Algebraic diagrammatic construction formalism with three-body interactions

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Background: Self-consistent Green’s function theory has recently been extended to the basic formalism needed to account for three-body interactions [A. Carbone, A. Cipollone, C. Barbieri, A. Rios, and A. Polls, Phys. Rev. C 88, 054326 (2013)]. The contribution of three-nucleon forces has then been included in \textit{ab initio} calculations on nuclear matter and isotopic chains of finite nuclei.

Purpose: Practical applications across post Hartree-Fock methods have mostly considered the contribution of three-nucleon interactions in an effective way, as averaged two-nucleon forces. We derive the working equations for all possible two- and three-nucleon terms that enter the expansion of the self-energy, including interaction-irreducible (i.e. not averaged) three-nucleon diagrams.

Methods: We employ the algebraic diagrammatic construction up to third order as the organization scheme for generating a non perturbative self-energy, in which ring (particle-hole) and ladder (particle-particle) diagrams are resummed to all orders.

Results: We derive expressions of the static and dynamic self-energy up to third order, by taking into account also the set of diagrams required when the skeleton expansion of the single-particle propagator is not assumed. A hierarchy of importance among different diagrams is revealed, and a particular emphasis is given to a third-order diagram (see Fig. 2c) which is expected to play a significant role among those featuring an interaction-irreducible three-nucleon force.

Conclusion: A consistent formalism to resum at infinite order correlations induced by three-nucleon forces in the self-consistent Green’s function theory is now available, and ready to be implemented in the many-body solvers. Work is in progress to include the first interaction-irreducible three-nucleon diagram in calculations of closed-shell medium-mass nuclei.

I. INTRODUCTION

Three-body interactions play a prominent role in determining the behaviour of strongly interacting quantum systems \cite{1}. For instance, three-nucleon forces are necessary to reproduce the saturation of infinite matter as well as to determine the structure and location of the driplines in neutron rich isotopes. Hence, they have been implemented in most of the post-Hartree-Fock approaches that are currently used to study medium mass isotopes, such as self-consistent Green’s function (SCGF) theory \cite{2,3}, the coupled cluster method \cite{4,5}, and the in-medium similarity renormalization group \cite{6,7}. In all of these methods, one typically proceeds by performing a normal ordering of the Hamiltonian, or a similar averaging, so that the dominant effect of three-nucleon forces (3NFs) can be taken into account as an effective nucleon-nucleon force (2NF). Advances of the above many-body methods, with the concurrent introduction of chiral two- and three-nucleon interactions based on the symmetries of QCD \cite{8,9}, have led recently to remarkable successes in nuclear \textit{ab initio} theory \cite{10,11,12}. Presently, the major sources of error in first-principle predictions are originating from uncertainties of the nuclear Hamiltonian.

However, the expected progress in the next-generation realistic interactions will eventually require further developments of the many-body formalisms.

The SCGF theory is a quantum many-body method that has been extensively applied to both condensed matter and nuclear systems \cite{2,13,17}. This approach relies on the solution of the Dyson equation, which is an exact restatement of the many-body Schrödinger equation and it allows for a diagrammatic expansion with respect to the nuclear interaction. However, for nuclear structure and reaction studies, a perturbative expansion is not sufficient due to the strong nature of the nuclear force and the importance of the long-range correlations, which affect the propagation of nucleons inside the medium. In practice, one must resort to an efficient method in which entire classes of correlations are resummed non perturbatively.

For this purpose, a major challenge is to find a scheme capable to organize the rapidly increasing number of Feynman diagrams entering the computation of Green’s functions, especially when 3NFs and many-nucleon interactions are present. Ideally, one should include different classes of Feynman diagrams at all orders, i.e. in a non-perturbative way: at the same time, one needs to keep under control the computational resources required by the many-body problem, even for those post-Hartree-Fock approaches scaling polynomially with the number of nucleons. A powerful tool complying with these requirements has been devised 30 years ago in the Green’s function theory applied to quantum chemistry, and it is referred to as algebraic diagrammatic construction (ADC) \cite{18,19}. Born as a method to include third-order self-energy diagrams that are necessary to reproduce affinities and ionisation energies, the ADC also allows the infinite resummation of specific classes of diagrams, such as the ladder and ring series. The general procedure is to impose the correct spectral representation of the self-energy and to require that it is also consistent with its perturbative expansion up to a given order $n$. 


The spectral representation implies that diagrams up to order \( n \) are actually taken as “seeds” for all-order resumptions. Hence, this generates a hierarchy of many-body truncations, labelled as ADC\((n)\), that is non perturbative and can be systematically improved.

The aim of this paper is to derive the entire set of working equations for the ADC\((3)\) self-energy, when 3NFs are present. The general formalism and diagrammatic rules for the SCGF theory with three-body interactions has been developed in Ref. 20. There it was shown that the number of Feynman diagrams to be calculated can be reduced by introducing averaged effective interactions (similarly to the normal ordering strategy mentioned above), so that one needs to consider only interaction-irreducible diagrams. Using the resulting effective 2NFs, a set of applications of the SCGF was put forward with computations of binding energies \([3, 21]\), spectral distributions and radii \([12, 22]\) for closed subshell isotopes of a nucleus in the same framework \([24]\).

