Perturbative Approach to Effective Shell-Model Hamiltonians and Operators

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ABSTRACT

The aim of this work is to present an overview of the derivation of the effective shell-model Hamiltonian and decay operators within many-body perturbation theory, and to show the results of selected shell-model studies based on their utilisation. More precisely, we report some technical details that are needed by non-experts to approach the derivation of shell-model Hamiltonians and operators starting from realistic nuclear potentials, in order to provide some guidance to shell-model calculations where the single-particle energies, two-body matrix elements of the residual interaction, effective charges and decay matrix elements, are all obtained without resorting to empirical adjustments. On the above grounds, we will present results of studies of double-$\beta$ decay of heavy-mass nuclei where shell-model ingredients are derived from theory, so to assess the reliability of such a way to shell-model investigations. Attention will be also focussed on the relevant aspects that are connected to the behavior of the perturbative expansion, whose knowledge is needed to establish limits and perspectives of this approach to nuclear structure calculations.

Keywords: Nuclear shell model, effective interactions, many-body perturbation theory, nuclear forces

1 INTRODUCTION

The present paper is devoted to the presentation of the formal details of the derivation of effective shell-model Hamiltonians ($H_{\text{eff}}$) and decay operators by way of a perturbative approach, and to review a large sample of its most recent applications to the study of spectroscopic properties of atomic nuclei. The goal of our work is to provide a useful tool for those practitioners who are interested in employing shell-model single-particle energies, two-body matrix elements, effective charges, magnetic-dipole and $\beta$-decay operators, which are produced by way of many-body theory, without resorting to parameters that are empirically adjusted to reproduce a selection of observables.
As is well known, the nuclear shell model (SM) is widely considered the basic theoretical tool for the microscopic description of nuclear structure properties. Nuclear shell model is based on the ansatz that each nucleon inside the nucleus moves independently from the others, in a spherically symmetric mean field plus a strong spin-orbit term. This first-approximation depiction of a nucleus is supported by the observation of “magic numbers” of protons and/or neutrons, corresponding to nuclei which are more tightly bound than their neighbors.

These considerations lead to depict the nucleons as arranging themselves into groups of energy levels, the “shells”, well separated from each other. The main product of the shell-model scheme is the reduction of the complex nuclear many-body problem to a very simplified one, where only a few valence nucleons interact in a reduced model space spanned by a single major shell above an inert core.

The cost that has to be paid for such a simplification is that shell-model wave functions, describing the independent motion of individual nucleons, do not include the correlations which are induced by the strong short-range bare interaction, and therefore could be very different from the real wave functions of the nuclei. The shell-model Hamiltonian, which will be introduced in the following section, contains one- and two-body components whose characterizing parameters, namely the single-particle (SP) energies and two-body matrix elements (TBMEs) of the residual interaction, account for the degrees of freedom that are not explicitly included in the truncated Hilbert space of the configurations. As a matter of fact, SP energies and TBMEs should be determined to include, in an effective way, the excitations both of core nucleons and of the valence nucleons into the shells above the model space.

The way to the effective SM Hamiltonian may follow two distinct paths.

One approach is phenomenological, that is the one- and two-body components of the Hamiltonian are adjusted to reproduce a selected 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]).

This has been, during seventy years and more of SM calculations, a very successful tool to reproduce a huge amount of data and to describe some of the most fundamental physical properties of the structure of atomic nuclei. In this regard, it is worth to mention the review by Caurier et al. [3] for an interesting discussion about the properties of the effective SM Hamiltonian; a few more references and discussion will be reported in the following section.

The alternative way to the construction of \( H_{\text{eff}} \) is to start from realistic nuclear forces - two- and three-body potentials (if possible) - and derive the effective Hamiltonian in the framework of the many-body theory, namely a \( H_{\text{eff}} \) whose eigenvalues belong to the set of eigenvalues of the full nuclear Hamiltonian, defined in the whole Hilbert space.

To this end, we need a similarity transformation which arranges, within the full Hilbert space of the configurations, a decoupling of the model space \( P \) where the valence nucleons are constrained from its complement \( Q = 1 - P \).

Nowadays, this may achieved within the framework of the \textit{ab initio} methods, which aim to solve the full Hamiltonian of \( A \) nucleons by employing controlled truncations of the accessible degrees of freedom. However, this approach is strictly constrained by the advance in computational power, and, even if successful, is currently confined to few nuclear mass regions. A comprehensive report of possible ways to tackle the problem of the derivation of \( H_{\text{eff}} \) starting from \textit{ab initio} methods can be found in Ref. [4], where the authors review also some SM applications and results.
Our work will be focused on the perturbative expansion of the effective SM Hamiltonian, that is grounded in the energy-independent linked-diagram perturbation theory [5], which has been extensively used in shell-model calculations during the last fifty years (see also review papers [6, 7]).

The earlier attempt along this line has been made by Bertsch [8], who employed as interaction vertices the matrix elements of the reaction matrix $G$ derived from the Kallio-Kolltveit potential [9] to study the role played by the core-polarization diagram at second order in perturbation theory, accounting for one-particle-one-hole ($1p - 1h$) excitations above the Fermi level of the core nucleons. The results of this work evidenced that the contribution of such a diagram to $H_{\text{eff}}$ was about 30% of the first-order two-body matrix element, when considering the open-shell nuclei $^{18}\text{O}$ and $^{42}\text{Sc}$ outside doubly-closed cores $^{16}\text{O}$ and $^{40}\text{Ca}$, respectively.

Then, it came the seminal paper by Tom Kuo and Gerry Brown [10], which is a true turning point in nuclear structure theory. It has indeed been the first successful attempt to perform a shell-model calculation starting from the free nucleon-nucleon (NN) Hamada-Johnston potential (HJ) [11], and resulted in a quantitative description of the spectroscopic properties of $sd$-shell nuclei.

The TBMEs of the $sd$-shell effective interaction in Ref. [10] were derived starting from the HJ potential, the hard-core component being renormalized via the calculation of the reaction-matrix $G$. The matrix elements of $G$ were then employed as interaction vertices of the perturbative expansion of $H_{\text{eff}}$, including terms up to second order in $G$.

The TBMEs obtained within this approach were used to calculate the energy spectra of $^{18}\text{O}$ and $^{18}\text{F}$ and provided good agreement with experiment. Moreover, these matrix elements, as well as those derived two years later for SM calculations in the $fp$ shell [12], have become the backbone of the fine tuning of successful empirical $H_{\text{eff}}$s such as the USD [13] and the KB3G potentials [3, 14].

The theoretical framework has evolved between the end of 1960s and beginning of 1970s, thanks to the introduction of the folded-diagrams expansion which has formally defined the correct procedure for the perturbative expansion of effective shell-model Hamiltonians [15, 16].

In the forthcoming sections we are going to present in detail the derivation of $H_{\text{eff}}$ and of consistent effective SM decay operators, according to the theoretical framework of the many-body perturbation theory. The core of our approach is the perturbative expansion of two vertex functions, the so-called $\hat{Q}$-box and $\hat{\Theta}$-box, in terms of irreducible valence-linked Goldstone diagrams. The $\hat{Q}$-box is then employed to solve non-linear matrix equations to obtain $H_{\text{eff}}$ by way of iterative techniques [17], while the latter together with the $\hat{\Theta}$-box are the main ingredients to derive the effective decay operators [18].

Our paper is organized as follows.

In the next section we will present a general overview of the SM eigenvalue problem, and of the derivation of the effective SM Hamiltonian.

In section 3 we will tackle the problem on the grounds of the Lee-Suzuki similarity transformation [17, 19], and in its sections we will introduce the iterative procedures to solve the decoupling equation which provide this similarity transformation into $H_{\text{eff}}$, both for degenerate and non-degenerate model spaces. Two sections will be devoted also to the perturbative expansion of the $\hat{Q}$-box vertex function and to the derivation of effective SM decay operators.

In section 4 we will show the results of investigations about the double-$\beta$ decay of $^{130}\text{Te}$ and $^{136}\text{Xe}$, and discuss the perturbative properties of $H_{\text{eff}}$ and effective shell-model decay operators.
In the last section, a summary of our present work will be reported.

## 2 GENERAL OVERVIEW

As mentioned in the Introduction, the shell model, introduced into nuclear physics seventy years ago [20, 21], is based on the assumption that, as a first approximation, each nucleon (proton or neutron) inside the nucleus moves independently in a spherically symmetric potential representing the average interaction with the other nucleons. This potential is usually described by a Woods-Saxon or harmonic oscillator (HO) potential including a strong spin-orbit term. The inclusion of the latter term is crucial providing single-particle states clustered in groups of orbits lying close in energy (shells). Each shell is well separated in energy from the others, and this enables to schematize the nucleus as an inert core, made up by shells filled up with neutrons and protons paired to a total angular momentum $J = 0^+$, plus a certain number of external nucleons, the so-called “valence” nucleons. This extreme single-particle shell model is able to successfully describe various nuclear properties [22], as, for instance, the angular momentum and parity of the ground-states in odd-mass nuclei. However, it is clear that to describe the low-energy structure of nuclei with two or more valence nucleons the “residual” interaction between the valence nucleons has to be considered explicitly, the term residual meaning that part of the interaction which is not taken into account by the central potential. The inclusion of the residual interaction removes the degeneracy of the states belonging to the same configuration and produces a mixing of different configurations.

Let us now use the simple nucleus $^{18}$O to introduce some common terminologies used in effective interaction theories.

Suppose we want to calculate the properties of the low-lying states in $^{18}$O. Then, we must solve the Schrödinger equation

$$H |\Psi_\nu \rangle = E_\nu |\Psi_\nu \rangle ,$$

where

$$H = H_0 + H_1 ,$$

and

$$H_0 = \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + U_i \right) ,$$

$$H_1 = \sum_{i<j=1}^{A} V_{ij}^{NN} - \sum_{i=1}^{A} U_i .$$

An auxiliary one-body potential $U_i$ has been introduced in order to break up the nuclear Hamiltonian as the sum of a one-body term $H_0$, which describes the independent motion of the nucleons, and the residual interaction $H_1$. It is worth pointing out that in the following, for sake of simplicity and without any loss of generality, we will assume that the interaction between the nucleons is described by a two-body force only, neglecting three-body contributions. The generalization of the formalism to include 3N forces may be found in Refs. [23, 24].

It is customary to choose an auxiliary one-body potential $U$ of convenient mathematical form, e.g. the harmonic oscillator potential

$$U = \sum_{i=1}^{A} \frac{1}{2} \omega r_i^2 .$$
In Fig. 1 we report the portion of the $H_0$ spectrum relevant for $^{18}\text{O}$.

![Energy shells which characterize the core, valence space, and empty orbitals for $^{18}\text{O}$](image)

**Figure 1.** Energy shells which characterize the core, valence space, and empty orbitals for $^{18}\text{O}$

We expect that the wave functions of the low-lying states in $^{18}\text{O}$ are dominated by components with a closed $^{16}\text{O}$ core (i.e. the $0s$ and $0p$ orbits are filled) and two neutrons in the valence orbits $1s$ and $0d$.

Thus, we choose a model space which is spanned by the vectors

$$|\Phi_i\rangle = \sum_{\alpha\beta \in \text{valence space}} C^i_{\alpha\beta} [a^\dagger_\alpha a^\dagger_\beta]|c\rangle,$$

where $|c\rangle$ represents the unperturbed $^{16}\text{O}$ core, as obtained by completely filling the $0s$ and $0p$ orbits

$$|c\rangle = \prod_{\alpha \in \text{filled shells}} a^\dagger_\alpha |0\rangle,$$

and the index $i$ stands for all the other quantum numbers needed to specify the state (e.g. the total angular momentum).

To sketch pictorially the situation, we report in Fig. 2 some SM configurations labeled in terms of particles and holes with respect to the $^{16}\text{O}$ core.

