsilon_{0} - QHQ}QH_{1}P$$

$$\hat{Q}_{1}(\epsilon_{0}) = -PH_{1}Q\frac{1}{\epsilon_{0} - QHQ}\omega_{1} \quad (29)$$

so that, for the next iteration $n = 2$, one has:

$$H_{1}^{\text{eff}}(\omega_{2}) = \left(1 + PH_{1}\frac{1}{\epsilon_{0} - QHQ}\omega_{1}\right)^{-1}\hat{Q}(\epsilon_{0}) =$$

$$= \frac{1}{1 - \hat{Q}_{1}(\epsilon_{0})}\hat{Q}(\epsilon_{0})$$

$$\omega_{2} = Q\frac{1}{\epsilon_{0} - QHQ}QH_{1}P - Q\frac{1}{\epsilon_{0} - QHQ}\omega_{1}H_{1}^{\text{eff}}(\omega_{2}) \quad (30)$$

Finally, the iterative form of the equation for the effective Hamiltonian within the LS approach reads:

$$H_{1}^{\text{eff}}(\omega_{n}) = \left[1 - \hat{Q}_{1}(\epsilon_{0})\sum_{m=2}^{n-1}\hat{Q}_{m}(\epsilon_{0})\prod_{k=n-m+1}^{n-1}H_{1}^{\text{eff}}(\omega_{k})\right]^{-1}\hat{Q}(\epsilon_{0}) \quad (31)$$
The KK and LS techniques to solve the decoupling equation do not necessarily provide the same effective Hamiltonian. In Ref. [6] it has been shown that, when converging, the KK iterative procedure provides an effective Hamiltonian whose eigenstates have the largest model space overlap, while the effective Hamiltonian obtained with the LS one has eigenvalues that are the lowest in energy.

It is worth noting that both procedures are constrained to choose an unperturbed Hamiltonian $H_0$ whose eigenstates belonging to the model space are degenerate in energy. In Ref. [19] an alternative approach to the standard KK and LS procedures has been proposed, which extends these methods to the non-degenerate case by introducing multi-energy $\hat{Q}$-boxes. However, this approach has proved to be quite complicated for practical applications, the only one appeared in the literature being that of Ref. [20].

In the following subsection, another method to calculate the shell-model effective Hamiltonian, recently derived by Suzuki et al. [7], will be outlined.

### 2.3. The $\hat{Z}(\epsilon)$ vertex function

From inspection of Eq. (18), which defines the $\hat{Q}$-box, it can be seen that when $\epsilon$ approaches one of the eigenvalues of $QHQ$, $\hat{Q}(\epsilon)$ has some poles, which can induce instabilities in the numerical derivation.

To overcome such difficulties, Suzuki et al. [7] have recently introduced an alternative vertex function $\hat{Z}(\epsilon)$ that is defined in terms of $\hat{Q}(\epsilon)$ and its first derivative:

$$\hat{Z}(\epsilon) \equiv \frac{1}{1 - \hat{Q}_1(\epsilon)} \left[ \hat{Q}(\epsilon) - \hat{Q}_1(\epsilon)(\epsilon - \epsilon_0)P \right].$$

(32)

In Ref. [7] it has been shown that $\hat{Z}(\epsilon)$ satisfies the following equation

$$\left[ \epsilon_0 + \hat{Z}(E_\alpha) \right] P|\Psi_\alpha\rangle = E_\alpha P|\Psi_\alpha\rangle \quad (\alpha = 1, \ldots, d),$$

(33)

which means that $H_{1\text{eff}}$ may be obtained calculating the $\hat{Z}$-box for those values of the energy, determined self-consistently, that correspond to the “true” eigenvalues $E_\alpha$.

To obtain the $E_\alpha$, let us now consider the eigenvalue problem

$$\left[ \epsilon_0 + \hat{Z}(\epsilon) \right] |\phi_k\rangle = F_k(\epsilon)|\phi_k\rangle \quad (k = 1, 2, \cdots, d),$$

(34)
where $F_k(\epsilon)$ are $d$ eigenvalues that depend on $\epsilon$. The true eigenvalues $E_\alpha$ may be determined by solving the following $d$ equations

$$\epsilon = F_k(\epsilon), \quad (k = 1, 2, \cdots, d).$$

Before discussing how to solve equations (34,35), let us point out some interesting properties of $\hat{Z}(\epsilon)$ and of the associated functions $F_k(\epsilon)$.

In the neighborhood of the poles of $\hat{Q}(\epsilon)$, the behavior of $\hat{Z}(\epsilon)$ is dominated by $\hat{Q}_1(\epsilon)$ and so it can be written $\hat{Z}(\epsilon) \approx (\epsilon - \epsilon_0)P$. This means that $\hat{Z}(\epsilon)$ has no poles and therefore the functions $F_k(\epsilon)$ are continuous and differentiable for any value of $\epsilon$.

Eqs. (34) may have spurious solutions, i.e. solutions that do not correspond to the true eigenvalues $E_\alpha$. However, in Ref. [7] it has been shown that the energy derivative of $F_k(\epsilon)$ becomes zero at $\epsilon = E_\alpha$, so the study of this derivative gives a criterion to get rid of the spurious solutions. In order to solve Eqs. (34) and (35), so as to derive the effective interaction, one may resort to both iterative and non-iterative methods.