While Ref. 20 introduced the set of self-energy diagrams up to third order, the necessary formalism for extending them to a non-perturbative approach has not yet been derived. We fill this gap here by deriving explicit expressions of the ADC\((3)\) based on the Feynman diagrams derived thereof. For this purpose we revisit the SCGF formalism in Sec. II with special emphasis on how 3NFs are incorporated in the self-energy expansion. Sec. III discusses the ADC method at order \( n \), i.e. ADC\((n)\), and we derive the working equations at second and third order, ADC\((2)\) and ADC\((3)\), in full detail. In this derivation, a hierarchy of importance among different self-energy diagrams emerges naturally: it is based on intermediate excitation energies embedded in each diagram topology. For the ADC\((3)\) we present in Sec. III diagrams that contain only two-particle-one-hole (2p1h) and two-hole-one-particle (2h1p) intermediate states with effective 2NFs or interaction-irreducible 3NFs. These diagrams collected in Fig. 4 are the dominant contributions to ADC\((3)\). Moreover, we present additional equations for a subset of diagrams with 3p2h and 3h2p intermediate states, according to a choice based on different topologies of diagrams obtained at third order. This will give a general overview of the formalism up to \( n=3 \). The remaining parts of the ADC\((3)\) equations do not introduce conceptually new contributions and are given in Appendix A. In Appendix B we display the angular momentum coupled form for the one diagram in Fig. (2c). This has not yet been included in calculations, but it could be added to current numerical implementations due to its relative importance among those with an irreducible 3NF. In Appendix C we derive additional non-skeleton Feynman diagrams, that are diagrams built from uncorrelated propagators, for both the static and dynamic self-energy. The entire set of equations derived in the ADC\((3)\) informs our conclusions, which are drawn in Sec. IV.

II. SCGF FORMALISM WITH 3NFs

Many-particle Green’s functions, also known in the literature as propagators or correlation functions, are at the heart of the SCGF formalism. The lowest order Green’s function is the one-body (1B) propagator describing the propagation of a particle (or an hole), that is formally created and annihilated by field operators \( a_\alpha^\dagger \) and \( a_\alpha \) in the quantum states \( \beta \) and \( \alpha \) respectively, i.e. \([25, 26]\)

\[
g_{\alpha\beta}(t - t') = -\frac{i}{\hbar} \langle \Psi_0^A \rvert T \left[ a_\alpha(t) a_\beta^\dagger(t') \right] \rvert \Psi_0^A \rangle . \tag{1}\]

The time interval \((t - t')\) of the propagation in Eq. (1) is ordered according to the action of the time-ordering operator \( T \), which obeys the Fermi statistics. To describe the propagation of two particles and two holes, we introduce also the two-body (2B) Green’s function,

\[
g_{\alpha\beta\gamma\delta}(t_\alpha, t_\beta, t_\gamma, t_\delta) = -\frac{i}{\hbar} \langle \Psi_0^A \rvert T \left[ a_\alpha(t_\alpha) a_\beta(t_\beta) a_\gamma(t_\gamma) a_\delta(t_\delta) \right] \rvert \Psi_0^A \rangle . \tag{2}\]

For our purposes, we consider the propagator of Eq. (1), which is defined with respect to the \( A \)-body ground state \( \rvert \Psi_0^A \rangle \). The latter is determined in turn as the lowest eigenvectors of the Schrödinger problem,

\[\hat{H} \rvert \Psi_n^A \rangle = E_n^A \rvert \Psi_n^A \rangle. \tag{3}\]

The Lehmann representation of the Green’s function is obtained by Fourier transforming Eq. (1) in the energy plane. It contains the relevant informations on the single particle dynamics,

\[g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A \rvert a_\alpha \rvert \Psi_n^A+1 \rangle \langle \Psi_n^A+1 \rvert a_\beta^\dagger \rvert \Psi_0^A \rangle}{\omega - (E_n^A+1 - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A \rvert a_\alpha \rvert \Psi_k^{-1} \rangle \langle \Psi_k^{-1} \rvert a_\beta \rvert \Psi_0^A \rangle}{\omega - (E_k^{-1} - E_0^A) - i\eta} . \tag{4}\]

In the denominator of Eq. (4) there are quasiparticle energies \( \varepsilon_n^+ \equiv (E_n^A+1 - E_0^A) \) and \( \varepsilon_k^- \equiv (E_0^A - E_k^{-1}) \), which are one-nucleon addition and removal energies. For transition amplitudes \( X_\beta^\alpha \) and \( Y_\alpha^k \) we use the notation

\[Z_{\alpha=n,k}^i \equiv \begin{cases} \langle \chi_{\alpha}^n \rangle^* \equiv \langle \Psi_0^A \rvert a_\alpha \rvert \Psi_0^A \rangle, \\ \langle \Psi_k^{-1} \rvert a_\alpha \rvert \Psi_0^A \rangle, \end{cases} \tag{5}\]

with the index \( i \) referring to both forward-in-time (\( n \)) and backward-in-time (\( k \)) processes. The first (second) overlap integral is related to the probability of adding
The 1B Green’s function is completely determined by solving the Dyson equation,

\[ g_{\alpha\beta}(\omega) = g_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} g_{\alpha\gamma}^{(0)}(\omega) \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega) , \]

which is a non-linear equation defining the irreducible self-energy \( \Sigma_{\gamma\delta}^*(\omega) \), where nuclear medium effects on the particle propagation are encoded. It corresponds to a set of irreducible Feynman diagrams, i.e. diagrams that cannot be divided into sub-diagrams by cutting a propagator line. The distinction between the unperturbed propagator \( g_{\alpha\beta}^{(0)}(\omega) \) and the correlated one \( g_{\alpha\beta}(\omega) \) in Eq. (6) results from the expansion with respect to the inter-particle interaction: \( g_{\alpha\beta}^{(0)}(\omega) \) is then the zeroth-order term in the expansion, that is the propagator with respect to the reference state, i.e.

\[ g_{\alpha\beta}^{(0)}(t-t') = -\frac{i}{\hbar} \langle \phi_0^A | T \left[ a_{\alpha}(t) a_{\beta}^\dagger(t') \right] | \phi_0^A \rangle . \]

From the derivation of the 1B propagator equation of motion, one can find the explicit separation of the irreducible self-energy in a part which is local in time \( \Sigma_{\alpha\beta}^\infty \) (static self-energy), and a energy dependent part \( \Sigma_{\alpha\beta}(\omega) \) (dynamic self-energy), containing the contributions from dynamical excitations in the system:

\[ \Sigma_{\alpha\beta}(\omega) = \Sigma_{\alpha\beta}^\infty + \Sigma_{\alpha\beta}(\omega) . \]

While for the discrete spectrum \( \Sigma_{\alpha\beta}(\omega) \) gives the coupling of the single-particle state with the collective configurations made by surrounding nucleons, in the continuum regime it describes the interaction of the nucleon projectile with a target nucleus. In this respect the energy dependent part of the self-energy is investigated as the microscopic counterpart of the dispersive optical model potentials.