To solve Eq. (1) using basis vectors like those shown in Fig. 2 amounts to diagonalizing the infinite matrix $H$ in Fig. 3. This is unfeasible, so we want to reduce this huge matrix to a smaller one, $H_{\text{eff}}$, requiring that the eigenvalues of the latter belong to the set of the eigenvalues of the former. The notation $|2p'\ 0h\rangle$ represents a configuration with a closed $^{16}\text{O}$ core plus 2 particles constrained interact in the $sd$ shell.

More formally, it is convenient to introduce the projection operators $P$ and $Q = 1 - P$ that project from the complete Hilbert space onto the model space and its complementary space (excluded space), respectively.

$P$ can be expressed in terms of the vectors in Eq. (6) as follows

$$P = \sum_{i=1}^d |\Phi_i\rangle\langle\Phi_i|,$$
The projection operators \( P \) and \( Q \) satisfy the properties
\[
P^2 = P, \quad Q^2 = Q, \quad PQ = QP = 0 .
\] (9)

The scope of the effective SM interaction theory is to transform the eigenvalue problem of Eq. (1) into a reduced model-space eigenvalue problem
\[
PH_{\text{eff}}P|\Psi_\alpha\rangle = (E_\alpha - E_C)P|\Psi_\alpha\rangle ,
\] (10)
where \( E_C \) is the true energy of the core; i.e. in the present case, the true ground-state energy of \(^{16}\text{O}\).

As mentioned in the Introduction, there are two main lines of attack to derive \( H_{\text{eff}} \):
- using a phenomenological approach
- starting from the bare nuclear interactions by means of a well-suited many-body theory.

In the phenomenological approach, empirical effective interactions containing adjustable parameters are introduced and modified to fit a certain set of experimental data or the two body-matrix elements themselves are treated as free parameters. This approach is very successful and we refer to several excellent reviews \([2, 3, 25, 26, 27]\) for a complete discussion on the topic.

Nowadays, there are several approaches to derive an effective SM Hamiltonian starting from the bare interaction acting among nucleons. As a matter of fact, aside the well-established approaches based on the

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**Figure 2.** Some \(^{18}\text{O}\) shell-model configurations

**Figure 3.** Representation of the matrices \( H \) and \( H_{\text{eff}} \) for \(^{18}\text{O}\)
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many-body perturbation theory [5] or on the Lee-Suzuki transformation [17, 19], novel non-perturbative methods like valence-space in-medium SRG (VS-IMSRG) [28], shell-model coupled cluster (SMCC) [29], or no-core shell-model (NCSM) with a core [30,31,32,33] based on the Lee-Suzuki similarity transformation, are now available. These non-perturbative approaches are firmly rooted in many-body theory and provide somehow different paths to $H_{\text{eff}}$. They can be derived in the same general theoretical framework expressing $H_{\text{eff}}$ as the result of a similarity transformation acting on the original Hamiltonian

$$H_{\text{eff}} = e^G H e^{-G},$$

(11)

where the transformation is parametrized as the exponential of a generator $G$, and is such that the decoupling condition is satisfied

$$Q H_{\text{eff}} P = 0.$$

(12)

In Ref. [4], it can be found a very detailed discussion showing how the different methods (perturbative and non-perturbative) can be derived in such a general framework and describing the corresponding approximation schemes employed in each approach.

As written in the Introduction, the aim of present review is to describe in detail the perturbative approach to the derivation of $H_{\text{eff}}$, topic that will be discussed in the next section. We refer to the already cited review paper by Stroberg et al [4] for an exhaustive description of the alternative methods.

3 THE PERTURBATIVE EXPANSION OF EFFECTIVE SHELL-MODEL OPERATORS

3.1 The Lee-Suzuki similarity transformation

Here, we will present the formalism of the derivation of the effective SM Hamiltonian, according to the similarity transformation introduced by Lee and Suzuki [19]. It is worth noting that this approach has been very successful since it is amenable of a straightforward perturbative expansion of $H_{\text{eff}}$ for open-shell systems outside a closed core, whereas in other approaches - such as, for example, the oscillator based effective theory (HOBET) proposed by Haxton and Song [34] or the coupled-cluster similarity transformation [35] - the factorization of the core configurations with respect to the valence nucleons is far more complicated to perform.

We start from the Schrödinger equation for the $A$-nucleon system, defined in the whole Hilbert space:

$$H |\Psi_\nu\rangle = E_\nu |\Psi_\nu\rangle .$$

(13)

As already mentioned, within the SM framework an auxiliary one-body potential $U$ is introduced to express the nuclear Hamiltonian as the sum of an unperturbed one-body mean-field term $H_0$, plus the residual interaction Hamiltonian $H_1$. The full Hamiltonian $H$ is then rewritten in terms of $H_0, H_1$, as reported in Eqs. (2,4).

According to the nuclear SM that we have introduced in the previous section, the nucleus may be depicted as a frozen core, composed by a number of nucleons which fill a certain number of energy shells generated by the spectrum of the one-body Hamiltonian $H_0$, plus a remainder of $n$ interacting valence nucleons moving in the mean field $H_0$. 

Frontiers
The large energy gap between the shells allows to consider the $A - n$ core nucleons, filling completely the shells which are the lowest in energy, as inert. The SP states accessible to the valence nucleons are those belonging to the major shell just placed (in energy) above the closed core. The configurations allowed by the valence nucleons within this major shell define a reduced Hilbert space, the model space, in terms of a finite subset of $d$ eigenvectors of $H_0$, as expressed in Eq. (6).

We then consider the projection operators $P$ (see Eq. (8)) and $Q = 1 - P$, which project from the complete Hilbert space onto the model space and its complementary space, respectively, and satisfy the properties in Eq. (9).

The goal of a SM calculation is to reduce the eigenvalue problem of Eq. (13) to the model-space eigenvalue problem

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

(14)

where $\alpha = 1, \ldots, d$ and $H_{\text{eff}}$ is defined only in the model space.

This means that we are looking for a new Hamiltonian $\mathcal{H}$ whose eigenvalues are the same of the Hamiltonian $H$ for the $A$-nucleon system, but satisfies the decoupling equation between the model space $P$ and its complement $Q$:

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

(15)

which guarantees that the desired effective Hamiltonian is $H_{\text{eff}} = P \mathcal{H} P$.

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

$$\mathcal{H} = X^{-1} H X .$$

(16)

Of course, the class of transformation operators $X$ that satisfy the decoupling equation (15) is infinite, and Lee and Suzuki [17, 19] have proposed an operator $X$ defined as $X = e^{\omega}$. Without loss of generality, $\omega$ can be chosen to satisfy the following properties:

$$\omega = Q \omega P ,$$

(17)

$$P \omega P = Q \omega Q = P \omega Q = 0 .$$

(18)

Eq. (17) implies that

$$\omega^2 = \omega^3 = \ldots = 0 .$$

(19)

According to the above equation, $X$ may be written as $X = 1 + \omega$, and consequently we have the following expression for $H_{\text{eff}}$:
The operator \( \omega \) may be calculated by solving the decoupling equation (15), and the latter may be rewritten as

\[
QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0 .
\] (21)

The above matrix equation is non-linear and, once the Hamiltonian \( H \) is expressed explicitly in the whole Hilbert space, it can be easily solved. Actually, this is not an easy task for nuclei with mass \( A > 2 \), and, as mentioned in the previous section, this approach has been employed only for light nuclei within the \textit{ab-initio} framework.

A successful way to the solution of Eq. (21) for SM calculations is the introduction of a vertex function, the \( \hat{Q} \)-box, which is suitable of a perturbative expansion.

We proceed now to explicit the \( \hat{Q} \)-box approach towards the derivation of \( H_{\text{eff}} \), and it is important to point out that in the following we assume our model space to be degenerate:

\[
PH_0 P = \epsilon_0 P .
\] (22)

Then, thanks to the decoupling equation (15), the effective Hamiltonian \( H_{\text{eff}}^1 = H_{\text{eff}} - PH_0 P \) can be expressed as a function of \( \omega \)

\[
H_{\text{eff}}^1 = PHP - PH_0 P = PH_1 P + PH_1 Q\omega .
\] (23)

The above identity, the decoupling equation (21), and the properties of \( H_0 \) and \( H_1 \) allow to define recursively the effective Hamiltonian \( H_{\text{eff}}^1 \).

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

\[
QHP = QH_1 P + QH_0 P = QH_1 P .
\] (24)

Then, the decoupling equation (21) can be rewritten in the following form:

\[
QH_1 P + QHQ\omega - \omega(PH_0 P + PH_1 P + PH_1 Q\omega) = QH_1 P + QHQ\omega - \omega(\epsilon_0 P + H_{\text{eff}}^1) = 0 .
\] (25)

Using this expression of the decoupling equation, we can write a new identity for the operator \( \omega \):

\[
\omega = Q\frac{1}{\epsilon_0 - QHQ}QH_1 P - Q\frac{1}{\epsilon_0 - QHQ}QH_1 Q\omega H_{\text{eff}}^1 .
\] (26)

Finally, we obtain a recursive equation by inserting Eq. (26) into the identity (23) which defines \( H_{\text{eff}}^1 \):
We define now the vertex function $\hat{Q}$-box as follows:

$$\hat{Q}(\epsilon) = PH_1 P + PH_1 Q \frac{1}{\epsilon_0 - QHQ} QH_1 P,$$  \hspace{1cm} (28)

that allows to express the recursive equation (27) as

$$H_{1}^{\text{eff}}(\omega) = \hat{Q}(\epsilon_0) - PH_1 Q \frac{1}{\epsilon_0 - QHQ} \omega H_{1}^{\text{eff}}(\omega).$$ \hspace{1cm} (29)

As can be seen from both Eqs. (28,29), configurations belonging to the $Q$ space that are close in energy to the unperturbed energy of model-space configurations (intruder states) may provide unstable solutions of Eq. (29). This is the so-called “intruder-state problem” as introduced in Ref. [36, 37] by Schucan and Weidenmüller. In the following sections we first show two possible iterative techniques to solve Eq. (29), as suggested by Lee and Suzuki[17]. These methods, which are based on the calculation of the $\hat{Q}$-box and its derivatives, are known as the Krencklawa-Kuo (KK) and the Lee-Suzuki (LS) techniques. In particular, we point out that in Ref. [17] the authors have shown that the Lee-Suzuki iterative procedure is convergent even when there are some intruder states.

Then, we will present other approaches that generalize the derivation of $H_{1}^{\text{eff}}$, based on the calculation of the $Q$-box, to unperturbed Hamiltonians $H_0$ which provide non-degenerate model spaces.

3.1.1 The Krencklawa-Kuo iterative technique

The Krencklawa-Kuo (KK) iterative technique for solving the recursive equation (29) traces back to the coupling of Eqs. (29) and (26), which provides the iterative equation:

$$H_{1}^{\text{eff}}(\omega_n) = \sum_{m=0}^{\infty} \left[ -PH_1 Q \left( \frac{-1}{\epsilon_0 - QHQ} \right)^{m+1} QH_1 P \right] \left[ H_{1}^{\text{eff}}(\omega_{n-1}) \right]^m. \hspace{1cm} (30)$$

The quantity inside the square brackets of Eq. (30), that will be dubbed from now on as $\hat{Q}_m(\epsilon_0)$, is proportional to the $m$-th derivative of the $\hat{Q}$-box calculated in $\epsilon = \epsilon_0$:

$$\hat{Q}_m(\epsilon_0) = -PH_1 Q \left( \frac{-1}{\epsilon_0 - QHQ} \right)^{m+1} QH_1 P = \frac{1}{m!} \left[ \frac{d^m \hat{Q}(\epsilon)}{d\epsilon^m} \right]_{\epsilon = \epsilon_0}. \hspace{1cm} (31)$$

We may then rewrite Eq. (30), according to the above identity, as:

$$H_{1}^{\text{eff}}(\omega_n) = \sum_{m=0}^{\infty} \frac{1}{m!} \left[ \frac{d^m \hat{Q}(\epsilon)}{d\epsilon^m} \right]_{\epsilon = \epsilon_0} \left[ H_{1}^{\text{eff}}(\omega_{n-1}) \right]^m = \sum_{m=0}^{\infty} \hat{Q}_m(\epsilon_0) \left[ H_{1}^{\text{eff}}(\omega_{n-1}) \right]^m. \hspace{1cm} (32)$$
The starting point of the KK iterative method is the assumption that \( H_{\text{eff}}^1(\omega_0) = \hat{Q}(\epsilon_0) \), which leads to rewrite Eq. (32) in the following form:

\[
H_{\text{eff}} = \sum_{i=0}^{\infty} F_i , \tag{33}
\]

where

\[
F_0 = \hat{Q}(\epsilon_0) \\
F_1 = \hat{Q}_1(\epsilon_0)\hat{Q}(\epsilon_0) \\
F_2 = \hat{Q}_2(\epsilon_0)\hat{Q}(\epsilon_0) + \hat{Q}_1(\epsilon_0)\hat{Q}_1(\epsilon_0)\hat{Q}(\epsilon_0) \\
... \tag{34}
\]

The above expression represent the well-known folded-diagram expansion of the effective Hamiltonian as introduced by Kuo and Krenciglowa, since in Ref. \[38\] the authors demonstrated the following operatorial identity:

\[
\hat{Q}_1\hat{Q} = -\hat{Q} \int \hat{Q} , \tag{35}
\]

where the integral sign corresponds to the so-called folding operation as introduced by Brandow in Ref. \[15\].