In the present paper we have employed a graphical non-iterative method to solve Eqs. (35), which we shall now describe.

As shown previously, the $F_k(\epsilon)$'s are continuous functions of the energy, therefore one of the well-known algorithms to solve nonlinear equations may be employed to determine the solutions of Eqs. (35) as the intersections of the graphs $y = \epsilon$ and $y = F_k(\epsilon)$.

More precisely, if we define the functions $f_k(\epsilon)$ as $f_k(\epsilon) = F_k(\epsilon) - \epsilon$, the solutions of Eqs. (35) can obtained by finding the roots of the equations $f_k(\epsilon) = 0$. To this end, from inspection of the graphs $y = \epsilon$ and $y = F_k(\epsilon)$, we determine for each intersection a small surrounding interval $[\epsilon_a, \epsilon_b]$ such that $f_k(\epsilon_a)f_k(\epsilon_b) < 0$. The assumption that $f_k(\epsilon)$ is monotone in this interval implies the existence of a unique root, that we can determine very accurately employing the secant method algorithm (see for instance Ref. [21]).

Once we have determined the true eigenvalues $E_\alpha$, the effective hamiltonian $H_1^{\text{eff}}$ is built up as

$$H_1^{\text{eff}} = \sum_{\alpha=1}^{d} \hat{Z}(E_\alpha)|\phi_\alpha\rangle\langle\tilde{\phi}_\alpha|,$$

where $|\phi_\alpha\rangle$ is the eigenvector obtained from Eq. (34) while $\langle\tilde{\phi}_\alpha|$ is the correspondent biorthogonal state ($\langle\tilde{\phi}_\alpha|\phi_{\alpha'}\rangle = \delta_{\alpha\alpha'}$).
In conclusion, it is worth pointing out that in the previous discussion we have considered the case of a degenerate unperturbed model space (i.e., $PH_0P = \epsilon_0P$). However, the above formalism can be easily generalized to the non-degenerate case replacing $\epsilon_0P$ with $PH_0P$ in Eqs. (32) and (34).

3. The perturbative approach to the shell-model $H^{eff}$

The present section is devoted to discuss details and problems of the derivation of a shell-model effective hamiltonian by way of the perturbative approach. More precisely, the $Q$-box is calculated perturbatively and then employed to derive the effective hamiltonian within the KK, LS, or $\hat{Z}$-box graphical approaches. It should be pointed out that the above techniques lead to effective hamiltonians whose matrix elements differ at most by a few keV when considering the KK and LS methods, while when using the $\hat{Z}$-box method the differences do not exceed 80 keV. This can be seen from inspection of Tables A.3 and A.4 that can be found in Appendix A.

3.1. The diagrammatic expansion of the $\hat{Q}$-box

The methods presented in the previous subsections are based on the calculation of the $\hat{Q}$-box function:

$$\hat{Q}(\epsilon) = PH_1P + PH_1Q \frac{1}{\epsilon - QHQ} QH_1P .$$

(37)

The term $1/(\epsilon - QHQ)$ can be expanded as a power series

$$\frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty} \frac{1}{\epsilon - QH_0Q} \left( \frac{QH_1Q}{\epsilon - QH_0Q} \right)^n ,$$

(38)

giving rise to a perturbative expression for the $\hat{Q}$-box. The diagrammatic representation of this perturbative expansion is a collection of diagrams that have at least one $H_1$-vertex, are irreducible (i.e., with at least one line not belonging to the model space between two successive vertices), and valence linked (i.e., are linked to at least one external valence line) [22].

Currently, realistic shell-model effective hamiltonians are derived for systems with one and two valence nucleons. The former provides the theoretical effective SP energies, while the two-body residual interaction $V^{eff}$ is obtained from the $H^{eff}$ of the two-valence-nucleon system using a subtraction procedure [23]. Up-to-date applications include in the $\hat{Q}$-box at most Goldstone
diagrams up to third order in $H_1$, which take into account up to $3p - 2h$ excitations for the one valence-nucleon system, and up to $4p - 2h$ excitations for the two valence-nucleon system. A comprehensive work concerning the evaluation of the linked Goldstone diagrams in an angular momentum coupled representation may be found in Ref. [24].

Figure 1: One-body first-order diagram. Graph (a) is the so-called self-energy diagram. Graph (b) represents the matrix element of the harmonic oscillator potential $U = \frac{1}{2}m\omega^2r^2$.

The one-body $\hat{Q}$-box diagram at first order in $H_1$ is reported in Fig. 1. All other $\hat{Q}$-box diagrams up to third order in $H_1$ can be found in Appendix B, and are reported in Fig. B.17 B.19 (one-body diagrams), and in Fig. B.18 B.20 B.21 B.22 (two-body diagrams).

From inspection of Fig. 1 it can be seen that the first-order one-body diagram is composed of the so-called self-energy diagram ($V$-insertion diagram) minus the auxiliary potential $U$-insertion. The $U$-insertion diagrams arise in the perturbative expansion owing to the presence of the $-U$ term in $H_1$.

The ($V - U$)-insertion diagrams turn out to be identically zero when employing a self-consistent Hartree-Fock (HF) auxiliary potential [20]. It is worth noting that in most applications the standard choice for the auxiliary potential is the harmonic-oscillator (HO) one, and that the ($V - U$)-insertion diagrams are neglected, assuming that the differences between the HO and the HF single-particle wavefunctions are negligible. In Subsection 3.4, we shall discuss about the contribution of these terms, comparing different effective hamiltonians derived starting from $\hat{Q}$-boxes with and without ($V - U$)-insertion diagrams.