Before proceeding with the application of the ADC formalism to the self-energy, we present in the next Section the main features of the concept of effective interaction, that allows an effective inclusion of 2NFs and 3NFs in the expansion of the propagator.

### A. Inclusion of the effective and interaction-irreducible 3NFs in the formalism

Let us consider first the nuclear Hamiltonian \( \tilde{H} \) with a kinetic energy part \( \tilde{T} \) and interaction operators in the 2NF and 3NF sector, denoted with \( \tilde{V} \) and \( \tilde{W} \) respectively,

\[ \tilde{H} = \tilde{T} + \tilde{V} + \tilde{W} . \]

Within approaches based on a mean-field approximation, it is customary to divide the Hamiltonian into two parts, \( \tilde{H} = H_0 + \tilde{H}_1 \), with \( H_0 \) being the mean field part and \( \tilde{H}_1 \) the residual interaction. In this way strongly interacting fermions are treated as a system of quasi-particles affected by an auxiliary potential \( \tilde{U} \), included in the mean field according to the definition \( H_0 = \tilde{T} + \tilde{U} \), plus the residual interaction \( \tilde{H}_1 \) which is added perturbatively. In the second quantization formalism the Hamiltonian reads then,

\[ \tilde{H} = \sum_{\alpha\beta} \tilde{h}_{\alpha\beta}^0 \tilde{a}_{\alpha}^\dagger \tilde{a}_{\beta} - \sum_{\alpha\beta} U_{\alpha\beta} \tilde{a}_{\alpha}^\dagger \tilde{a}_{\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\gamma,\beta\delta} \tilde{a}_{\alpha}^\dagger \tilde{a}_{\gamma}^\dagger \tilde{a}_{\delta} \tilde{a}_{\beta} + \frac{1}{36} \sum_{\alpha\beta\gamma\delta\eta} W_{\alpha\gamma\epsilon,\beta\delta\eta} \tilde{a}_{\alpha}^\dagger \tilde{a}_{\gamma}^\dagger \tilde{a}_{\delta} \tilde{a}_{\eta} \],

with \( \tilde{h}_{\alpha\beta}^0 = T_{\alpha\beta} + U_{\alpha\beta} \).

The Greek indexes \( \alpha, \beta, \gamma, \ldots \) label a complete set of single-particle states which define the model space used in the computation. In most cases one chooses this set as the one diagonalizing the unperturbed Hamiltonian \( H_0 \). The diagonalization gives the eigenvalues \( \varepsilon_{\alpha}^0 \) and allows to define \( \tilde{a}_{\alpha}^\dagger \) and \( \tilde{a}_{\alpha} \), the creation and annihilation operators for a particle in state \( \alpha \), as the field operators in the definition (4) of the Green’s function. However, we keep the general case here, with the matrix elements of the auxiliary 1B operator \( \tilde{U} \) given by \( U_{\alpha\beta} \). Equivalently, the antisymmetrized matrix elements of 2NFs and 3NFs are \( V_{\alpha\gamma,\beta\delta} \) and \( W_{\alpha\gamma\epsilon,\beta\delta\eta} \), respectively.

The expansion of the self-energy \( \Sigma_{\alpha\beta}(\omega) \) in Eq. (8) involves terms with individual contributions of the 1B potential, but also of 2NFs and 3NFs in Eq. (10). Of course, also terms containing combinations of different interactions are possible. The number of diagrams allowed by the Feynman diagrammatic rules is growing fast with the order of the expansion. A useful strategy is to consider only interaction-irreducible diagrams. Diagrams are considered interaction-reducible if the two interaction vertices obtained by cutting any interaction line are belonging to two disconnected diagrams. This happens when all the fermion lines leaving one interaction vertex return eventually to it. If the interaction vertex which is cut, had only one fermionic line looping over it, all the linked diagrams can then be included effectively by averaging the interaction vertex with a 1B Green’s function. Alternatively, when the cut interaction vertex had two fermionic lines the averaging is performed with a 2B Green’s function and so on. This process of averaging reduces the order of the interaction: For instance, a 2NF averaged on an interaction vertex with a 1B Green’s function gives rise to an effective 1B operator.

In Ref. [20] it is shown that diagrammatic series can be reduced to a smaller set of diagrams by excluding all interaction-reducible diagrams. The averaging procedure described above amounts to define an effective Hamiltonian up to 3NFs,

\[ \tilde{H}_1 = \tilde{U} + \tilde{V} + \tilde{W} , \]

where \( \tilde{U} \) and \( \tilde{V} \) represent effective interaction operators. As long as only interaction-irreducible diagrams are con-
sidered, the use of $\tilde{H}_1$ is equivalent to the interaction-reducible expansion based on Eq. \ref{eq:10} (see Section II of \ref{ref:20} for details).

Explicit expressions for effective 1B and 2N interaction operators are:

$$\tilde{U} = \sum_{\alpha\beta} \tilde{U}_{\alpha\beta} a^\dagger_{\alpha} a_{\beta},$$  \hspace{1cm} (12)

with

$$\tilde{U}_{\alpha\beta} = -U_{\alpha\beta} + \sum_{\gamma\delta} V_{\alpha\gamma,\beta\delta} \rho_{\gamma\delta} + \frac{1}{4} \sum_{\delta\eta} W_{\alpha\gamma\epsilon,\beta\delta\eta} \Gamma_{\delta\eta;\gamma\epsilon},$$  \hspace{1cm} (13)

and

$$\tilde{V} = \frac{1}{4} \sum_{\alpha\beta} \left[ V_{\alpha\gamma,\beta\delta} + \sum_{\epsilon\eta} W_{\alpha\gamma\epsilon,\beta\delta\eta} \rho_{\epsilon\eta} \right] a^\dagger_{\alpha} a^\dagger_{\beta} a_{\delta} a_{\beta},$$  \hspace{1cm} (14)

where, in the averaging of 2NFs and 3NFs, one- and two-body reduced density matrices of the many-body system are produced,

$$\rho_{\gamma\delta} = \langle \Psi_0^A | a^\dagger_{\alpha} a_{\beta} | \Psi_0^A \rangle = -i \hbar g_{\gamma\delta}(t - t^+),$$  \hspace{1cm} (15)

$$\Gamma_{\delta\eta;\gamma\epsilon} = \langle \Psi_0^A | a^\dagger_{\alpha} a^\dagger_{\beta} a_{\eta} a_{\delta} | \Psi_0^A \rangle = i \hbar g_{\delta\eta;\gamma\epsilon}(t - t^+),$$  \hspace{1cm} (16)

respectively. The two-body density of Eq. \ref{eq:14} is obtained when the opportune limits are taken in the time arguments of the 2B Green’s function in Eq. \ref{eq:2}.