3.1.2 The Lee-Suzuki Iterative Technique

The Lee-Suzuki (LS) technique is another iterative procedure which can be carried out by rearranging Eq. (29) in order to obtain an explicit expression of the effective Hamiltonian \( H_{\text{eff}}^1 \) in terms of the operators \( \omega \) and \( \hat{Q} \) \[17\]:

\[
H_{\text{eff}}^1(\omega) = \left(1 + PH_1Q\frac{1}{\epsilon_0 - QHQ} \omega \right)^{-1} \hat{Q}(\epsilon_0) . \tag{36}
\]

The iterative form of the above equation is the following:

\[
H_{\text{eff}}^1(\omega_n) = \left(1 + PH_1Q\frac{1}{\epsilon_0 - QHQ} \omega_{n-1} \right)^{-1} \hat{Q}(\epsilon_0) , \tag{37}
\]

and we may also write an iterative expression of Eq. (26):

\[
\omega_n = Q\frac{1}{\epsilon_0 - QHQ}QH_1P - Q\frac{1}{\epsilon_0 - QHQ}\omega_{n-1}H_{\text{eff}}^1(\omega_n) . \tag{38}
\]

The standard procedure is to start the iterative procedure by choosing \( \omega_0 = 0 \), so that we may write:
\[ H_{1}^{\text{eff}}(\omega_{1}) = \hat{Q}(\epsilon_{0}) \]
\[ \omega_{1} = Q \frac{1}{\epsilon_{0} - QHQ} QH_{1}P. \]

It can be demonstrated, by performing some algebra, the following identity:
\[ \hat{Q}_{1}(\epsilon_{0}) = -PH_{1}Q \frac{1}{\epsilon_{0} - QHQ} Q \frac{1}{\epsilon_{0} - QHQ} QH_{1}P = -PH_{1}Q \frac{1}{\epsilon_{0} - QHQ} \omega_{1}, \quad (39) \]

then, for the following iteration \( n = 2 \) we have:
\[ H_{1}^{\text{eff}}(\omega_{2}) = \left( 1 + PH_{1}Q \frac{1}{\epsilon_{0} - QHQ} \omega_{1} \right)^{-1} \hat{Q}(\epsilon_{0}) = \]
\[ = \frac{1}{1 - \hat{Q}_{1}(\epsilon_{0})} \hat{Q}(\epsilon_{0}) \]
\[ \omega_{2} = Q \frac{1}{\epsilon_{0} - QHQ} QH_{1}P - Q \frac{1}{\epsilon_{0} - QHQ} \omega_{1} H_{1}^{\text{eff}}(\omega_{2}). \quad (40) \]

Finally, the LS iterative expression of \( H_{\text{eff}} \) is the following:
\[ H_{1}^{\text{eff}}(\omega_{n}) = \left[ 1 - \hat{Q}_{1}(\epsilon_{0}) \sum_{m=2}^{n-1} \hat{Q}_{m}(\epsilon_{0}) \prod_{k=n-m+1}^{n-1} H_{1}^{\text{eff}}(\omega_{k}) \right]^{-1} \hat{Q}(\epsilon_{0}). \quad (41) \]

It is important to point out that KK and LS iterative techniques, which allow the solution of the decoupling equation 25 in principle do not provide the same \( H_{\text{eff}} \). Suzuki and Lee have shown that the KK iterative approach provides an effective Hamiltonian whose eigenstates have the largest overlap with the model space ones, and that \( H_{\text{eff}} \) obtained employing the LS technique has eigenvalues that are the lowest in energy among those belonging to the set of the full Hamiltonian \( H \) [17].

Both procedures we have presented are are limited to employ an unperturbed Hamiltonian \( H_{0} \) whose model-space eigenstates are degenerate in energy. However, in Ref. [32] the authors have introduced an alternative approach to the standard KK and LS techniques, whose goal is to extend these methods to the non-degenerate case by introducing multi-energy \( \hat{Q} \)-boxes. Actually, this approach is quite involved for practical applications, the only one existing in the literature being that in Ref. [40].

In the following sections, we outline two methods [41, 42] to derive effective SM Hamiltonians which may be implemented straightforwardly to employ \( H_{0} \) that are non-degenerate within the model space.

### 3.1.3 The Kuo-Krenciglowa technique extended to non-degenerate model spaces

The extended Kuo-Krenciglowa (EKK) method is an extension of the KK iterative technique to derive a \( H_{\text{eff}} \) within non-degenerate model spaces [41, 43].
We will now summarize the EKK method as follows.

First, a shifted Hamiltonian $\tilde{H}$ is introduced in terms of an energy parameter $E$

$$\tilde{H} = H - E. \quad (42)$$

Then, we rewrite Eq. (25) in terms of $\tilde{H}$:

$$\left(E - QHQ\right)\omega = QH_1P - \omega P\tilde{H}P - \omega PH_1Q\omega = QH_1P - \omega \tilde{H}_{\text{eff}}. \quad (43)$$

Eq. (43) may be solved by way of an iterative procedure, analogously to the KK technique, in terms of the $\tilde{Q}$-box and its derivatives, as defined in Eqs. (28) and (31), respectively.

The effective Hamiltonian $\tilde{H}_{\text{eff}}$ at the $n$-step of the iterative procedure may be then expressed as follows [41]:

$$\tilde{H}^{(n)}_{\text{eff}} = \tilde{H}_{\text{BH}}(0) + \sum_{k=1}^{\infty} \tilde{Q}_k(0) \left[ \tilde{H}^{(n-1)}_{\text{eff}} \right]^k, \quad (44)$$

where $\tilde{H}_{\text{BH}}$ is the solution of the Bloch-Horowitz equation [44]:

$$\tilde{H}_{\text{BH}}(E) = P \tilde{H}P + PH_1Q \frac{1}{E - QHQ} QH_1P. \quad (45)$$

We observe that the EKK method does not require $H_0$ to be degenerate within the model space, and has been therefore applied to derive $H_{\text{eff}}$ in a multi-shell valence space [45, 46] and in Gamow SM calculations with realistic $NN$ potentials [47, 48].

It is worth pointing out that, since $\tilde{H}_{\text{eff}} = \lim_{n \to \infty} \tilde{H}^{(n)}_{\text{eff}}$, we can write

$$\tilde{H}_{\text{eff}} = \tilde{H}_{\text{BH}}(0) + \sum_{k=1}^{\infty} \tilde{Q}_k(0) \left[ \tilde{H}_{\text{eff}} \right]^k, \quad (46)$$

Eq. (46) may be interpreted as a Taylor series expansion of $\tilde{H}_{\text{eff}}$ around $\tilde{H}_{\text{BH}}$, and the parameter $E$ corresponds to a shift of the origin of the expansion, and a resummation of the series [45]. As a matter of fact, because of Eq. (42) we may express $\tilde{H}_{\text{eff}}$ as

$$H_{\text{eff}} = \tilde{H}_{\text{eff}} + E = H_{\text{BH}}(0) + \sum_{k=1}^{\infty} \tilde{Q}_k(0) \left[ \tilde{H}_{\text{eff}} \right]^k, \quad (47)$$

Now, both sides of the above equation will be independent of $E$, providing that the summation is carried out at infinity, and the parameter $E$ may be tuned to accelerate the convergence of the series, when in practical applications a numerical partial summation needs to be employed and a perturbative expansion of the $\tilde{Q}$-box is carried out [45].
3.1.4 The $\hat{Z}(\epsilon)$ vertex function

Suzuki and coworkers in Ref. [42] have proposed an approach to the derivation of $H_{\text{eff}}$ that aims to avoid the divergencies of the $\hat{Q}$-box vertex function, if a non-degenerate model space in considered. In fact, the definition of the $\hat{Q}$-box in Eq. (28) evidences that if $\epsilon$ approaches one of the eigenvalues of $QHQ$, then instabilities may arise if one employs a numerical derivation, since these eigenvalues are poles for $\hat{Q}(\epsilon)$.

We now sketch out the procedure of Ref. [42] and, for the sake of simplicity, consider the case of a degenerate unperturbed model space (i.e., $PH_0P = \epsilon_0 P$).

A new vertex function $\hat{Z}(\epsilon)$ is introduced and defined in terms of $\hat{Q}(\epsilon)$ and its first derivative as follows:

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

(48)

It can be demonstrated that $\hat{Z}(\epsilon)$ satisfies the following equation [42]:

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

(49)

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

To calculate $E_\alpha$, we solve the following eigenvalue problem

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

(50)

where $F_k(\epsilon)$ are $d$ eigenvalues that depend on $\epsilon$. Then, the true eigenvalues $E_\alpha$ can be obtained through the solution of the $d$ equations

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

(51)

First, it is worth pointing out some fundamental properties of $\hat{Z}(\epsilon)$ and of the associated functions $F_k(\epsilon)$ and then we proceed to discuss the solution of the equations (50,51).

The behavior of $\hat{Z}(\epsilon)$ in proximity of the poles of $\hat{Q}(\epsilon)$ is dominated by $\hat{Q}_1(\epsilon)$, and we may write $\hat{Z}(\epsilon) \approx (\epsilon - \epsilon_0)P$. This means that $\hat{Z}(\epsilon)$ has no poles and therefore $F_k(\epsilon)$ are continuous and differentiable functions for any value of $\epsilon$.

Eqs. (51) may have solutions that do not correspond to the true eigenvalues $E_\alpha$, namely spurious solutions. In Ref. [42] it has been shown that, since the energy derivative of $F_k(\epsilon)$ approaches to zero at $\epsilon = E_\alpha$, the study of this derivative provides a criterion to locate and reject spurious solutions. The solution of Eqs. (50) and (51), that are necessary to derive the effective interaction, may be obtained employing both iterative and non-iterative methods.

We describe here a graphical non-iterative method to solve Eqs. (51).
As mentioned before, the \( F_k(\epsilon) \)'s are continuous functions of the energy, therefore the solutions of Eqs. \( (51) \) may be determined as the intersections of the graphs \( y = \epsilon \) and \( y = F_k(\epsilon) \) employing one of the well-known algorithms to solve nonlinear equations.

More precisely, if we define the functions \( f_k(\epsilon) \) as \( f_k(\epsilon) = F_k(\epsilon) - \epsilon \), the solutions of Eqs. \( (51) \) can obtained by finding the roots of the equations \( f_k(\epsilon) = 0 \). From inspection of the graphs \( y = \epsilon \) and \( y = F_k(\epsilon) \), we can locate for each intersection a small surrounding interval \([\epsilon_a, \epsilon_b]\) where \( f_k(\epsilon_a)f_k(\epsilon_b) < 0 \).

The assumption that \( f_k(\epsilon) \) is a monotone function within this interval implies the existence of a unique root, which can be accurately determined by means of the secant method algorithm (see for instance Ref. \[49\]).