As we pointed out before, in the existing literature the effective hamiltonians are derived taking into account in the $\hat{Q}$-box at most diagrams up to the third order, being computationally prohibitive to go to higher-order.

In order to have a better estimate of the value to which the perturbation series should converge, it is helpful to resort to the Padè approximant the-
ory \[25, 26\], and to calculate the Padè approximant \([2|1]\) of the \(\hat{Q}\)-box, as suggested in \[27\]:

\[
[2|1] = V_{Qbox}^0 + V_{Qbox}^1 + V_{Qbox}^2 (1 - (V_{Qbox}^2)^{-1} V_{Qbox}^3)^{-1},
\]

(39)

where \(V_{Qbox}^n\) is the square non-singular matrix representing the \(n\)th-order contribution to the \(\hat{Q}\)-box in the perturbative expansion.

In the following subsections we show results which we have obtained calculating \(H_{\text{eff}}\) for two valence nucleons outside \(^4\)He doubly-closed core in the \(p\)-shell model space, and using two potentials based on the chiral perturbation theory at next-to-next-to-next-to-leading order. One is the well-known \(N^3\)LO potential derived by Entem and Machleidt \[12, 13\], that is characterized by a smooth gaussian cutoff around 2.5 fm\(^{-1}\). The other potential, dubbed \(N^3\)LOW \[14\], has a sharp cutoff with a smaller value \(\Lambda = 2.1\) fm\(^{-1}\). In both cases, for protons the Coulomb force has been explicitly added.

### 3.2. Convergence with respect to the intermediate-state space

The \(Q\) space that enters the definition of the \(\hat{Q}\)-box in Eq. \[18\] is infinite, representing the complement of the model space in the whole Hilbert space. This implies that in the calculation of the diagrams composing the \(\hat{Q}\)-box one should perform an infinite sum over the intermediate states between successive vertices. This is unfeasible, so the space of the intermediate states has obviously to be truncated. A well established procedure is to introduce an energy truncation, i.e. the intermediate states whose unperturbed excitation energy is greater than a fixed value \(E_{\text{max}}\) are disregarded. \(E_{\text{max}}\) has to be chosen sufficiently large to ensure that the results are almost independent from its value.

In this regard, it is appropriate to mention the papers by Vary \textit{et al.} \[28\], Kung \textit{et al.} \[29\], and Sommermann \textit{et al.} \[30\], where the convergence rate of the sum over intermediate-particle states in the second-order core polarization contribution to the effective shell-model interaction was studied, using realistic potentials renormalized by way of the Brueckner theory \[31\].

In Figs. 2 and 3, the theoretical energies of the yrast states in \(^6\)Li relative to \(^4\)He are reported as a function of \(E_{\text{max}}\), expressed in terms of the number of oscillator quanta \(N_{\text{max}}\). The energies reported in Figs. 2,3 have been calculated using an effective hamiltonian derived from the \(N^3\)LO and \(N^3\)LOW potentials respectively, including in the \(\hat{Q}\)-box diagrams up to the second order in \(H_1\).
Figure 2: Theoretical energies of $^6$Li yrast states relative to $^4$He, obtained with the N$^3$LO potential, as a function of $N_{\text{max}}$ (see text for details).

Figure 3: Same as in Fig. 2 for N$^3$LOW.

From inspection of Fig. 2 it can be seen that convergence is reached with the N$^3$LO potential when including intermediate states whose unperturbed
excitation energy is less than $E_{\text{max}} = 20 \hbar \omega$, with $\hbar \omega = 19$ MeV. This value of the harmonic oscillator parameter is close to the one provided by the expression \[32\] $\hbar \omega = 45A^{-1/3} - 25A^{-2/3}$ for $A = 4$.

A faster convergence can be obtained using the N$^3$LLOW potential, since, as shown in Fig. 3, the energies are practically stable from $E_{\text{max}} = 10 \hbar \omega$ on. This is related to the fact that the two potentials are characterized by largely different cutoffs, N$^3$LLOW being a low-momentum potential.

In most applications a subtraction procedure \[23\] is used so as to retain from $H_{\text{eff}}^1$ only the effective two-body interaction $V_{\text{eff}}$, while the SP energies are taken from experiment.

We have therefore found it worthwhile to study the convergence properties of $V_{\text{eff}}$ when enlarging the space of intermediate states. To this end, we have kept fixed the set of SP energies, using the one obtained from the effective hamiltonians with the largest number of intermediate states, and calculated the energies of the yrast states in $^6$Li relative to $^4$He, using effective two-body interactions $V_{\text{eff}}$ that correspond to different values of $N_{\text{max}}$.

The results are shown in Figs. 4 and 5 for the N$^3$LO and N$^3$LLOW potentials respectively.

Figure 4: Theoretical energies of $^6$Li yrast states relative to $^4$He, obtained with the N$^3$LO potential, as a function of $N_{\text{max}}$ (see text for details).

Comparing these figures with the previous Figs. 2 and 3 it can be seen
that a faster convergence is obtained. This may support the choice of smaller intermediate state spaces when the SP energies are not derived theoretically but taken, for instance, from experiment.