When the irreducible self-energy is computed with the effective Hamiltonian of Eq. \ref{eq:11}, many-body effects incorporated in the SCGF formalism go beyond standard mean-field approaches, such as the normal ordering procedure. As shown by Eqs. \ref{eq:15} and \ref{eq:16}, density matrices are indeed obtained from correlated propagators, i.e. they are not computed from the reference state.

The separation in Eq. \ref{eq:10} into a simple unperturbed Hamiltonian $H_0$ and an interacting part is instrumental in applying the perturbation expansion to the Green’s function and in deriving the corresponding rules for Feynman diagrams. For the irreducible self-energy, all one-particle irreducible, skeleton and interaction-irreducible diagrams up to third order have been derived in Ref. \ref{ref:20}.

Considering the decomposition of Eq. \ref{eq:9}, the irreducible static self-energy $\Sigma^\infty_{\alpha\beta}$ is given by the 1B effective interaction, i.e.

$$\Sigma^\infty_{\alpha\beta} = \tilde{U}_{\alpha\beta}.$$  \hspace{1cm} (17)

The subtraction of $\tilde{U}$ in Eq. \ref{eq:12} implies that the $\Sigma^\infty_{\alpha\beta}$ is independent from the choice of the reference state or, in other words, independent from the partition of the Hamiltonian in the mean field part and residual part.

The energy dependent part $\Sigma_{\alpha\beta}(\omega)$ is expanded in terms of the residual interaction. Within the skeleton expansion, when single-particle propagators are correlated, the irreducible self-energy up to third order is given by the static part of Eq. \ref{eq:17}, two second-order diagrams of Fig. \ref{fig:1} and 17 third-order diagrams of Figs. \ref{fig:2} and \ref{fig:5} composing the dynamic part of the self-energy. In this approximation, the energy-dependent part of the self-energy contains only effective 2NFs and irreducible 3NFs as interaction insertions. Without propagator renormalization, when one considers the diagrammatic expansion with reference propagators $g^{(0)}(t, t')$ as internal fermionic lines, other diagrams with different topologies must be included to take into account explicitly additional correlations in both the static and dynamic part of the self-energy. These diagrams, containing also the effective 1B interaction, are presented in Appendix C.

In Fig. \ref{fig:1} we show the only two one-particle irreducible, skeleton and interaction-irreducible diagrams at second order. The two diagrams thereof imply different sets of intermediate state configuration (ISC), which is a multiparticle-multihole, or multihole-multiparticle, excitation produced by the interaction and propagating within the nuclear medium. The diagram in Fig. \ref{fig:1a} involves two-particles–one-hole (2p1h) and two-holes–one-particle (2h1p) ISCs, but it is computed with the 2N effective interaction of Eq. \ref{eq:14} instead of the original 2NF and hence it contains effectively the contribution of the 3NF $\tilde{W}$.

The diagram in Fig. \ref{fig:1b} arises instead from an interaction-irreducible 3NF. There are two reasons to assume that this contribution is less important than the one in Fig. \ref{fig:1a} first, 3NFs are generally weaker than corresponding 2NFs (typically, $<\tilde{W}> \approx \frac{1}{m} <\tilde{V}>$ for nuclear interactions \cite{23}); second, the diagram in Fig. \ref{fig:1b} involves $3p2h$ and $3h2p$ ISCs, which are at higher energies and therefore expected to play a minor role at the Fermi surface due to phase space arguments.

By the same token, we may expect that the three diagrams shown in Fig. \ref{fig:2} are the dominant ones among the 17 one-particle irreducible, skeleton and interaction-irreducible self-energy diagrams appearing at third order in the expansion of $\Sigma_{\alpha\beta}(\omega)$. While all diagrams in Fig. \ref{fig:2} involve 2p1h and 2h1p ISCs, diagrams in Figs. \ref{fig:2a} and \ref{fig:2b} contain only effective 2NFs. These two diagrams have been already included in actual calculations for nuclear matter and for finite nuclei \cite{22,23,24,25,26}.

![FIG. 1. One-particle irreducible, skeleton and interaction-irreducible self-energy diagrams appearing at second order in the expansion of Eq. (3), using the effective Hamiltonian of Eq. (11). The wiggly lines represent the 2N effective interaction of Eq. (14), while the long-dashed lines represent the interaction-irreducible 3NF $\tilde{W}$.](image-url)
and following, we will consider explicitly 2 in-time multihole-multiparticle configurations. In the note forward-in-time multiparticle-multihole (backward-in-time multiparticle-multiparticle) configurations.

\[ \langle q \rangle \equiv (n_1, n_2, n_3, k_1, k_5) \]

\[ \langle q' \rangle \equiv (n_6, n_7, n_8, k_9, k_{10}) \]

for forward-in-time terms, and

\[ s \equiv (k_1, k_2, n_3) \]

\[ s' \equiv (k_4, k_5, n_6) \]

\[ u \equiv (k_1, k_2, k_3, n_4, n_5) \]

\[ u' \equiv (k_6, k_7, k_8, n_9, n_{10}) \]

for backward-in-time terms.