After we have determined the true eigenvalues \( E_\alpha \), the effective Hamiltonian \( H_{1b}^{\text{eff}} \) is constructed as

\[
H_{1b}^{\text{eff}} = \sum_{\alpha=1}^{d} \hat{Z}(E_\alpha)|\phi_\alpha\rangle \langle \tilde{\phi}_\alpha|, \tag{52}
\]

where \( |\phi_\alpha\rangle \) is the eigenvector obtained from Eq. \( (50) \) while \( \langle \tilde{\phi}_\alpha| \) is the correspondent biorthogonal state (\( \langle \tilde{\phi}_\alpha|\phi_{\alpha'}\rangle = \delta_{\alpha\alpha'} \)).

As we have mentioned at the beginning of this section, we have considered the case of a degenerate unperturbed model space (i.e., \( PH_0P = \epsilon_0P \)), but the above formalism can be easily generalized to the non-degenerate case replacing \( \epsilon_0P \) with \( PH_0P \) in Eqs. \( (48-50) \).

### 3.2 The diagrammatic expansion of the \( \hat{Q} \)-box vertex function

The methods to derive \( H_{\text{eff}} \), which have been presented in the previous sections, need the calculation of the \( \hat{Q} \)-box function vertex function:

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

For our purpose, the term \( 1/(\epsilon - QHQ) \) should be expanded as a power series

\[
\frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty} \frac{1}{\epsilon - QH_0Q} \left( \frac{QH_1Q}{\epsilon - QH_0Q} \right)^n, \tag{53}
\]

leading to a perturbative expansion of the \( \hat{Q} \)-box. It is useful to employ a diagrammatic representation of this perturbative expansion, which is a collection of Goldstone diagrams that have at least one \( H_1 \)-vertex, are irreducible - namely at least one line between two successive vertices does not belong to the model space - and are linked to at least one external valence line (valence linked) \[16\].

The standard procedure for most perturbative derivations of \( H_{\text{eff}} \) is to deal with systems with one and two valence nucleons, but later we will also show our way to include contributions from three-body diagrams that come into play when more than two valence nucleons are considered. \( H_{\text{eff}}^{1b} \) of single valence-nucleon nuclei provides the theoretical effective SP energies, while TBMEs of the residual interaction \( V_{\text{eff}} \) are obtained from the \( H_{\text{eff}}^{2b} \) for systems with two valence nucleons. This can be achieved by a subtraction procedure \[50\], namely removing from \( H_{\text{eff}}^{2b} \) the diagonal component of the effective SP energies, derived from the \( H_{\text{eff}}^{1b} \) of the one valence-nucleon systems.
A useful tool, for those who want acquire a sufficient knowledge about the calculation of $\hat{Q}$-box diagrams in an angular momentum coupled representation, is the paper by Kuo and coworkers in Ref. [51].

It is worth pointing out that in current literature the effective SM Hamiltonians are derived accounting for $\hat{Q}$-box diagrams at most up to the third order in perturbation theory, since it is computationally highly demanding to perform calculations including complete higher-order sets of diagrams. A complete list can be found in Ref. [52], Appendix B, and it is a collection of 43 one-body and 135 two-body diagrams. It should be pointed out that lists of diagrams may be easily obtained using algorithms which generate order-by-order Hugenholtz diagrams for perturbation theory applications (see, for example, Ref. [53]).

![Figure 4. Two-body ladder diagram at third order in perturbation theory. Arrow lines represent incoming/outcoming and intermediate particle states. Wavy lines indicate interaction vertices.](image)

Since the aim of present work is to support practitioners with useful tips to derive effective SM Hamiltonians within the perturbative approach, we are going to show some selected examples of $\hat{Q}$-box diagrams and their analytical expression. Our first example is the third-order ladder diagram $V_{ladder}$ shown in Fig. 4 and to explicit its expression we will use the proton-neutron angular-momentum coupled representation for the TBMEs of the input $V_{NN}$:

$$\langle 1, 2; J | V_{NN} | 3, 4; J \rangle \equiv \langle n_1 l_1 j_1 t_{z_1}, n_2 l_2 j_2 t_{z_2}; J | V_{NN} | n_3 l_3 j_3 t_{z_3}, n_4 l_4 j_4 t_{z_4}; J \rangle .$$

The TBMEs elements of the input potential $V_{NN}$ are antisymmetrized but not normalized to ease the calculation of the $\hat{Q}$-box diagrams, $n_m, l_m, j_m, t_{z_m}$ indicate the orbital and isospin quantum numbers of the SP state $m$.

The analytical expression of $V_{ladder}$ is:

$$\langle a, b; J | V_{ladder} | c, d; J \rangle = + \frac{1}{4} \sum_{p_1 p_2 p_3 p_4} \frac{\langle a, b; J | V_{NN} | p_1, p_2; J \rangle \langle p_1, p_2; J | V_{NN} | p_3, p_4; J \rangle \langle p_3, p_4; J | V_{NN} | c, d; J \rangle}{[\epsilon_0 - (\epsilon_{p_1} + \epsilon_{p_2})][\epsilon_0 - (\epsilon_{p_3} + \epsilon_{p_4})]},$$

where $\epsilon_m$ denotes the unperturbed single-particle energy of the orbital $j_m$, $\epsilon_0$ is the so-called starting energy, namely the unperturbed energy of the incoming particles $\epsilon_0 = \epsilon_c + \epsilon_d$. 

This is a provisional file, not the final typeset article
We point out that the factor $+1/4$ is related to the rules that characterize the calculation of overall factors in $\hat{Q}$-box Goldstone diagrams; for any diagram we have a phase factor

$$(-1)^{n_h+n_l+n_c+n_{exh}}$$

whose value is determined by the total number of hole lines ($n_h$), the total number of closed loops ($n_l$), the total number of crossings of different external lines as they trace through the diagrams ($n_c$), and the total number of external hole lines which continuously trace through the diagrams ($n_{exh}$) [51]. There is also a factor $(1/2)^{n_{ep}}$, that accounts of the number of pairs of lines which start together from one interaction vertex and end together to another one ($n_{ep}$).

The diagram in Fig. 4 exhibits $n_h = n_l = n_c = n_{exh} = 0$, consequently the phase is positive. The number of pairs of particles starting and ending together in the same vertices is $n_{ep} = 2$, and consequently the overall factor is $+1/4$.

![Diagram](image)

**Figure 5.** Two-body $3p-1h$ diagram at third order in perturbation theory. Arrow lines represent incoming/outcoming and intermediate particle/hole states. Wavy lines indicate interaction vertices.

The factorization of Goldstone diagrams such as the ladder one in Fig. 4 is quite simple in terms of its interaction vertices. There is a large class of diagrams, as for example the three-particle-one-hole diagram ($3p-1h$) in Fig. 5, which require some considerations in order to provide a straightforward factorization.

The factorization may be easily performed by taking into account that the interaction operator $V_{NN}$ transforms as a scalar under rotation, and so introducing the following cross-coupling transformation of the TBMEs:

$$\langle a, b; J | V_{NN} | c, d; J \rangle_{CC} = \frac{1}{\hat{J}} \sum_{J'} \hat{J}' X \left( \begin{array}{ccc} j_c & j_a & J \\ j_d & j_b & J' \end{array} \right) \langle a, b; J' | V_{NN} | c, d; J' \rangle, \quad (56)$$

where $\hat{x} = (2x + 1)^{1/2}$. $X$ is the so-called standard normalized 9-$j$ symbol, expressed as follows in terms of the Wigner 9-$j$ symbol [54]:

$$X \left( \begin{array}{ccc} r & s & t \\ u & v & w \\ x & y & z \end{array} \right) = \hat{t} \hat{w} \hat{x} \hat{y} \left( \begin{array}{ccc} r & s & t \\ u & v & w \\ x & y & z \end{array} \right).$$
The orthonormalization properties of the $X$ symbol allow then to write the direct-coupled TBMEs in terms of the cross-coupled TBMEs:

$$\langle a, b; J|V_{NN}|c, d; J \rangle = \frac{1}{J} \sum_{J'} J' X j_{c} j_{d} J j_{a} j_{b} J \langle a, b; J'|V_{NN}|c, d; J' \rangle_{CC}$$ (57)

Eqs. (56,57) help to perform the factorization of diagram in Fig. 5; first a rotation according Eq. (57) transforms the direct coupling to the total angular momentum $J$ into the cross-coupled one $J'$ (diagram A going into diagram $A_1$ in Fig. 5). This allows to cut the inner loop and factorize the diagram into two terms, a ladder component $(\alpha)$ and a cross-coupled matrix element $(\beta)$ (diagram $A_2$ in Fig. 5):

$$(\alpha) = \langle a, p_3; J'|A|c, h; J' \rangle_{CC}$$

$$\langle h, b; J'|V_{NN}|p_3, d; J' \rangle_{CC}$$ (58)

Then, we transform the ladder diagram (A) back to a direct coupling to $J''$ by way of Eq. (56), and factorize it into the TBMEs (I) and (II) (diagram $A_3$ in Fig. 5):

$$(I) = \langle a, p_3; J''|V_{NN}|p_1, p_2; J'' \rangle$$

$$(II) = \langle p_1, p_2; J''|V_{NN}|c, h; J'' \rangle$$

The analytical expression of the diagram in Fig. 5 is the following:

$$\langle a, b; J|V_{3p1h}|c, d; J \rangle = -\frac{1}{2} \frac{1}{J} \sum_{h p_1 p_2 p_3} \sum_{J', J''} J'' X j_{c} j_{d} J j_{a} j_{b} J \langle a, b; J'|V_{NN}|p_1, p_2; J' \rangle X j_{h} j_{p_1} J' j_{h} j_{p_2} J' \langle h, b; J'|V_{NN}|p_3, d; J' \rangle_{CC} \langle a, p_3; J''|V_{NN}|p_1, p_2; J'' \rangle \langle p_1, p_2; J''|V_{NN}|c, h; J'' \rangle$$

The factor $(-1/2)$ accounts the fact that $n_{ep} = 1, n_h = n_l = 1$, and that an extra-phase factor $(-1)^{n_{ph}}$ is needed for the total number of cut of particle-hole pairs ($n_{ph}$) [51], since in order to factorize the diagram we have cut the inner loop.

It is important pointing out that there are other three diagrams with the same topology as the one in Fig. 5 which corresponds to the exchange of the external incoming and outcoming particles.

Let us now turn our attention to one-body diagrams.

First of all, we consider the contribution of diagrams such as the one in Fig. 6.

The diagram in Fig. 6 is the so-called $(V-U)$-insertion diagram, and is composed of the self-energy diagram $(V$-insertion diagram) minus the auxiliary potential $U$-insertion. The $U$-insertion diagrams are due to the presence of the $-U$ term in $H_1$. The analytical expression of this diagrams is the following:
\[ \langle a\|[V-U]\]|b\rangle = \frac{\delta_{ja,jb}}{2Ja + 1} \sum_{Jh} (2J + 1) \langle ja, h; J|V|jb, h; J \rangle - \langle a\|[U]\]|b\rangle \] (59)

Figure 6. \((V-U)\)-insertion diagram. Graph (A) is the self-energy diagram. Graph (B) represents the matrix element of the harmonic oscillator potential \(U = \frac{1}{2}m\omega^2 r^2\).

The calculation of the self-energy diagram A has been performed by coupling the external lines to a scalar, which leads the SP total angular momentum and parity \(Ja, jb\) being identical. Then, we cut the inner hole line and, since SP states \(a, b\) are coupled to \(J = 0^+\), we apply the transformation in Eq. (56) for \(J = 0^+\).

Since the standard choice for the auxiliary potential is the harmonic-oscillator (HO) one, it appears also the reduced matrix element of \(U = \frac{1}{2}m\omega^2 r^2\) between SP states \(a, b\) (graph B).