From now on, our calculations will refer to an intermediate state space with $N_{max} = 22$ and $N_{max} = 18$ for the N$^3$LO and N$^3$LOW potentials, respectively.

It is worth noting that the use of a second-order $\hat{Q}$-box does not imply a loss of generality of the foregoing discussion, since both at second and third order in the $\hat{Q}$-box expansion the $Q$ space is spanned by the same particle-particle, 3-particle 1-hole, and 4-particle 2-hole excitations. Therefore the conclusions drawn previously still hold for an effective hamiltonian derived including diagrams up to third order in the $\hat{Q}$-box expansion.

Concluding this subsection, we would like to point out that an alternative approach to the study of the convergence with respect to the intermediate-state space could be to sum at all orders the ladder diagrams of the perturbative expansion by calculating the Brueckner reaction-matrix $G$ of the N$^3$LO potential.

However, this is not an easy task, since to manage the operator $Q_{2p} = 1 - P$ in the integral equation that defines the $G$ matrix,
\[ G(\omega) = V_{NN} - V_{NN}Q_{2p}\frac{1}{\omega - H_0}Q_{2p}G(\omega) \quad , \tag{40} \]

would mean to handle matrix elements of the \( NN \) potential \( V_{NN} \) in a very large space spanned by the HO wavefunctions.

A way to simplify the calculation of the \( G \) matrix is to resort to the so-called \( G_T \) matrix \[33\], for which plane waves are used as intermediate states:

\[ G_T(\omega) = V_{NN} - V_{NN}Q_{2p}\frac{1}{\omega - Q_{2p}TQ_{2p}}Q_{2p}G_T(\omega) \quad . \tag{41} \]

A main advantage of the \( G_T \) matrix is that an exact treatment of the projection operator \( Q_{2p} \) can be done employing the Tsai-Kuo method \[34\].

By renormalizing the \( N^3 \)LO potential with the \( G_T \) matrix procedure, we have calculated the energies of the yrast states in \( ^6 \)Li relative to \( ^4 \)He, using effective hamiltonians derived at the second order in \( H_1 \), as a function of \( N_{\text{max}} \). The energies are reported in Fig. \( \text{6} \) (case (a)), and compared with the results previously shown in Fig. \( \text{2} \) (case (b)).

![Figure 6: Theoretical energies of \( ^6 \)Li yrast states relative to \( ^4 \)He, obtained with the \( G_T \) matrix derived from the \( N^3 \)LO potential, as a function of \( N_{\text{max}} \) (see text for details).](image-url)
From inspection of Fig. 6, it is evident that the renormalization of the N³LO potential strongly reduce the dependence on the number of intermediate states of the perturbative expansion of $H_{\text{eff}}$, and consequently a faster convergence with respect to $N_{\text{max}}$ is reached. One has to keep in mind, however, that, since the Brueckner reaction matrix is energy dependent, the results (a) are slightly dependent on the choice of the starting energy $\epsilon_0$ in Eq. (19).

3.3. Order-by-order convergence

Now, it is time to focus our attention on the dependence of the effective hamiltonian on the order at which the perturbative expansion of the $\hat{Q}$-box is arrested.

Historically, this problem was faced first in Ref. [35], where some selected third-order and few fourth-order terms in the $G$ matrix were calculated, and the convergence order-by-order of the perturbation series was investigated.

As mentioned in Subsec. 3.1 we have derived effective hamiltonians using $\hat{Q}$-boxes at second order ($H_{\text{eff}}^{2nd}$) and third order ($H_{\text{eff}}^{3rd}$) in perturbation theory. Besides, we have also derived effective hamiltonians calculating the Padè approximant $[2|1]_{25,26}$ of the $\hat{Q}$-box ($H_{\text{Padè}}^{\text{eff}}$). The matrix elements of the latter can be found in the Tables in Appendix A.

Figure 7: Theoretical energies of $^{6}$Li yrast states relative to $^{4}$He, obtained with $H_{\text{eff}}^{1st}$, $H_{\text{eff}}^{2nd}$, $H_{\text{eff}}^{3rd}$, and $H_{\text{Padè}}^{\text{eff}}$ derived from the N³LO potential (see text for details). In the right side of the figure, where an expanded scale is adopted, the $H_{\text{eff}}^{1st}$ results are omitted.
Actually, in the definition of the Padé approximant [2|1] (see Eq. (39)) also the contribution at first order in $H_1$ comes into play, so it is worth to consider also the results obtained using only the diagram of Fig. 1 for the one-body hamiltonian, plus the $NN$ bare potential ($H_{1st}^{\text{eff}}$).

In Figs. 7 and 8 we report the energies of $^6\text{Li}$ yrast states with respect to $^4\text{He}$, obtained with the $N^3\text{LO}$ and $N^3\text{LOW}$ potentials, respectively, and calculated with $H_{1st}^{\text{eff}}, H_{2nd}^{\text{eff}}, H_{3rd}^{\text{eff}}$, and $H_{\text{Pade}}^{\text{eff}}$.

The large difference between the results with $H_{1st}^{\text{eff}}$ and those obtained taking into account the correlations with the core and the shells above the model space ($H_{2nd}^{\text{eff}}, H_{3rd}^{\text{eff}}$) evidences the poor description provided by the bare $NN$ potential without any renormalization due to long-range correlations.