For instance, \( M_{\alpha \beta} = M_{(n_1, n_2, k_3) \alpha} \) connects a single-particle state of index \( \alpha \) to an intermediate state composed by a 2p1h configuration, whereas more complicated coupling matrices such as \( M_{\alpha \beta} = M_{(n_1, n_2, n_3, k_4, k_5) \alpha} \) involve 3p2h configurations. Eq. (18) can be seen as an expansion on the ISC space, because the sums include in principle all multi-particle-multi-hole states for a particle addition or removal.

Coupling matrices need to be antisymmetric with respect to permutation of particle indexes and hole indexes. Terms in ADC(2) are all antisymmetric, while some terms in ADC(3) must be antisymmetrized through permutation operators. For those terms which do not require the application of these antisymmetrization operators, it is convenient to order the indexes in Eqs. (19-20) as presented in Eqs. (19-20), defining for instance \((n_1 \leq n_2, k_3), (n_1 \leq n_2 \leq n_3, k_4 \leq k_5), \) and so on. This is very important for practical implementation, owing to the reduction of the dimension of the ADC(3) matrix when single-particle indexes are properly ordered. All the working equations for coupling and interaction matrices presented below do not assume ordered indexes, therefore they are based on the ISC notation as presented in Eqs. (19-20).

ISC energies are diagonal matrices in these indexes. For nucleon addition, with \( M + 1 \) particles and \( M \) holes, \((M + 1)pMh, \) we have,

\[ E^+_{jj'} = E^+_{jj} = \text{diag}(\epsilon^+_n, \epsilon^+_n, \ldots, \epsilon^+_n, \epsilon^+_n, \epsilon^+_n, \epsilon^+_n) \]

\[ -\epsilon^+_{k_1} - \epsilon^+_{k_2} - \cdots - \epsilon^+_{k_{M'}} \] (21)

while for the nucleon removal ISC,

\[ E^-_{kk'} = E^-_{kk} = \text{diag}(\epsilon^-_n, \epsilon^-_n, \ldots, \epsilon^-_n, \epsilon^-_n, \epsilon^-_n, \epsilon^-_n) \]

\[ -\epsilon^-_{k_1} - \epsilon^-_{k_2} - \cdots - \epsilon^-_{k_{M'}} \] (22)

In order to solve for the 1B propagator of Eq. (4), it is useful to recast the Dyson equation in a matrix form, allowing in this way a more efficient computation of 1B propagator eigenvalues. To see this point, we have to start again from the Dyson equation (1) and regard the 1B propagator as a meromorphic function on the complex energy plane. This function has simple poles and residues given by one-nucleon addition (or removal) energies and transition amplitudes, respectively. We can
then find a relation among the transition amplitudes of Eq. (5), by extracting them as residues of the propagator

\[ Z_{\alpha}^i (Z_{\beta}^j)^\dagger = \frac{1}{\hbar \omega - \varepsilon_{\alpha}^{(0)}} \sum_{\delta} \Sigma_{\alpha \delta}^\star (\omega) Z_{\delta}^i (Z_{\beta}^j)^\dagger \bigg|_{\hbar \omega = \varepsilon_{\alpha}}, \]  

(23)

in the Dyson equation. This gives,

\[ Z_{\alpha}^i Z_{\beta}^j = \frac{1}{\hbar \omega - \varepsilon_{\alpha}^{(0)}} \sum_{\delta} \Sigma_{\alpha \delta}^\star (\omega) Z_{\delta}^i Z_{\beta}^j \bigg|_{\hbar \omega = \varepsilon_{\alpha}}, \]

(24)

where \( \varepsilon_{\alpha}^{(0)} \) are one-nucleon addition and removal energies of the unperturbed propagator, obtained from the eigenvalues of \( H_0 \).

By using the decomposition of Eq. (18) we obtain the relation,

\[ Z_{\alpha}^i = \frac{1}{\hbar \omega - \varepsilon_{\alpha}^{(0)}} \sum_{\delta} \Sigma_{\alpha \delta}^\star (\omega) Z_{\delta}^i \bigg|_{\hbar \omega = \varepsilon_{\alpha}}, \]

(25)

which contains both forward-in-time and backward-in-time solutions of the propagator. In the last equality of Eq. (24) we have introduced the vectors \( W_j^i \) and \( W_k^i \), defined as

\[ W_j^i = W_j (\omega) \bigg|_{\hbar \omega = \varepsilon_{\alpha}}, \]

and

\[ W_k^i = W_k (\omega) \bigg|_{\hbar \omega = \varepsilon_{\alpha}}, \]

respectively. As it is going to be clear below, these components are introduced in order to make the Dyson matrix independent of the energy \( \hbar \omega \).

The matrix whose diagonalization gives the eigenspectra of the \( |\Psi_n^{A+1}\rangle \) and \( |\Psi_n^{A-1}\rangle \) systems, and the transition amplitudes of the 1B propagator, is then,

\[ \begin{pmatrix} Z_{\alpha}^i \\ W_r^i \\ W_s^i \\ W_q^i \\ \vdots \end{pmatrix} \begin{pmatrix} \varepsilon_{\alpha}^{(0)} + \Sigma_{\alpha \delta}^\star \\ M_{\alpha \beta}^\dagger \\ N_{\alpha s} \\ M_{\alpha q}^\dagger \\ N_{\alpha u} \end{pmatrix} = \begin{pmatrix} \alpha \beta \\ \delta_{r r'} \\ \beta s' \\ \alpha i \\ \alpha \end{pmatrix} \begin{pmatrix} Z_{\delta}^j \\ W_r^j \\ W_s^j \\ W_q^j \\ \vdots \end{pmatrix}, \]

(27)

where the empty entries in the matrix are zero, meaning that the forward-in-time and backward-in-time sectors are not coupled together, and the dots stay for the self-energy terms with ISCs beyond the 3p2h and 3h2p configurations.