It is worth pointing out that the diagonal contributions of \((V-U)\)-insertion diagrams, for SP states belonging to the model space, correspond to the first order contribution of the perturbative expansion of the effective SM Hamiltonian of single valence-nucleon systems \(H^{1b}_{\text{eff}}\).

Moreover, \((V-U)\)-insertion diagrams turn out to be identically zero when employing a self-consistent Hartree-Fock (HF) auxiliary potential [40], and in Ref. [52] it has been discussed the important role played by these terms, comparing different effective Hamiltonians derived starting from \(\hat{Q}\)-boxes with and without contributions from \((V-U)\)-insertion diagrams.

Now, we will show an example of one-body diagram and comment briefly its analytical calculation.

We consider the diagram as reported in Fig. 7 while the complete list of third-order one-body diagrams can be found in Ref. [52] Fig. B.19.

We dub this diagram \(V_{2p1h}\), since between the upper interaction vertices they appear two particles and 1 hole as intermediate states. This belongs to the group of non-symmetric diagrams, which occur always in pairs giving equal contributions. Its analytical expression is:
Figure 7. An example of one-body diagram (see text for details).

\[
\langle j \| V_2 p_1 h \| j \rangle = -\frac{1}{2j+1} \sum_{J=0}^{J'=0+} \frac{2J+1}{(2J+1)} \frac{\langle j, h_2; J \| V_{NN} | p_1, p_2; J \rangle \langle p_1, p_2; J \| V_{NN} | h_1, h_2; J \rangle \langle h_1 \| V-U \| j \rangle}{[\epsilon_0 - (\epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_2})][\epsilon_0 - (\epsilon_j + \epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_1} - \epsilon_{h_2})]},
\]

(60)

\(\epsilon_0 = \epsilon_j\) being the unperturbed SP energy of the incoming particle \(j\).

In order to factorize the diagram, we have first cross-coupled the incoming and outcoming model-space states \(j\) to \(J'=0^+\) (diagram \(A_1\) in Fig. 7). Then we cut the hole-line \(h_2\) and, by way of Eq. (56), we obtain a sum of two-body diagrams which are direct-coupled to the total angular momentum \(J\) [51] (diagram \(A_2\) in Fig. 7). These operations are responsible of the factors \(1/(2j+1)\) and \((2J+1)\), the overall factor \(1/2\) is due to the pair of particle lines \(p_1, p_2\) starting and ending at same vertices, and the minus sign comes from the 2 hole lines and 1 loop appearing in the diagram. The factorization accounts also of the \((V-U)\) insertion \(\langle h_1 \| V-U \| j \rangle\).

As mentioned before, this diagrammatics is valid to derive \(H_{\text{eff}}\) for one- and two-valence nucleon systems, and things are different and more complicated if one would like to derive \(H_{\text{eff}}\) for system with three or more valence nucleons.

Actually, none of available SM codes can perform the diagonalization of SM Hamiltonians with three-body components, apart from BIGSTICK SM code [55] but only for light nuclei.

In order to include the contribution to \(H_{\text{eff}}\) from \(\hat{Q}\)-box diagrams with at least three incoming and outcoming valence particles, we resort to the so-called normal-ordering decomposition of the three-body component of a many-body Hamiltonian [56]. To this end, we include in the calculation of the \(\hat{Q}\)-box also second-order three-body diagrams, which, for those nuclei with more than 2 valence nucleons, account for the interaction via the two-body force of the valence nucleons with core excitations as well as with virtual intermediate nucleons scattered above the model space (see Fig. 8).

For each topology reported in Fig. 8 there are nine diagrams, corresponding to the possible permutations of the external lines. The analytical expressions of the second-order three-body contributions is reported in Ref. [57], and we derive from those expressions a density-dependent two-body term.

To this end, we calculate, for each \((A, B)\) topology, nine one-loop diagrams, namely the graph \((\alpha)\) in Fig. 9. Their explicit form, in terms of the three-body graphs \((A, B)\), is:
Figure 8. Second-order three-body diagrams. The sum over the intermediate lines runs over particle and hole states outside the model space, shown by A and B, respectively. For the sake of simplicity, for each topology we report only one of the diagrams which correspond to the permutations of the external lines.

Figure 9. Density-dependent two-body contribution that is obtained from a three-body one. \( \alpha \) is obtained by summing over one incoming and outgoing particle of the three-body graphs A reported in Fig. 8.

\[
\langle (j_a j_b)_J | V^\alpha | (j_c j_d)_J \rangle = \sum_{m, J'} \rho_m \frac{j^2}{J^2} \langle [(j_a j_b)_J, j_m]_J | V^{A,B} | [(j_c j_d)_J, j_m]_J \rangle ,
\]

where the summation over \( m \)-index runs in the model space. \( \rho_m \) is the unperturbed occupation density of the orbital \( m \) according to the number of valence nucleons.

Finally, the perturbative expansion of the \( \hat{Q} \)-box contains one- and two-body diagrams up to third order in \( V_{NN} \), and a density-dependent two-body contribution accounting for three-body second-order diagrams [58, 57].

It should be pointed out that the latter term depends on the number of valence protons and neutrons, thus leading to the derivation of specific effective shell-model Hamiltonians, that differ only for the two-body matrix elements.

### 3.3 Effective shell-model decay operators

In the shell-model approach, we are interested not only in calculating energies, but also the matrix elements of operators \( \Theta \) representing physical observables (e.g. e.m. transition rates, multipole moments, ...).

Since the wave-functions \( |\psi_\alpha\rangle \) obtained diagonalizing \( H_{\text{eff}} \) are not the true ones \( |\Psi_\alpha\rangle \), but their projections onto the chosen model space \( (|\psi_\alpha\rangle = P|\Psi_\alpha\rangle) \), it is obvious that one has to renormalize \( \Theta \) to take into
account the neglected degrees of freedom corresponding to the $Q$-space. In other words, one has to consider the short range correlation “wounds” inflicted by the bare interaction on the SM wave functions. Formally, one wants to derive an effective operator $\Theta_{\text{eff}}$ such that

$$
\langle \tilde{\Psi}_\alpha | \Theta | \Psi_\beta \rangle = \langle \tilde{\psi}_\alpha | \Theta_{\text{eff}} | \psi_\beta \rangle.
$$

(62)

The perturbative expansion of effective operators has been approached since the earliest attempts to employ realistic potentials for SM calculations, and among many they should be mentioned the fundamental and pioneering studies carried out by L. Zamick for the problematics of electromagnetic transitions [59, 60, 61] and I. S. Towner for the study of the quenching of spin-operator matrix elements [62, 63].

In present section we discuss the formal structure of non-Hermitian effective operators, as introduced by Suzuki and Okamoto in Ref. [18]. More precisely, we provide an expansion formula for the effective operators in terms of the $\hat{\Theta}$-box, that analogously to the $\hat{Q}$-box in the effective interaction theory (see Sec. 3), is the building block for constructing effective operators.

According to Eq. (20) (and keeping in mind that $\omega \equiv Q\omega P$), we may write $H_{\text{eff}}$ as

$$
H_{\text{eff}} = PH(P + \omega),
$$

(63)

so that we can express the true eigenstates $|\Psi_\alpha\rangle$ and their orthonormal counterparts $\langle \tilde{\Psi}_\alpha |$ as

$$
|\Psi_\alpha\rangle = (P + \omega)|\psi_\alpha\rangle \quad \langle \tilde{\Psi}_\alpha | = \langle \tilde{\psi}_\alpha |(P + \omega^\dagger)(P + \omega^\dagger).
$$

(64)

On the other hand, a general effective operator expression in the bra-ket representation is given by

$$
\Theta_{\text{eff}} = \sum_{\alpha\beta} |\psi_\alpha\rangle \langle \tilde{\Psi}_\alpha | \Theta | \Psi_\beta \rangle \langle \tilde{\psi}_\beta |,
$$

(65)

where $\Theta$ is a general time-independent Hermitian operator. Therefore we can write $\Theta_{\text{eff}}$ in an operator form as

$$
\Theta_{\text{eff}} = (P + \omega^\dagger\omega)^{-1}(P + \omega^\dagger)\Theta(P + \omega).
$$

(66)

It is worth noting that Eq. (62) holds independently of the normalization of $|\Psi_\alpha\rangle$ and $|\psi_\alpha\rangle$, but if the true eigenvectors are normalized, then $\langle \tilde{\Psi}_\alpha | = \langle \Psi_\alpha |$ and the $|\psi_\alpha\rangle$ should be normalized in the following way

$$
\langle \tilde{\psi}_\alpha |(P + \omega^\dagger\omega)|\psi_\alpha\rangle = 1.
$$

(67)

To explicitly calculate $\Theta_{\text{eff}}$, we introduce the $\hat{\Theta}$-box defined as

$$
\hat{\Theta} = (P + \omega^\dagger)\Theta(P + \omega),
$$

(68)

so that $\Theta_{\text{eff}}$ can be factorized as

$$
\Theta_{\text{eff}} = (P + \omega^\dagger\omega)^{-1}\hat{\Theta}.
$$

(69)

The derivation of $\Theta_{\text{eff}}$ is divided in two parts: the calculation of $\hat{\Theta}$ and the one of $\omega^\dagger\omega$.
According to Eq. (68) and taking into account the expression of $\omega$ in terms of $H_{\text{eff}}$

$$\omega = \sum_{n=0}^{\infty} (-1)^n \left(\frac{1}{\epsilon_0 - QHQ}\right)^{n+1} QH_1 P (H_{\text{eff}}^1)^n,$$

we can write

$$\hat{\Theta} = \hat{\Theta}_{PP} + (\hat{\Theta}_{PQ} + \text{h.c.}) + \hat{\Theta}_{QQ},$$

where

$$\hat{\Theta}_{PP} = P\hat{\Theta}P,$$

$$\hat{\Theta}_{PQ} = P\hat{\Theta}\omega P = \sum_{n=0}^{\infty} (H_{\text{eff}}^1)^n \hat{\Theta}_n,$$

$$\hat{\Theta}_{QQ} = \omega\hat{\Theta}_{PP}\omega = \sum_{n,m=0}^{\infty} (H_{\text{eff}}^1)^n \hat{\Theta}_{nm}(H_{\text{eff}}^1)^m,$$

and $\hat{\Theta}_m$, $\hat{\Theta}_{mn}$ have the following expressions:

$$\hat{\Theta}_m = \frac{1}{m!} \frac{d^m}{d\epsilon^m} \hat{\Theta}(\epsilon) \bigg|_{\epsilon = \epsilon_0},$$

$$\hat{\Theta}_{mn} = \frac{1}{m!n!} \frac{d^m}{d\epsilon_1^m} \frac{d^n}{d\epsilon_2^n} \hat{\Theta}(\epsilon_1; \epsilon_2) \bigg|_{\epsilon_1 = \epsilon_0, \epsilon_2 = \epsilon_0},$$

with

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

$$\hat{\Theta}(\epsilon_1; \epsilon_2) = PH_1 Q \frac{1}{\epsilon_1 - QHQ} Q\hat{\Theta} Q \frac{1}{\epsilon_2 - QHQ} QH_1 P.$$

As regards the product $\omega^\dagger \omega$, using the definition (31), we can write

$$\omega^\dagger \omega = -\sum_{n=1}^{\infty} \sum_{m=1}^{\infty} ((H_{\text{eff}}^1)^\dagger)^{n-1} \hat{\Theta}(\epsilon_0)_{n+m-1} (H_{\text{eff}}^1)^{m-1}.$$

Expressing $H_{\text{eff}}^1$ in in terms of the $\hat{Q}$-box and its derivatives (see Eqs. (33,34)), the above quantity may be rewritten as

$$\omega^\dagger \omega = -\hat{Q}_1 + (\hat{Q}_2 \hat{Q} + \text{h.c.}) + (\hat{Q}_3 \hat{Q} \hat{Q} + \text{h.c.}) + (\hat{Q}_2 \hat{Q}_1 \hat{Q} + \text{h.c.}) + \cdots$$