Comparing the results shown in the right sides of both figures, we observe that the differences in the energies obtained with $H_{2nd}^{\text{eff}}$ and $H_{3rd}^{\text{eff}}$ are less notable using the low-momentum $N^3\text{LOW}$ potential. This traces back to the fact that the $N^3\text{LO}$ potential, even though its gaussian cutoff is around 2.5 fm$^{-1}$, exhibits some repulsion in the intermediate range, while the $N^3\text{LOW}$ potential is a real low-momentum potential.

This is testified by the fact that in nuclear matter the $N^3\text{LO}$ potentials saturates, while the $N^3\text{LOW}$ potential does not; in Fig. 9 we report the energy per nucleon in symmetric nuclear matter obtained from a Brueckner-Hartree-Fock calculation. Obviously, the larger repulsive components of the $N^3\text{LO}$ potential influence negatively the order-by-order convergence.
It is worth pointing out, however, that both potentials lead to results obtained with $H_{\text{Pade}}$ that are very close to those with $H_{3\text{rd}}^{\text{eff}}$, thus supporting the hypothesis of a weak dependence of the results on higher-order $\hat{Q}$-box perturbative terms.

On the above grounds, in the following discussions we will employ only effective hamiltonians derived by calculating the Padè approximant $[2|1]$ of the $\hat{Q}$-box.

Finally, it is appropriate to draw attention to the papers by Hjorth-Jensen et al. [36, 37, 38, 39] where, within the framework of the folded-diagram theory, the inclusion of the third-order diagrams in the $G$-matrix in the calculation of the $\hat{Q}$-box was studied and the order-by-order convergence of the effective interaction was examined. The main finding of Ref. [39] was that the effects of third-order contributions in the $T = 1$ channel are almost negligible.

3.4. Dependence on the harmonic-oscillator parameter

As we have mentioned before, the shell-model effective hamiltonian is derived using the harmonic-oscillator potential as the auxiliary potential $U$.

Since we truncate the number of intermediate states and arrest the perturbative expansion of the $\hat{Q}$-box at a certain order, this introduces a dependence on the value of the harmonic-oscillator parameter.
In order to study this dependence, we have derived from the N^3LO potential three effective hamiltonians using ℏω = 18, 19, and 20 MeV, respectively. In Fig. 10, the theoretical energies of the yrast states in ^6Li are reported as a function of ℏω; case (a) refers to effective hamiltonians derived including in the \( \hat{Q} \)-boxes diagrams up to second order in perturbation theory. Case (b) refers to effective hamiltonians derived including all third-order diagrams in the \( \hat{Q} \)-box, and then calculating its Padé approximant [2|1].

From inspection of Fig. 10 it can be observed that while the eigenvalues of the second-order effective hamiltonians retain a significative dependence on the harmonic-oscillator parameter, the effective hamiltonians derived calculating the Padè approximant [2|1] of the \( \hat{Q} \)-box are far less dependent on ℏω. It is worth to note, however, that in case (a) the relative spectra of ^6Li are almost independent of ℏω.

The results shown in Fig. 10 highlight the need to include higher-order terms in the perturbative expansion of the \( \hat{Q} \)-box. In this connection, for the sake of completeness we compare the results obtained in case (b) with those obtained without including second- and third-order \( (V - U) \)-insertion diagrams in the \( \hat{Q} \)-boxes, i.e. taking into account only the first-order one (see Fig. 11). In Fig. 11, the theoretical energies of the yrast states in ^6Li obtained with this procedure (case (c)) are reported and compared with (b).
The results reported in Fig. 11 show that without including consistently order by order the \((V - U)\)-insertion diagrams in the \(\tilde{Q}\)-box, a relevant dependence on \(\hbar \omega\) may be introduced.

Finally, it should be mentioned that in the works in Refs. [40, 41], the role of \((V - U)\)-insertion diagrams has been investigated.

3.5. An application of the \(\tilde{Z}\)-box graphical method: \((0 + 2) \hbar \omega\) shell-model calculations

Starting from a HO unperturbed hamiltonian, it is natural to extend our calculations for the \(p\)-shell model space to a \((0 + 2) \hbar \omega\) one, which includes the \(sd\)-shell orbitals too. In such a case, the unperturbed hamiltonian yields a non-degenerate model space, the \(p\) and \(sd\) orbitals being separated by \(\Delta E = \hbar \omega\).

In Subsec. 2.3 it has been shown that the \(\tilde{Z}\)-box graphical method provides a simple way to derive effective hamiltonians for non-degenerate model spaces. We have therefore found it interesting to employ it to obtain a realistic effective shell-model hamiltonian for the \(psd\) model space.
To this end, we have calculated the Padè approximant $[2|1]$ of the $\hat{Q}$-box as a function of the energy $\epsilon$, starting from the chiral $\text{N}^3\text{LO}$ potential. The $\hat{Q}(\epsilon)$ has been then employed to calculate the vertex-function $\hat{Z}(\epsilon)$, as defined by Eq. (32). The $\hat{Z}(\epsilon)$ is the building block of the graphical method we have described in Subsec. 2.3 to derive $H_{\text{eff}}$, whose equations have been solved using the secant method algorithm (see Fig. 12).