The matrix on the r.h.s. of Eq. (27) is energy-independent, whereas the components \( W_j^i \) of the eigenvectors are functions of the corresponding eigenvalue \( \varepsilon_i \), as it is apparent from definitions (25,26). The diagonalization of the self-energy matrix leads to the extraction of all the poles of the propagator at once, while the normalization of the \( i \)-th eigenvector is required according to,

\[ \sum_{\alpha \beta} Z_{\alpha}^i Z_{\beta}^i + \sum_j (W_j^i)^\dagger W_j^i + \sum_k (W_k^i)^\dagger W_k^i = 1. \]

(28)

The general dependence on \( \varepsilon_i \) of the eigenproblem in Eq. (27) requires an iterative search for the solutions, that in turn implies a severe growth in the dimension of the self-energy matrix. This can be handled by projecting the space of the energy configurations to a smaller Krylov subspace, and then multi-pivot Lanczos-type algorithm can be applied, as illustrated in Ref. [32].
III. GENERAL OUTLINE OF THE ADC(n) METHOD

The irreducible self-energy \( \Sigma_{\alpha\beta}(\omega) \) is the object of the ADC formalism applied in this work. Its expression as a product of matrices in Eq. (18) is the most general analytic form that is consistent with the causality principle and the known Lehmann representation.

Our task is then to find expressions for coupling and interaction matrices including the correlations due to 2NFs and 3NFs. The ADC(\( n \)) strategy consists in deriving explicit expressions of the coupling and interaction matrices by expanding Eq. (18) in powers of 2NFs and 3NFs and then to compare with the Goldstone-Feynman expansion of Eq. (31) with the calculated expression for Goldstone-removal \( \epsilon \) and for backward-in-time coupling matrices, gives the minimal expressions for interaction matrices including the correlations due to 2NFs and/or 3NF, and for backward-in-time coupling matrices,

\[
M_{j\alpha} = M_{j\alpha}^{(1)} + M_{j\alpha}^{(1)} + M_{j\alpha}^{(1)} + \ldots, \quad (29)
\]

where the term \( M_{j\alpha}^{(1)} \) is of \( n \)th order in 2NF and/or 3NF, and for backward-in-time coupling matrices,

\[
N_{\alpha k} = N_{\alpha k}^{(1)} + N_{\alpha k}^{(1)} + N_{\alpha k}^{(1)} + \ldots. \quad (30)
\]

By plugging the two expansions of Eqs. (29-30) into Eq. (18), we obtain the corresponding expansion for the energy-dependent irreducible self-energy up to third order (first order contributions are all included in \( \Sigma_{\alpha\beta}^{\infty} \)).

\[
\begin{align*}
\tilde{\Sigma}_{\alpha\beta}(\omega) &= \sum_j M_{j\alpha j}^{(1)} \left[ \frac{1}{\hbar \omega - E_j^\alpha + i\eta} \right] M_{j\beta j}^{(1)} \\
&+ \sum_j M_{j\alpha j}^{(1)} \left[ \frac{1}{\hbar \omega - E_j^\alpha + i\eta} \right] C_{jj'} \left[ \frac{1}{\hbar \omega - E_{j'}^\beta + i\eta} \right] M_{j'\beta j'}^{(1)} + \ldots \\
&+ \sum_j N_{\alpha k j}^{(1)} \left[ \frac{1}{\hbar \omega - E_k^\delta - i\eta} \right] N_{k\beta j}^{(1)} + \ldots,
\end{align*}
\]

(31)

for both forward-in-time and backward-in-time self-energy parts. The comparison of the formal expansion of Eq. (31) with the calculated expression for Goldstone-type diagrams, gives the minimal expressions for interaction and coupling matrices in terms of the transition amplitudes \( Z_{\alpha i} \) and the one-nucleon addition \( E_{\alpha}^{n} \) and removal \( \epsilon \) energies of the 1B propagator \( g_{\alpha\beta}(\omega) \) of Eq. (1).

By looking at the expansion in Eq. (31), we see that the third-order terms containing the interaction matrices \( C_{jj'} \) and \( D_{kk'} \) do not retain the same analytic form as Eq. (18), which is based on the Lehmann representation of the propagator itself. In order to recover this analytic form in terms of self-energy poles, one must introduce higher-order terms and perform a resummation of those diagrams up to infinite order: this resummation gives the non-perturbative character of the method, that takes into account at all orders several types of diagrams, particle-particle and hole-hole ladders, and particle-hole rings, as well as other resummations induced by 3NFs.

Then one can solve the Dyson equation by simply diagonalizing Eq. (27), with the possibility to resort to the Lanczos algorithm, if the dimensionality of the problem requires a reduction to the Krylov subspace.

A. ADC method at second order: ADC(2)

In this Section we present the explicit expressions of coupling and interaction matrices entering in the ADC(2) formalism. The two second order diagrams shown in Fig. 1 are sufficient to define the ADC(2) approximation scheme. Coupling and interaction matrices required to build the ADC(3) are introduced in Section III B and Appendix A. Unless otherwise stated, for coupling and interaction matrices we adopt the Einstein’s convention to build the ADC(2) formalism. The two second order diagrams shown in Fig. 1 are sufficient to define the ADC(2) approximation scheme. Coupling and interaction matrices required to build the ADC(3) are introduced in Section III B and Appendix A.
different orders according to the expansions in Eqs. (29) and (30). Within a given order, coupling matrices can also differ with respect to the kind of interaction (2NF and/or 3NF) appearing in the term. For this reason we specify in the notation an extra superscript distinguishing different coupling matrices at the same order.

For instance, at second order we will encounter a coupling matrix \( M_{\gamma\alpha}^{(1a)} \) containing a 2N interaction linked to a \( r = (n_1, n_2, k_3) \) ISC, \( M_{q\alpha}^{(1b)} \) containing a 3N interaction linked to a \( q = (n_1, n_2, n_3, k_4, k_5) \) ISC, and so on. The extra superscript with Latin letter corresponds to the labeling of diagrams in the Figures.