Putting together Eq. (77) and (80), we can write the final perturbative expansion form of the effective operator $\Theta_{\text{eff}}$

$$\Theta_{\text{eff}} = (P + \hat{Q}_1 \hat{Q}_1 + \hat{Q}_2 \hat{Q} + \cdots) \times (\chi_0 + \chi_1 + \chi_2 + \cdots),$$
where
\[
\chi_0 = (\hat{\Theta}_0 + \text{h.c.}) + \hat{\Theta}_{00}, \tag{82}
\]
\[
\chi_1 = (\hat{\Theta}_1 \hat{Q} + \text{h.c.}) + (\hat{\Theta}_{01} \hat{Q} + \text{h.c.}), \tag{83}
\]
\[
\chi_2 = (\hat{\Theta}_1 \hat{Q}_1 + \text{h.c.}) + (\hat{\Theta}_2 \hat{Q}\hat{Q} + \text{h.c.}) + (\hat{\Theta}_{02} \hat{Q}\hat{Q} + \text{h.c.}) + \hat{Q}\hat{\Theta}_{11} \hat{Q}. \tag{84}
\]

\[
\ldots
\]

It is worth enlightening the strong link existing between $H_{\text{eff}}$ and any effective operator. This is achieved by inserting the identity $\hat{Q}\hat{Q}^{-1} = 1$ in Eq. (81), so to obtain the following expression:

\[
\Theta_{\text{eff}} = (P + \hat{Q}_1 + \hat{Q}_1 \hat{Q}_1 + \hat{Q}_2 \hat{Q} + \hat{Q}\hat{Q}_2 + \cdots) \hat{Q}\hat{Q}^{-1} \times (\chi_0 + \chi_1 + \chi_2 + \cdots) = H_{\text{eff}}\hat{Q}^{-1}(\chi_0 + \chi_1 + \chi_2 + \cdots). \tag{85}
\]

In actual calculations the $\chi_n$ series is arrested to a finite order and the starting point is the derivation of a perturbative expansion of $\hat{\Theta}_0 \equiv \hat{\Theta}(\epsilon_0)$ and $\hat{\Theta}_{00} \equiv \hat{\Theta}(\epsilon_0; \epsilon_0)$, including diagrams up to a finite order in the perturbation theory, consistently with the expansion of the $\hat{Q}$-box. The issue of the convergence of the $\chi_n$ series and of the perturbative expansion of $\hat{\Theta}_0$ and $\hat{\Theta}_{00}$ will be extensively treated in section 4.1.

In Fig. 10 we report all the diagrams up to second order appearing in the $\hat{\Theta}_0$ expansion for a one-body operator $\Theta$.

![Figure 10. One-body second-order diagrams included in the perturbative expansion of $\hat{\Theta}_0$. The asterisk indicates the bare operator $\Theta$.](image)

The evaluation of the diagrams involved in the derivation of $\Theta_{\text{eff}}$ follows the same rules described in the previous section. In the following, therefore, we will just outline the procedure to calculate such diagrams with one $\Theta$ vertex.

Let us suppose that the operator $\Theta$ transforms like a spherical tensor of rank $\lambda$, component $\mu$:

\[
\Theta \equiv T^\lambda_\mu, \tag{86}
\]

with

\[
(T^\lambda_\mu)^\dagger = (-1)^{\lambda-\mu}T^\lambda_{-\mu}. \tag{87}
\]
By using the Wigner-Eckart theorem, it is possible to express any transition matrix element in terms of a reduced transition element
\[
\langle j_a | T^\lambda | j_b \rangle = (-1)^{\lambda - \mu} \langle j_a | T^\lambda_{\mu} | j_b \rangle ,
\]
where in the r.h.s. of Eq. (88) \( j_b \) is coupled to \( j_a \) to a total angular momentum and projection equal to \( \lambda \) and \(-\mu\), respectively, and we have assumed, without any lack of generality, that we are dealing with single-particle states.

Therefore, we evaluate each diagram as a contribution to the reduced matrix element of the effective operator. To be more explicit, we consider as an example the calculation of the following second-order diagram that takes into account the renormalization of the operator due to 1p-1h core excitations.

The first step is to couple \( j_b \) and \( j_a \) to a total angular momentum equal to \( \lambda \). This enables to factorize the diagram as the product of a cross-coupled matrix element of the interaction and the reduced matrix element of the operator (see right-hand side of Fig. 11).

Explicitly, we can evaluate the diagram as
\[
\langle j_a | \Theta_{2p1h} | j_b \rangle = - \sum_{p,h} (-1)^{j_p + j_h - \lambda} \langle j_a, p; \lambda | V_{NN} | j_b, h; \lambda \rangle_{CC} \langle h | T^\lambda_p | p \rangle \epsilon_0 - (\epsilon_a + \epsilon_b - \epsilon_h) .
\]

The minus sign in front of the value is due to the fact that \( n_h = n_l = 1 \), and that an extra-phase factor \((-1)^{n_{ph}}\) is needed for the total number of cut of particle-hole pairs \( (n_{ph}) \) [51], since we have cut the inner loop to factorize the diagram.

4 APPLICATIONS

We present in this section a specific example of SM calculations which have been performed by employing effective SM Hamiltonian a decay operators derived from realistic nuclear potentials within the many-body perturbation theory.

It should be noted that this kind of calculations have been carried out since the middle of 1960s, but the spirit has been mostly to retain only the TBMEs, since the single-body component of \( H_{eff} \) has not been considered enough accurate to provide SM results in a good agreement with experiment. A large sample of calculations which are framed in such a successful approach can be found in previous reviews on this topic [6, 7].
We have sampled in this work the results of a calculation where both SP energies and TBMEs, that are needed to diagonalize the SM Hamiltonian, have been obtained by deriving $H_{\text{eff}}$ according to the procedures that have been reported in the previous section. Besides $H_{\text{eff}}$, the many-body perturbation theory has been employed to derive consistently effective operators to calculate electromagnetic transition rates and Gamow-Teller (GT) strengths without resorting to empirical effective charges or quenching factors for the axial coupling constant $g_A$.

There are some motivations that lead to perform SM calculations by deriving and employing all SM parameters - SP energies, TBMEs, effective transition and decay operators - starting from realistic nuclear forces:

- the need to study the soundness of many-body perturbation theory in order to provide reliable SM parameters;
- to investigate the ability of classes of nuclear potentials to describe nuclear structure observables;
- the opportunity to compare and benchmark SM calculations with other nuclear structure methods which employ realistic potentials.

The goal of these studies is to test the reliability of such an approach to the nuclear shell model, especially its predictiveness that is crucial to describe physical phenomena that are not yet at hand experimentally.

### 4.1 The double-$\beta$ decay around doubly-closed $^{132}\text{Sn}$

Neutrinoless double-$\beta$ ($0\nu\beta\beta$) decay is an exotic second-order electroweak process predicted by extensions of the Standard Model of particle physics. Observation of such a process would show the non-conservation of lepton number, and evidence that neutrinos have a Majorana mass component (see Refs. [64, 65] and references therein).

In the framework of light-neutrino exchange, the half life for the $0\nu\beta\beta$ decay is inversely proportional to the square of the effective Majorana neutrino mass $\langle m_\nu \rangle$:

$$\left[ T_{1/2}^{0\nu} \right]^{-1} = G_{0\nu}^{0\nu} \left| M_{0\nu}^{0\nu} \right|^2 g_A^2 \left( \frac{\langle m_\nu \rangle}{m_e} \right)^2,$$

where $g_A$ is the axial coupling constant, $m_e$ is the electron mass, $G_{0\nu}^{0\nu}$ is the so-called phase-space factor (or kinematic factor), and $M_{0\nu}^{0\nu}$ is the nuclear matrix element (NME), that is connected to the wave functions of the nuclei involved in the decay.

At present, the phase-space factors for nuclei that are possible candidates for $0\nu\beta\beta$ decay may be calculated with great accuracy [66, 67]. Therefore, it is crucial to have precise values of the NME, both to improve the reliability of the $0\nu\beta\beta$ lifetime predictions - fundamental ingredient to design new experiments - and to extract neutrino properties from the experimental results, when they will become available.

Several nuclear structure models are exploited to provide NME values as precise as possible, the most largely employed being, at present, the Interacting Boson Model (IBM) [68, 69, 70], the Quasiparticle Random-Phase Approximation (QRPA) [71, 72, 73, 74], Energy Density Functional methods [75], the Covariant Density Functional Theory [76, 77, 78], the Generator-Coordinate Method (GCM) [79, 80, 81, 82], and the Shell Model (SM) [83, 84, 85, 86, 87].
All the above models use a truncated Hilbert space to overcome the computational complexity, and each of them can be more efficient than another for a specific class of nuclei. However, when comparing the calculated NMEs obtained with different approaches, it can be shown that, at present, the results can differ by a factor of two or three (see for instance the review in Ref. [88]).

In Ref. [89], it has been reported on the calculation of the $0\nu\beta\beta$-decay NME for $^{48}\text{Ca}$, $^{76}\text{Ge}$, $^{82}\text{Se}$, $^{130}\text{Te}$, and $^{136}\text{Xe}$ in the framework of the realistic SM, where $H_{\text{eff}}$s and $0\nu\beta\beta$-decay effective operators are consistently derived starting from a realistic $NN$ potential, the high-precision CD-Bonn potential [90].

It is worth mentioning that the above work is not the first example of such an approach, since it has been pioneered by Kuo and coworkers [91, 92], and more recently pursued by Holt and Engel [93].

In present work, we will restrict ourselves to present the results obtained in Ref. [89] for the heavy-mass nuclei around $^{132}\text{Sn}$, $^{130}\text{Te}$ and $^{136}\text{Xe}$. At present, these nuclei are under investigation as $0\nu\beta\beta$-decay candidates by some large experimental collaborations. The possible $0\nu\beta\beta$ decay of $^{130}\text{Te}$ is investigated both by the EXO-200 collaboration at the Waste Isolation Pilot Plant in Carlsbad, New Mexico, [95], and by the KamLAND-Zen collaboration in the Kamioka mine in Japan [96].

The starting point of the SM calculation is the high-precision CD-Bonn $NN$ potential [90], whose non-perturbative behavior induced by its repulsive high-momentum components is healed resorting to the so-called $V_{\text{low-k}}$ approach [97].

This provides a smooth potential which preserves exactly the onshell properties of the original $NN$ potential up to a chosen cutoff momentum $\Lambda$. As in other SM studies [98] [99] [100] [101], the value of the cutoff has been chosen as $\Lambda = 2.6$ fm$^{-1}$, since the role of missing three-nucleon force (3NF) decreases by enlarging the $V_{\text{low-k}}$ cutoff [99]. In fact, in Ref. [99] it has been shown that $H_{\text{eff}}$s derived from $V_{\text{low-k}}$s with small cutoffs ($\Lambda = 2.1$ fm$^{-1}$) own SP energies in a worse agreement with experiment, and also an unrealistic shell-evolution behavior. This characteristic may be ascribed to larger impact of the induced 3NF, which becomes less important by enlarging the cutoff.

We have experienced that $\Lambda = 2.6$ fm$^{-1}$, within a perturbative expansion of the $\hat{Q}$-box, is an upper limit, since a larger cutoff worsens the order-by-order behavior of the perturbative expansion, and at the end of present section it is reported a study of the perturbative properties of $H_{\text{eff}}$ and of the effective decay operators derived using this $V_{\text{low-k}}$ potential.

The Coulomb potential is explicitly taken into account in the proton-proton channel.

The shell-model effective hamiltonian $H_{\text{eff}}$ has been derived within the framework of the many-body perturbation theory as described in section 3, including diagrams up to third order in $H_1$ in the $\hat{Q}$-box-expansion, while all the effective operators, both one- and two-body, have been obtained consistently using the approach described in section 3.3, including diagrams up to third order in perturbation theory in the evaluation of the $\Theta$-box and arresting the $\chi_n$ series in Eq. (81) to $\chi_2$.

The effective hamiltonian and operators are defined in a model space spanned by the five $0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2}$ proton and neutron orbitals outside the doubly-closed $^{100}\text{Sn}$ core. The single-particle (SP) energies, and the two-body matrix elements (TBMEs) of $H_{\text{eff}}$ can be found in Ref. [101].