We have to recall now that, when dealing with a $(0 + 2) \hbar \omega$ model space, the results of the diagonalization of the shell-model hamiltonian are affected by the spurious center-of-mass motion [42]. The procedure we have followed to separate in energy the excitations due to the internal degrees of freedom from those with spurious center-of-mass components is the one suggested by Gloeckner and Lawson in Ref. [43].
Thus we have diagonalized the modified shell-model hamiltonian $H'$

$$H' = H_{\text{eff}} + H_{\beta},$$

where $H_{\beta}$ is $\beta$ times the center-of-mass excitation energy of the $A$-nucleon system

$$H_{\beta} = \beta \left\{ \frac{\left( \sum_{i=1}^{A} p_i \right)^2}{2Am} + \frac{m\omega^2}{2A} \left( \sum_{i=1}^{A} r_i \right)^2 - \frac{3}{2} \hbar \omega \right\}. \quad (43)$$

The spurious components are pushed up in energy by increasing the parameter $\beta$, so that one can assume that the low-energy spectrum is free from the above components. Usually, the parameter $\beta$ is expressed as a power of ten $\beta = 10^\alpha$, and the hamiltonian $H'$ is diagonalized increasing $\alpha$ until the low-energy eigenvalues are stable.

In Fig. 13 we report our results for the yrast states of $^6$Li as a function of the $\alpha$ parameter, and compare the positive parity spectrum with the one reported in Fig. 7 corresponding to the $0\hbar\omega$ $p$-shell model space, using the LS method where the Padè approximant of the $Q$-box has been calculated.
From inspection of Fig. 13, it can be observed that the results are quite stable for $\alpha \geq 1.5$. Moreover, it should be noticed that the yrast $4^+, 5^+, 1^-$, and $4^-$ states have not been reported since they turn out to be strongly affected by center-of-mass spuriosity.

Finally, it is worth to note that yrast $0^+, 1^+, 2^+$, and $3^+$ are in an excellent agreement with those calculated within the $0 \hbar \omega$ model space.

4. Comparison of realistic shell model with \textit{ab initio} calculations

In the previous subsections we have shown how the approximations involved in the derivation of realistic shell-model effective hamiltonians may be kept under control by way of some convergence checks.

However, to study the accuracy of these approximations one should compare the final results with those provided by an approach that gives an “exact” solution of the Schrödinger equation (1).

To this end, we will compare in this subsection our results obtained for the $p$-shell nuclei starting from the N$^3$LO potential with those provided from the \textit{ab initio} no-core shell model (NCSM) [15, 10].

All the results shown in the previous subsections have been obtained starting from a $A$-body hamiltonian which is not translationally invariant:

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V_{ij}^{NN}.$$  \hfill (44)

In order to compare realistic shell model with NCSM we have to employ a purely intrinsic Hamiltonian, so we have to remove the center of mass kinetic energy from the hamiltonian of Eq. (44).
We rewrite the intrinsic hamiltonian as follows:

\[ H_{\text{int}} = (1 - \frac{1}{A}) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} \left( V_{ij}^{NN} - \frac{p_i p_j}{m A} \right) = \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + U_i \right) + \left[ \sum_{i<j=1}^{A} \left( V_{ij}^{NN} - U_i - \frac{p_i^2}{2m A} - \frac{p_i p_j}{m A} \right) \right] = H_0 + H_1. \] 

In Fig. 14 the calculated energies of the yrast states in $^6$Li relative to $^4$He are reported. Results labelled with (a) refer to a shell-model calculation with an effective hamiltonian derived from Eq. (44), while the spectrum (b) corresponds to an effective hamiltonian derived from the translationally invariant hamiltonian of Eq. (45). The NCSM spectrum is obtained using the value of the binding energy as calculated in Ref. [10], combined with the calculated excitation energies reported in Ref. [15], and is calculated with respect to the $^4$He ground state energy provided by the N$^3$LO potential [44].

From inspection of Fig. 14 it is evident the need to employ a purely intrinsic hamiltonian when dealing with light nuclei. Moreover, it can be observed that the agreement between the shell-model results and the NCSM ones is quite good.
At this point it is worth to remind that our shell-model effective hamiltonian is derived for a system with only two valence-nucleons. This implies that using this hamiltonian to study nuclei with $n > 2$ valence nucleons, one introduces an approximation due to neglect the 3-, 4-, .. $n$-body components that arise in $H_1^{\text{eff}}$, even if the original hamiltonian contains only a two-body force.

With this remark in mind, we compare in Fig. 15 the ground-state energies, relative to $^4\text{He}$, for the $N = Z$ nuclei with mass $6 \leq A \leq 12$ calculated within the framework of the realistic shell model (dot-dashed line) and of the NCSM (dotted line), with the experimental ones (continuous line) [45].

Figure 15: Ground-state energies for $N = Z$ nuclei with mass $6 \leq A \leq 12$. 

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The shell-model ground state energy for $^6\text{Li}$ is close to the one derived with the NCSM as already shown in Fig. 14, while the discrepancy between the calculated values becomes more significant going from $^{10}\text{B}$ to $^{12}\text{C}$. This can be related to the many-body ($>2$) components of $H_1^{\text{eff}}$, whose role grows with the number of valence nucleons.

Fig. 16 shows the theoretical RSM and NCSM relative spectra of $^{10}\text{B}$ compared with the experimental one [46]. From this figure it can be seen that the RSM excitation energies are in good agreement with the NCSM ones, the largest discrepancy being less than 1 MeV.