In order to illustrate the ADC procedure, we write first the entire expressions for all the Goldstone diagrams in second order Feynman diagram of Fig. 1. Then we display the formulas of the coupling matrices that can be singled out from the self-energy expressions. The equation for the dynamic self-energy in Fig. 1a reads,

\[
\Sigma_1^{(1a)}(\omega) = \frac{1}{2} \sum_{n_1, n_2, n_3} \left( \sum_{k_1, k_2} \frac{\lambda^{n_1} \lambda^{n_2} \lambda^{n_3} \lambda^{k_1} \lambda^{k_2} \lambda^{k_3}}{\hbar \omega - (\varepsilon_{n_1} + \varepsilon_{n_2} + \varepsilon_{k_3} + i\eta)} + \sum_{k_1, k_2} \frac{\lambda^{k_2} \lambda^{k_3}}{\hbar \omega - (\varepsilon_{k_1} + \varepsilon_{k_2} + \varepsilon_{n_3} - i\eta)} \right) V_{\mu\nu,\alpha\lambda}. \tag{32}
\]

Being already in the Lehmann form of Eq. (18), we can read directly from Eq. (32) the forward-in-time contribution to the ADC(2) coupling matrix,

\[
M_{\gamma\alpha}^{(1a)} = \frac{1}{\sqrt{2}} \lambda^{n_1} \lambda^{n_2} \lambda^{n_3} V_{\mu\nu,\alpha\lambda}, \tag{33}
\]

while in the backward-in-time channel we have

\[
N_{\alpha\gamma}^{(1a)} = \frac{1}{\sqrt{2}} \lambda^{k_1} \lambda^{k_2} \lambda^{n_3} V_{\mu\nu,\alpha\lambda}, \tag{34}
\]

that couples the effective 2NF with the 2h2p ISC. It is also clear that the interaction matrices \( C_{jj'} \) and \( D_{kk'} \) are zero in ADC(2). The representations of Eqs. (33-34) as fragments of Goldstone diagrams are depicted in Figs. 3a and 4a respectively.

The equation for the energy-dependent self-energy with 3NFs in Fig. 1b reads,

\[
\Sigma_1^{(1b)}(\omega) = \frac{1}{12} W_{\alpha\gamma,\delta,\tau} \left( \sum_{k_1, k_2, k_3, k_4} \frac{\lambda^{n_1} \lambda^{n_2} \lambda^{n_3} \lambda^{k_1} \lambda^{k_2} \lambda^{k_3} \lambda^{k_4}}{\hbar \omega - (\varepsilon_{n_1} + \varepsilon_{n_2} + \varepsilon_{n_3} + \varepsilon_{k_4} - i\eta)} \right) \left( \sum_{j_1, j_2, j_3, j_4} \frac{\lambda^{j_1} \lambda^{j_2} \lambda^{j_3} \lambda^{j_4}}{\hbar \omega - (\varepsilon_{j_1} + \varepsilon_{j_2} - \varepsilon_{k_3} - \varepsilon_{k_4} - i\eta)} \right) W_{\mu\nu,\lambda,\beta\eta}. \tag{35}
\]

The coupling matrix that links the 3NF to 3p2h ISCs is found in the diagram of Fig. 1b and it is read from Eq. (35). Its expression is,

\[
M_{q\alpha}^{(1b)} = \frac{1}{\sqrt{12}} \lambda^{n_1} \lambda^{n_2} \lambda^{n_3} \lambda^{k_1} \lambda^{k_2} \lambda^{k_3} W_{\mu\nu,\lambda,\alpha\eta}, \tag{36}
\]

while the corresponding matrix linked to the 3h2p ISC is,

\[
N_{\alpha\gamma}^{(1b)} = \frac{1}{\sqrt{12}} W_{\alpha\gamma,\mu\nu,\lambda} \lambda^{k_1} \lambda^{k_2} \lambda^{n_4} \lambda^{n_5}. \tag{37}
\]

Eq. (37) is also found in the diagram of Fig. 1b and in the second term of Eq. (35). Their graphical representations as fragments of Goldstone diagrams are depicted in Figs. 3b and 4b.

The four coupling matrices in Eqs. (33-34) and (36-37) along with their complex conjugates, complete the set of matrices found in the irreducible Goldstone diagrams of the self-energy at second order, which are given by the first and fourth rows in Eq. (31). Their graphical representations as building blocks of Goldstone diagrams are found in Figs. 3 and 4. All these matrices enter as building blocks of the ADC construction at second and third order in the expansion with respect to the nuclear interaction. To summarize, the ADC(2) approximation for Eq. (18) requires the following terms,

\[
M_{\gamma\alpha}^{(ADC(2))} = M_{\gamma\alpha}^{(1a)} + M_{q\alpha}^{(1b)}, \tag{38}
\]

\[
N_{\alpha\gamma}^{(ADC(2))} = N_{\alpha\gamma}^{(1a)} + N_{\alpha\gamma}^{(1b)}, \tag{39}
\]

\[
C_{jj'} = 0, \tag{40}
\]

\[
D_{kk'} = 0. \tag{41}
\]

There are no interaction matrices \( C_{jj'} \) and \( D_{kk'} \), in the
ADC(2), because coupling matrices are linked directly without any intermediate interaction insertion. This is not true anymore in the ADC(3), where matrices $M^{(1a)}$ and $N^{(1a)}$ are linked through interaction matrices $C_{j,j'}$ and $D_{pk}$, respectively, as it is the case for self-energy terms on third and sixth lines of Eq. (31).

**B. ADC method at third order: ADC(3)**

In this Section we present explicit expressions of the coupling and interaction matrices entering in the ADC formalism at third order, for the three diagrams shown in Fig. 2 and for the four diagrams appearing first in each row of Fig. 5. These diagrams contribute to Goldstone diagrams ($rr'$) and ($ss'$) of Eq. (27), corresponding to 2p1h and 2h1p ISCs, which are the simplest configurations to be excited in the Fock space. The diagrams depicted in Figs. 2a-2b are the dominant ones at third order, given that only 2N interactions are present. The diagram in Fig. 2a contains instead a 3NF, but it can nonetheless play a significant role, because its Goldstone diagrams feature only 2p1h and 2h1p ISCs.