Before showing the results for the $0\nu\beta\beta$ NME obtained in Ref. [89], it is worth checking the reliability of the adopted approach. To this end, we present here some results obtained for the calculation of quantities
for which there exist an experimental counterpart to compare with. Namely, we show some selected results for the electromagnetic properties, GT strength distributions and $2\nu\beta\beta$ decays in $^{130}$Te and $^{136}$Xe, that are reported in Refs. [101, 102].

In Figs. [12] and [13] they are shown the experimental [103, 104] and calculated low-energy spectra and $B(E2)$s of parent and grand-daughter nuclei involved in double-beta-decay of $^{130}$Te and $^{136}$Xe, respectively.

![Figure 12](image1.png)

**Figure 12.** Experimental and calculated spectra of $^{130}$Te and $^{130}$Xe. The arrows are proportional to the $B(E2)$ strengths, whose values are reported in $e^2$fm$^4$. Reproduced from Ref. [102].

![Figure 13](image2.png)

**Figure 13.** Same as in Fig. [12] but for $^{136}$Xe and $^{136}$Ba. Reproduced from Ref. [102].

From the inspection of Figs. [12] and [13] it can be seen that the comparison between theory and experiment, as regards the low-lying excited states and the $B(E2)$ transition rates, is quite good for $^{130}$Te, $^{136}$Xe, and $^{136}$Ba, while it is less satisfactory for $^{130}$Xe, whose theoretical spectrum is expanded when compared with the observed one. As regards the electromagnetic properties, in Ref. [102] they are calculated also some $B(M1)$ strengths and magnetic dipole moments using an effective spin-dependent $M1$ operator, and the comparison with the available data (see Tables VII and IX in Ref. [102]) evidences a good agreement.

Two different kinds of experimental data related to GT decay are available in $^{130}$Te and $^{136}$Xe: GT-strength distributions, and the NMEs involved in $2\nu\beta\beta$ decays.

The GT strength $B(GT)$ can be extracted from the GT component of the cross section at zero degree of intermediate energy charge-exchange reactions, following the standard approach in the distorted-wave Born approximation (DWBA) [105, 106]:

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\[ \frac{d \sigma^{GT}(0^\circ)}{d \Omega} = \left( \frac{\mu}{\pi \hbar^2} \right)^2 \frac{k_f}{k_i} N_D^{\sigma \tau} |J_{\sigma \tau}|^2 B(GT) \right. \quad (91) \]

where \( N_D^{\sigma \tau} \) is the distortion factor, \(|J_{\sigma \tau}|\) is the volume integral of the effective \( NN \) interaction, \( k_i \) and \( k_f \) are the initial and final momenta, respectively, and \( \mu \) is the reduced mass.

On the other hand, the experimental \( 2\nu\beta\beta \) NME \( M_{GT}^{2\nu} \) can be extracted from the observed half life \( T_{1/2}^{2\nu} \) of the parent nucleus

\[ T_{1/2}^{2\nu}^{-1} = G^{2\nu} |M_{GT}^{2\nu}|^2 \]  \quad (92)

Both the above quantities can be calculated in terms of the matrix elements of the GT\(^{-}\) operator

\[ B(GT) = \left| \langle \Phi_f \| \sum_j \tilde{\sigma}_j \tau_j^- \| \Phi_i \rangle \right|^2, \quad (93) \]

\[ M_{GT}^{2\nu} = \sum_n \frac{(0^+_n \| \tilde{\sigma} \tau^- \| 1^+_n)(1^+_n \| \tilde{\sigma} \tau^- \| 0^+_n)}{E_n + E_0} \]  \quad (94)

where \( E_n \) is the excitation energy of the \( J^\pi = 1^+_n \) intermediate state, \( E_0 = \frac{1}{2} Q_{\beta\beta}(0^+) + \Delta M \), \( Q_{\beta\beta}(0^+) \) and \( \Delta M \) being the \( Q \) value of the \( \beta\beta \) decay and the mass difference between the daughter and parent nuclei, respectively. The nuclear matrix elements in Eqs. (93) and (94) are calculated within the long-wavelength approximation, including only the leading order of the Gamow-Teller operator in a nonrelativistic reduction of the hadronic current.

In Ref. [102], the GT strength distributions and the \( 2\nu\beta\beta \) NMEs have been calculated for \( ^{130}\text{Te} \) and \( ^{136}\text{Xe} \) using an effective spin-isospin dependent GT operator, derived consistently with \( H_{\text{eff}} \) by following the procedure described in section 3.3.

Fig. 14 shows the theoretical running sums of the GT strengths \( \Sigma B(GT) \), calculated with both bare and effective GT operators, reported as a function of the excitation energy, and compared with the available data extracted from \(^{(3}\text{He},t)\) charge-exchange experiments [107, 108], for \( ^{130}\text{Te} \) and \( ^{136}\text{Xe} \). From its inspection, it can be seen that, in both nuclei, the GT-strength distributions calculated using the bare GT operator overestimate the experimental ones by more than a factor of two. Including the many-body renormalization of the GT operator brings the predicted GT strength distribution into much better agreement with that extracted from experimental data.

In Ref. [102] the NMEs \( M_{GT}^{2\nu} \) involved in the decay of \( ^{130}\text{Te} \) and \( ^{136}\text{Xe} \) are calculated using the definition in Eq. (94), by means of the Lanczos strength-function method as in Ref. [3]. The results obtained with the bare GT operator and with the effective one are reported in Table 1 and compared with the experimental values [109].

The effective operator induces a relevant quenching of the calculated NME, 47% for \( ^{130}\text{Te} \) and 37% for \( ^{136}\text{Xe} \) decay, leading to a quite good agreement with the experimental value in both nuclei, that is of the same quality as that of other shell-model calculations where all parameters (SP energies and TBMEs) have been fitted to experiment and a quenching factor \( q \) has been introduced to reproduce GT data (see for...
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Figure 14. Running sums of the $B(GT)$ strengths as a function of the excitation energy $E_x$ up to 3 MeV, and 4.5 MeV respectively for $^{130}\text{Te}$ and $^{136}\text{Xe}$. Reproduced from Ref. [102].

Table 1. Experimental [109] and calculated NME of the $2\nu\beta\beta$ decay (in MeV$^{-1}$) for $^{130}\text{Te}$ and $^{136}\text{Xe}$.

| Decay           | NME$_{\text{Expt}}$ | bare | effective |
|-----------------|----------------------|------|-----------|
| $^{130}\text{Te} \rightarrow ^{130}\text{Xe}$ | 0.031 ± 0.004        | 0.131 | 0.061     |
| $^{136}\text{Xe} \rightarrow ^{136}\text{Ba}$ | 0.0181 ± 0.0007      | 0.0910 | 0.0341    |

example Ref. [110]). The overall agreement between theory and experiment shows the present capability of the many-body perturbation theory to derive consistently effective Hamiltonians and transition operators that are able to reproduce quantitatively the observed spectroscopic and decay properties, without resorting to any empirical adjustment, such as the quenching of the axial coupling constant $g_A$. This supports the reliability of this approach to calculate the NME involved in $0\nu\beta\beta$, whose results have been reported in Ref. [89], and are shortly recollected in the following.

The $0\nu\beta\beta$ two-body operator for the light-neutrino scenario can be expressed in the closure approximation (see for instance Refs. [111, 112]) in terms of the neutrino potentials $H_\alpha$ and form functions $h_\alpha(q)$ ($\alpha = F$, GT, or $T$) as follows

$$\Theta_{\text{GT}} = \vec{\sigma}_1 \cdot \vec{\sigma}_2 H_{\text{GT}}(r)\tau_1^- \tau_2^-$$

$$\Theta_F = H_F(r)\tau_1^- \tau_2^-$$

$$\Theta_T = [3 (\vec{\sigma}_1 \cdot \hat{r}) (\vec{\sigma}_1 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2] H_T(r)\tau_1^- \tau_2^-,\quad (97)$$

$$H_\alpha(r) = \frac{2R}{\pi} \int_0^\infty j_{n_\alpha}(qr)h_\alpha(q^2)qdq$$

$$q + \langle E \rangle.\quad (98)$$

The value of the parameter $R$ is $R = 1.2 A^{1/3} \text{ fm}$, the $j_{n_\alpha}(qr)$ are the spherical Bessel functions, $n_\alpha = 0$ for Fermi and Gamow-Teller components, $n_\alpha = 2$ for the tensor one. The explicit expression of neutrino
form functions $h_\alpha(q)$ may be found in Ref. [89], and the average energies $\langle E \rangle$ are evaluated as in Refs. [111,112].

Apart from effects related to sub-nucleonic degrees of freedom, that have not been taken into account in Ref. [89], the 0νββ-decay operator has to be renormalized to take into account both the degrees of freedom that are neglected in the adopted model space and the contribution of the short-range correlations (SRC). The latter arise since the action of a two-body decay operator on an unperturbed (uncorrelated) wave function, as the one used in the perturbative expansion of $\Theta_{\text{eff}}$, differs from the action of the same operator on the real (correlated) nuclear wave function.

It is worth pointing out that the calculations for 2νββ decay are not affected by this renormalization, since, as mentioned before, we retain only the leading order of the long-wavelength approximation which corresponds to a zero-momentum-exchange ($q=0$) process. On the other hand, the inclusion of higher-order contributions or corrections due to the sub-nucleonic structure of the nucleons [113,114,115,116] would connect high- and low-momentum configurations and this renormalization should be carried out for the two-neutrino emission decay too.

In Ref. [117] the inclusion of SRC has been realized by means of an original approach [117] that is consistent with the $V_{\text{low}}$-procedure. The 0νββ operator $\Theta$, expressed in the momentum space, is renormalized by way of the same similarity transformation operator $\Omega_{\text{low}}$ that defines the $V_{\text{low}}$ potential. This enables to consider effectively the high-momentum (short range) components of the $NN$ potential, in a framework where their direct contribution is not explicitly considered above a cutoff $\Lambda$. The resulting $\Theta_{\text{low}}$ vertices are then employed in the perturbative expansion of the $\hat{\Theta}$-box to calculate $\Theta_{\text{eff}}$ using Eq. (85). More precisely, the perturbative expansion has considered diagrams up to third order in perturbation theory, including the ones related to the so-called Pauli blocking effect (see Fig. 2 in Ref. [89]), and the $\chi_n$ series has been arrested to $\chi_2$.

In Ref. [89] the contribution of the tensor component of the neutrino potential (Eq. (97)) is neglected, and therefore the total nuclear matrix element $M_{0\nu}$ is expressed as

\[ M_{0\nu} = M^{0\nu}_{\text{GT}} - \left( \frac{g_V}{g_A} \right)^2 M^{0\nu}_{\text{F}}, \]

where $g_A = 1.2723$, $g_V = 1$ [118], and the matrix elements between the initial and final states $M_{0\alpha}$ are calculated within the closure approximation

\[ M_{0\alpha} = \sum_{j_n,j_p,j_{n'}} \langle \hat{f} | a_p^\dagger a_n^\dagger a_{p'}^\dagger a_{n'} | \hat{i} \rangle \times \langle j_p,j_{p'} | \Theta_\alpha | j_n,j_{n'} \rangle. \]

The calculated NMEs using the 0νββ-decay effective operator are reported in Table 2 and compared with the values obtained with the bare operator without any renormalization.

The most striking feature that can be inferred from the inspection of Table 2 is that the effects of the renormalization of the 0νββ-decay operator are far less relevant than those observed in the 2νββ-decay sector.