![Figure 16: Theoretical and experimental spectra for $^{10}\text{B}$. The theoretical energies have been obtained using the N$^3$LO potential within a realistic shell-model framework (RSM) and via a NCSM calculation (NCSM).](image)

It should be noted that in Ref. [10] it has been pointed out how the contribution of a three-body force improves significantly the reproduction by the theory of both ground state and excitation energies.

5. Summary and remarks

This paper has been devoted to present the current status of the derivation of a shell-model effective hamiltonian within the perturbative approach, starting from a realistic $NN$ potential.
As we have already emphasized, the core of this approach is the perturbative expansion of the well-known $Q$-box vertex function. Therefore, we have focused our attention on the problems arising from the calculation of the $Q$-box perturbative series. We have tackled different questions, all of them dealing with the convergence properties (truncation of the intermediate-state space, order-by-order convergence, dependence on the HO parameter).

At present, it is practically unfeasible to calculate contributions to the perturbative expansion beyond the third order ones. Thus we have presented results obtained by using the theory of the Padé approximants, starting from two different $NN$ chiral potentials that are characterized by different offshell properties. Comparing the results obtained with effective hamiltonians derived calculating the $Q$-box at third order in perturbation theory and those obtained calculating the corresponding $[2|1]$ Padé approximant, we conclude that modern chiral $NN$ potentials provide effective hamiltonians scarcely dependent on higher-order contributions.

The foregoing conclusion is also borne out by the comparison of shell-model results obtained with an effective hamiltonian derived from the chiral $N^3$LO potential with those provided by ab initio NCSM calculations for some $p$-shell nuclei.

Finally, we have applied the recently introduced $Z$-box graphical method to derive a realistic effective hamiltonian for the $(0 + 2) \hbar \omega psd$ model space. The results show the versatility of this new method, which may be easily applied to non-degenerate model spaces.

We hope that the discussions and results given in this paper may provide useful guide to calculating shell-model realistic effective hamiltonians.

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Appendix A. Effective hamiltonians

Table A.1: Single-particle energies (in MeV) of different effective hamiltonians derived from the N$^3$LO potential and calculating the Padé approximant [21] of the $\hat{Q}$-box. Labels LS, $\hat{Z}$-box, and $A = 6$ indicate SP energies obtained using the LS iterative technique, the $\hat{Z}$-box graphical method, and starting from a purely intrinsic hamiltonian for $A = 6$ (see Sec. 4), respectively.

| $nlj$ | $T_z$ | LS  | $\hat{Z}$-box | $A = 6$ |
|-------|-------|-----|---------------|---------|
| 0$p_{3/2}$ | 1/2  | 4.593 | 4.543 | 2.747 |
| 0$p_{1/2}$ | 1/2  | 7.449 | 7.512 | 5.886 |
| 0$p_{3/2}$ | -1/2 | 3.915 | 3.904 | 2.052 |
| 0$p_{1/2}$ | -1/2 | 7.077 | 7.163 | 5.720 |

Table A.2: Same as in Table A.1 for the N$^3$LOW potential.

| $nlj$ | $T_z$ | LS  | $\hat{Z}$-box | $A = 6$ |
|-------|-------|-----|---------------|---------|
| 0$p_{3/2}$ | 1/2  | 4.941 | 4.925 | 3.083 |
| 0$p_{1/2}$ | 1/2  | 7.647 | 7.755 | 5.655 |
| 0$p_{3/2}$ | -1/2 | 4.001 | 3.987 | 2.126 |
| 0$p_{1/2}$ | -1/2 | 6.954 | 6.892 | 5.186 |
Table A.3: Two-body matrix elements (in MeV) of different effective hamiltonians derived calculating the Padé approximant [21] of the $Q$-box from the N³LO potential. They are antisymmetrized, and normalized by a factor $1/\sqrt{(1+\delta_{j_a,j_b})(1+\delta_{j_c,j_d})}$. Labels are the same as in Table A.1.

| $n_{a}l_{a}j_{a}$ | $n_{b}l_{b}j_{b}$ | $n_{c}l_{c}j_{c}$ | $n_{d}l_{d}j_{d}$ | $J$ | $T_z$ | LS | Z-box | $A = 6$ |
|-------------------|-------------------|-------------------|-------------------|-----|------|----|-------|---------|
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 0 1 | -1.954 | -1.926 | -2.298 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 0 1 | -3.636 | -3.630 | -3.804 |
| 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 0 1 | 0.727 | 0.725 | 0.358 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 1 1 | 0.611 | 0.615 | 0.425 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 2 1 | -0.879 | -0.876 | -1.056 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 2 1 | -1.677 | -1.704 | -1.737 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 2 1 | -1.824 | -1.887 | -2.163 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 0 -1 | -2.746 | -2.742 | -3.062 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 0 -1 | -3.754 | -3.760 | -3.958 |
| 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 0 -1 | 0.021 | -0.030 | -0.400 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 1 -1 | 0.135 | 0.111 | -0.054 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 2 -1 | -1.367 | -1.370 | -1.564 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 2 -1 | -1.747 | -1.783 | -1.832 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 2 -1 | -2.205 | -2.295 | -2.538 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 0 0 | -2.656 | -2.642 | -2.976 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 0 0 | -3.751 | -3.809 | -3.932 |
| 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 0 0 | 0.121 | 0.085 | -0.271 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 1 0 | -1.902 | -1.889 | -2.366 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 1 0 | 3.615 | 3.659 | 3.680 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 1 0 | -3.581 | -3.619 | -3.698 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 1 0 | 2.794 | 2.832 | 3.072 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 1 0 | -3.046 | -3.085 | -3.352 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ | 1 0 | 3.224 | 3.301 | 3.347 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ | 1 0 | 1.096 | 1.128 | 1.153 |
| 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ | 1 0 | -3.109 | -3.209 | -3.422 |
| 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 1 0 | -1.143 | -1.205 | -1.247 |
| 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ | 1 0 | -2.113 | -2.166 | -2.850 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 2 0 | -1.369 | -1.370 | -1.554 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 2 0 | -1.230 | -1.252 | -1.286 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ | 2 0 | 1.207 | 1.227 | 1.285 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ | 2 0 | -4.280 | -4.331 | -4.760 |
| 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ | 2 0 | -2.062 | -2.134 | -2.281 |
| 0 $p_{1/2}$ 0 $p_{3/2}$ 0 $p_{1/2}$ 0 $p_{3/2}$ | 2 0 | -4.373 | -4.423 | -4.876 |
| 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ 0 $p_{3/2}$ | 3 0 | -5.137 | -5.118 | -5.565 |
Table A.4: Same as in Table A.3 for the N³LOW potential.

| $n_a l_a j_a$ | $n_b l_b j_b$ | $n_c l_c j_c$ | $n_d l_d j_d$ | $J$ | $T_z$ | LS | Z-box | $A = 6$ |
|---------------|---------------|---------------|---------------|-----|-------|-----|-------|--------|
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 0   | 1     | -2.828 | -2.815 | -3.221 |
| 0p₃/2        | 0p₃/2        | 0p₁/₂        | 0p₃/2        | 0   | 1     | -3.554 | -3.585 | -3.800 |
| 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 0   | 1     | -0.425 | -0.394 | -0.894 |
| 0p₃/2        | 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 1   | 1     | 0.478  | 0.486  | 0.291  |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 2   | 1     | -0.896 | -0.899 | -1.111 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 2   | 1     | -1.893 | -1.906 | -1.971 |
| 0p₃/2        | 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 2   | 1     | -2.077 | -2.109 | -2.447 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 0   | -1    | -3.573 | -3.554 | -3.892 |
| 0p₃/2        | 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 0   | -1    | -3.779 | -3.788 | -3.995 |
| 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 0   | -1    | -1.033 | -1.014 | -1.477 |
| 0p₃/2        | 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 1   | -1    | 0.042  | 0.042  | 0.161  |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 2   | -1    | -1.399 | -1.400 | -1.620 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₁/₂        | 2   | -1    | -1.985 | -1.987 | -2.064 |
| 0p₃/2        | 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 2   | -1    | -2.478 | -2.498 | -2.791 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 0   | 0     | -3.523 | -3.508 | -3.862 |
| 0p₃/2        | 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 0   | 0     | -3.743 | -3.759 | -3.957 |
| 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 0   | 0     | -0.987 | -0.966 | -1.436 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 1   | 0     | -2.283 | -2.254 | -2.676 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₁/₂        | 1   | 0     | 3.631  | 3.626  | 3.682  |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₁/₂        | 1   | 0     | -3.542 | -3.536 | -3.661 |
| 0p₃/2        | 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 1   | 0     | 2.737  | 2.759  | 3.130  |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 1   | 0     | -3.462 | -3.439 | -3.709 |
| 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 0p₃/2        | 1   | 0     | 3.486  | 3.464  | 3.520  |
| 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 0p₃/2        | 1   | 0     | 1.183  | 1.197  | 1.098  |
| 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 0p₃/2        | 1   | 0     | -3.444 | -3.423 | -3.656 |
| 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 1   | 0     | -1.273 | -1.288 | -1.254 |
| 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 0p₁/₂        | 1   | 0     | -3.277 | -3.264 | -3.918 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 2   | 0     | -1.396 | -1.400 | -1.616 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₁/₂        | 2   | 0     | -1.393 | -1.396 | -1.453 |
| 0p₃/2        | 0p₃/2        | 0p₁/₂        | 0p₃/2        | 2   | 0     | 1.372  | 1.375  | 1.461  |
| 0p₃/2        | 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 2   | 0     | -4.678 | -4.693 | -5.098 |
| 0p₃/2        | 0p₁/₂        | 0p₁/₂        | 0p₃/2        | 2   | 0     | -2.055 | -2.041 | -2.285 |
| 0p₁/₂        | 0p₃/2        | 0p₁/₂        | 0p₃/2        | 2   | 0     | -4.675 | -4.690 | -5.090 |
| 0p₃/2        | 0p₃/2        | 0p₃/2        | 0p₃/2        | 3   | 0     | -5.569 | -5.568 | -6.014 |
Appendix B. Diagrammatics

Figure B.17: One-body second-order diagrams. The asterisk indicates non-symmetric diagrams, which occur always in pairs giving equal contributions. For the sake of simplicity we report only one of them.

Figure B.18: Two-body diagrams up to second order in perturbation theory. For the sake of simplicity, for each topology we report only one of the diagrams which correspond to the exchange of the external pairs of lines.
Figure B.19: Same as Fig. B.17 but for third-order diagrams.
Figure B.20: Same as Fig. B.18 but for third-order diagrams.
Figure B.21: Same as Fig. B.20.
Figure B.22: Same as Fig. B.20.
Abstract

Keywords:

1.