A long standing issue related with the calculation of $M^{0\nu}$ is the possible interplay between the derivation of the effective one-body GT operator and the renormalization of the two-body GT component of the 0νββ operator, some authors presuming that the same empirical quenching introduced to reproduce the
Table 2. Calculated values of $M^{0\nu}$ for $^{130}\text{Te}$ and $^{136}\text{Xe}$ decay. The first column corresponds to the results obtained employing the bare $0\nu\beta\beta$-decay operator, the second one to the calculations performed with $\Theta_{\text{eff}}$.

| Decay         | bare operator | $\Theta_{\text{eff}}$ |
|---------------|---------------|------------------------|
| $^{130}\text{Te} \rightarrow ^{130}\text{Xe}$ | 3.27          | 3.16                   |
| $^{136}\text{Xe} \rightarrow ^{136}\text{Ba}$ | 2.47          | 2.39                   |

observed GT-decay properties (single-$\beta$ decay strengths, $M^{2\nu}_{\text{GT}}$, etc.) should be also employed to calculate $M^{0\nu}$ (see for instance Refs. [119, 120]). Actually, the comparison of the results in Tables 1 and 2 shows that the mechanisms which rule the microscopic derivation of the one-body single-$\beta$ and the two-body $0\nu\beta\beta$ decay effective operators lead to a considerably different renormalization, at variance with the above hypothesis.

SM calculations of this section have been performed by employing, as interaction vertices of the perturbative expansion of the $\hat{Q}$-box, a realistic potential derived from the high-precision CD-Bonn $NN$ potential [90]. This potential is characterized by a strong repulsive behavior in the high-momentum regime, so, as mentioned before, it has been renormalized by deriving a low-momentum $NN$ potential using the $V_{\text{low}-k}$ approach [97].

As in other SM studies [98, 99, 100, 101], the value of the cutoff has been chosen as $\Lambda = 2.6$ fm$^{-1}$, since the role of missing three-nucleon force (3NF) decreases by enlarging the $V_{\text{low}-k}$ cutoff [99]. This value, within a perturbative expansion of the $\hat{Q}$-box, is an upper limit, since a larger cutoff worsens the order-by-order behavior of the perturbative expansion. Here, we report some considerations about the properties of the perturbative expansion of $H_{\text{eff}}$ and the SM effective transition operator, when this “hard” $V_{\text{low}-k}$ is employed to derive SM Hamiltonian and operators.

Studies of the perturbative properties of the SP energy spacings and TBMEs are reported in Refs. [99] and [121], where $H_{\text{eff}}$ has been derived within the model space outside $^{132}\text{Sn}$ and starting from the “hard” $V_{\text{low}-k}$. However, in Ref. [122] it can be found a systematic investigation of the convergence properties of theoretical SP energy spectra, TBMEs, and $2\nu\beta\beta$ NMEs as a function both of the dimension of the intermediate-state space and the order of the perturbative expansion. Moreover, in Ref. [89] they are also reported the convergence properties of the perturbative expansion of the effective $0\nu\beta\beta$-decay operator with respect to the number of intermediate states, and the truncation both of the order of $\chi_n$ operators and the perturbative order of the diagrams.

Here, we sketch out briefly these results in order to assess the reliability of realistic SM calculation performed starting from a “hard” $V_{\text{low}-k}$.

The model space employed for the SM calculations reported in Ref. [122] is spanned by the five proton and neutron orbitals $0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2}$ outside the doubly-closed $^{100}\text{Sn}$, in order to study the $2\nu\beta\beta$ decay of $^{130}\text{Te}$ and $^{136}\text{Xe}$.

In Fig. 15 it can be found the behavior of the calculated SP spectrum of $^{101}\text{Sn}$, with respect to the $0g_{7/2}$ SP energy, as a function of the maximum allowed excitation energy of the intermediate states expressed in terms of the oscillator quanta $N_{\text{max}}$.

From the inspection of Fig. 15 it is clear that the results achieve convergence at $N_{\text{max}} = 14$, which justifies the choice, for the perturbative expansion of the effective SM Hamiltonian and decay operators, to
include intermediate states with an unperturbed excitation energy up to \( E_{\text{max}} = N_{\text{max}} \hbar \omega \) with \( N_{\text{max}} = 16 \) \cite{101,122,102,89}.

As regards the order-by-order convergence of the SP energies, in Fig. 15 the calculated neutron SP energies, using a number of intermediate states corresponding to \( N_{\text{max}} = 16 \), are reported as a function of the order of the perturbative expansion up to the third order. They are also and compared with the Padé approximant \([2|1]\) of the \( \hat{Q}\)-box, which estimates the value to which the perturbative series may converge. The results at third order are very close to those obtained with the Padé approximant, indicating that the truncation at third order should be a reasonable estimate of the sum of the series.

As regards the TBMEs, we report in Fig. 16 and the neutron-neutron diagonal \( J^{\pi} = 0^+ \) TBMEs as a function both of \( N_{\text{max}} \) and of the perturbative order. These TBMEs, which contain the pairing properties of the effective Hamiltonian, are the largest in size of the calculated matrix elements and the most sensitive to the behavior of the perturbative expansion.

From the inspection of Fig. 16 the convergence with respect to \( N_{\text{max}} \) appears to be very fast for diagonal matrix elements \( (1d_5/2)^2 \), \( (1d_3/2)^2 \), and \( (2s_1/2)^2 \), while those corresponding to orbitals lacking of their own spin-orbit partner, \( (0g_7/2)^2 \) and \( (0h_{11/2})^2 \), show a slower convergence. The order-by-order convergence, as shown in Fig. 16 is quite satisfactory, and again the results at third order are very close to those obtained with the Padé approximant. Therefore, the conclusion is that \( H_{\text{eff}} \), calculated from a \( V_{\text{low-k}} \) with a cutoff equal to 2.6 fm\(^{-1}\) by way of a perturbative expansion arrested at third order, is a good estimate of the sum of its perturbative expansion, both for the one- and two-body components.

Now, we focus the attention on the perturbative expansion of the GT effective operator \( \hat{G}_{\text{eff}} \).

The selection rules of the GT operator, that characterize a spin-isospin-dependent decay, drive a fast convergence of the matrix elements of its SM effective operator with respect to \( N_{\text{max}} \). In fact, if the perturbative expansion is arrested at second order, their values do not change from \( N_{\text{max}} = 2 \) on \cite{62}, and at third order in perturbation theory their third decimal digit values do not change from \( N_{\text{max}} = 12 \) on.

In Table 3 the results of the calculated NME of the \( 2\nu\beta\beta \) decays \(^{130}\text{Te}_{\text{g.s.}} \rightarrow ^{130}\text{Xe}_{\text{g.s.}} \) and \(^{136}\text{Xe}_{\text{g.s.}} \rightarrow ^{136}\text{Ba}_{\text{g.s.}} \), obtained with effective operators at first, second, and third order in perturbation
Figure 16. Neutron-neutron diagonal $J^\pi = 0^+$ TBMEs as a function of $N_{\text{max}}$ (left-hand side) of the perturbative order (right-hand side). Reproduced from Ref. [122] under the Creative Commons CC BY license.

theory ($\chi_n$ series in Eq. (85) is arrested to $\chi_0$), are reported and compared with the experimental results [109].

Table 3. Order-by-order $M_{2\nu}^{GT}$s (in MeV$^{-1}$) for $^{130}$Te and $^{136}$Xe [122].

| Decay          | 1st ord $M_{2\nu}^{GT}$ | 2nd ord $M_{2\nu}^{GT}$ | 3rd ord $M_{2\nu}^{GT}$ | Expt.          |
|----------------|--------------------------|--------------------------|--------------------------|----------------|
| $^{130}$Te $\rightarrow$ $^{130}$Xe | 0.142                    | 0.040                    | 0.044                    | 0.031 $\pm$ 0.004 |
| $^{136}$Xe $\rightarrow$ $^{136}$Ba | 0.0975                   | 0.0272                   | 0.0285                   | 0.0181 $\pm$ 0.0007 |

As can be seen, also the order-by-order convergence of the $M_{2\nu}^{GT}$s is very satisfactory, since the results change for both transitions about 260% from the first- to second-order calculations, while the change is 9% and 5% from the second- to third-order results for $^{130}$Te and $^{136}$Xe decays, respectively. This suppression of the third-order with respect to the second-order contribution is favoured by the mutual cancelation of third-order diagrams.

In Ref. [89] it has been performed also a study about the convergence properties of the effective decay-operator $\Theta_{\text{eff}}$ for the $0\nu\beta\beta$ decay, with respect the truncation of the $\chi_n$ operators, the number of intermediate states which have been accounted for the perturbative expansion, as well as the order-by-order behavior up to third order in perturbation theory.

In Fig. [17] the results of the calculated values of $M^{0\nu}$ for the $^{76}$Ge $\rightarrow$ $^{76}$Se decay are drawn as a function of the maximum allowed excitation energy of the intermediate states expressed in terms of the oscillator quanta $N_{\text{max}}$, and they are reported including $\chi_n$ contributions up to $n = 2$. We can see that the $M^{0\nu}$'s values are convergent from $N_{\text{max}} = 12$ on and that contributions from $\chi_1$ are quite relevant, those from $\chi_2$ being almost negligible.
It is worth pointing out that, according to expressions (84), $\chi_3$ is defined in terms of the first, second, and third derivatives of $\Theta_0$ and $\Theta_{00}$, as well as on the first and second derivatives of the $Q$-box. This means that one could estimate $\chi_3$ being about one order of magnitude smaller than $\chi_2$ contribution.

On the above grounds, in Ref. [89] the effective SM $0\nu\beta\beta$-decay operator has been obtained including in the perturbative expansion up to third-order diagrams, whose number of intermediate states corresponds to oscillator quanta up to $N_{\text{max}} = 14$, and up to $\chi_2$ contributions.

Now, in order to consider the order-by-order convergence behavior in Fig. 18 are reported the calculated values of $M^{0\nu}$, $M^{0\nu}_{\text{GT}}$, and $M^{0\nu}_{F}$ for $^{130}\text{Te}$, and $^{136}\text{Xe}$ $0\nu\beta\beta$ decay, respectively, at first, second-, and third-order in perturbation theory. We compare the order-by-order results also with their Padé approximant [2|1], as an indicator of the quality of the perturbative behavior [123].

It is worth pointing out that the perturbative behavior is ruled by the Gamow-Teller component, the Fermi matrix element $M^{0\nu}_{F}$ being only slightly affected by the renormalization procedure. Moreover, if the order-by-order perturbative behavior of the effective SM $0\nu\beta\beta$-decay operator is compared with the single
\( \beta \)-decay one, we observe a less satisfactory perturbative behavior for the calculation of \( M^0_{0\nu} \), the difference between second- and third-order results being about 30\% for \(^{130}\text{Te},^{136}\text{Xe} \) 0\( \nu \beta \beta \) decays.

5 SUMMARY

This paper has been devoted to a general presentation of the perturbative approach for deriving effective shell-model operators, namely the SM Hamiltonian and decay operators.

First, we have presented the theoretical framework, which is essentially based on the perturbative expansion of a vertex function, the \( \hat{Q} \)-box for the effective Hamiltonian and the \( \hat{\Theta} \)-box for effective decay operators, whose calculation is pivotal within the Lee-Suzuki similarity transformation. The iterative procedures to solve recursive equations that provide effective shell-model Hamiltonians have been presented in detail, as well as tips that could be useful to calculate the Goldstone diagrams emerging within the perturbative expansion of the above-mentioned vertex functions.

In the last section, we have shown the results of a shell-model study carried out using only single-particle energies, two-body matrix elements of the residual interaction, and effective decay operators derived from a realistic nuclear potential, without any empirical adjustment. This is a part of a large set of investigations which aim to assess the relevance of such an approach to the study of nuclear structure. The versatility of shell-model calculations is grounded on the ability to reproduce experimental results for mass regions ranging from light nuclei - \(^4\text{He} \) core \([23, 52]\) - up to heavy mass systems - nuclei around \(^{132}\text{Sn} \) \([121]\) -, as well as to describe exotic and rare phenomena such as the Borromean structure \([124]\), quadrupole collectivity \([98, 100]\), or the double-\( \beta \) decay process \([101, 102, 89]\) without resorting to empirical adjustments to data.

This testifies the liveliness of this theoretical tool, and could be inspiring for further fruitful investigations in a near and long-distance future.

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