Each row in Fig. 5 collects a different topology of diagrams in terms of number of effective 2NFs and interaction-irreducible 3NFs entering in diagrams. In general, these diagrams are less important compared to the ones in Fig. 2 because they feature at least a 3p2h and a 3h2p ISC in all their Goldstone contributions. For forward-in-time (backward-in-time) diagrams, topologies in the first and second row of Fig. 5 couple 2p1h (2h1p) ISCs to 3p2h (3h2p) ISCs. They are linked by $C_{r'\eta} (D_{s'u})$ and $C_{q'r} (D_{u's})$, accounting for off-diagonal entries of Eq. (27). Within these two kind of topologies, diagrams in the first row contain only one 3NF, therefore they are expected to be more important than the ones in the second row, each featuring two 3NFs. Finally, the last two rows in Fig. 5 introduce the diagonal coupling between ISCs with five fermionic lines, 3p2h for forward-in-time diagrams and 3h2p for backward-in-time diagrams, corresponding respectively to entries $(qq')$ and $(uu')$ of Eq. (27). Again, there is a hierarchy between the two topologies, with those in the fourth row being less important due to the presence of three 3NFs.

The first four diagrams in each row are assumed as emblematic for each topology, and treated in the present Section. The remnant coupling and interaction matrices composing third-order diagrams and not presented in this Section, are displayed in Appendix A.

Coupling and interaction matrices are fully antisymmetrized with respect to their particle and hole indexes. In order to show this explicitly, we introduce the following antisymmetrizer operators. Given a function depending on up to three particle or hole indexes, i.e. $f(i,j,h) \equiv f(n_i,n_j,n_h)$ or $f(i,j,h) \equiv f(k_i,k_j,k_h)$, the antisymmetric permutation operator of a pair of indexes is introduced,

$$A_{ij} f(i,j,h) \equiv f(i,j,h) - f(j,i,h).$$  \hfill (42)

For 3p2h and 3h2p configurations, it is useful to define the cyclic permutation operator as

$$P_{ijk} f(i,j,h) \equiv f(i,j,h) + f(h,i,j) + f(j,h,i),$$  \hfill (43)

and the permutation operator acting on three indexes, that is

$$A_{ijk} f(i,j,h) \equiv f(i,j,h) + f(h,i,j) + f(j,h,i) - f(i,h,j) - f(j,i,h) - f(h,j,i).$$  \hfill (44)

Coupling matrices appearing at third order contain two interaction operators, which can be the interaction-irreducible 3NF and/or the effective 2NF. For the sake of clarity, we write in a compact form pieces of diagram containing one interaction, whose vertices are not connected to any external fermion line. These terms are indeed the cluster operators included in the exponential Ansatz of the coupled-cluster wave function [33]. Without assuming the Einstein’s convention of summing over repeated indices, we write them as,

$$t_{k_1}^{n_1} \equiv \sum_{\alpha\beta} \lambda_{\alpha}^{n_1} \bar{U}_{\alpha\beta} \gamma_{\beta}^{k_1} \frac{1}{\epsilon_{k_2} - \epsilon_{n_1}^{+}},$$  \hfill (45)

with the effective one-body potential of Eq. (12),

$$t_{k_3 k_4}^{n_1 n_2} \equiv \sum_{\alpha\beta \gamma \delta} \lambda_{\alpha}^{n_1} \gamma_{\beta}^{n_2} \bar{V}_{\alpha\beta,\gamma\delta} \gamma_{\delta}^{k_3} \gamma_{\gamma}^{k_4} \frac{1}{\epsilon_{k_3} + \epsilon_{k_4} - \epsilon_{n_1}^{+} - \epsilon_{n_2}^{+}},$$  \hfill (46)
with the effective 2NF of Eq. (14), and we introduce another definition,

\[ t_{n_1 n_2 n_3}^{k_4 k_5 k_6} = \sum_{\alpha, \beta, \gamma, \mu, \nu, \lambda} \lambda^n_\alpha \lambda^n_\beta \lambda^n_\gamma W_{\alpha \beta \gamma, \mu \nu \lambda} \gamma^k_\mu \gamma^k_\nu \gamma^k_\lambda, \]

for the term with the interaction-irreducible 3NF.

1. ADC(3) matrices for Feynman diagrams in Fig. 2

At third order in the ADC, we consider first the subset of coupling matrices and interaction matrices which are linked to 2\( p_1 h \) and 2\( h_1 p \) ISC configurations, the ADC(3) approximation for Eq. (18) requires the following terms,

\[ M^{(I\alpha)}_{j\alpha} = M^{(I\alpha a)}_{j\alpha} + M^{(I\alpha b)}_{j\alpha} + M^{(I\alpha c)}_{j\alpha}, \]
\[ N_{\alpha k}^{(I)} = N_{\alpha a}^{(Ia)} + N_{\alpha s}^{(Ib)} + N_{\alpha s}^{(Ic)}, \]
\[ C_{j j'} = C_{pp}^{j j'} + C_{ph}^{j j'} + C_{3N}^{j j'}, \]
\[ D_{k k'} = D_{ss}^{h k} + D_{ss}^{h p} + D_{ss}^{3N}, \]

that complement the ones already introduced in Eqs. (38-41) at second order.

We introduce now explicit expressions for the r.h.s. of Eqs. (48-51), and start by presenting coupling matrices composed by two effective 2NFs connecting to 2\( p_1 h \) ISC configuration. By using the definition in Eq. (46) we have the matrices,

\[ M^{(I\alpha a)}_{j\alpha} = \frac{1}{2\sqrt{2}} t_{n_1 n_2}^{k_4 k_5} (\gamma^k_\mu \gamma^k_\nu) \gamma^k_\lambda \tilde{V}_{\mu, \nu, \alpha, \lambda}, \]

FIG. 5. As in Fig. 1 but for third-order diagrams with 3\( p_2 h \) and 3\( h_2 p \) intermediate state configurations.
Other coupling matrices containing one effective 2NF and one interaction-irreducible 3NF, we present here the complex conjugates of Eqs. (54) and (55), while the coupling matrix (c) to the complex conjugate of Eq. (57).

Among coupling matrices containing one effective 2NF and one interaction-irreducible 3NF, we present here the ones appearing in the self-energy diagram of Fig. 2c that is

$$\mathbf{M}_{\alpha s}^{(Ic)} = \frac{1}{2\sqrt{2}} t_{k_{1}k_{2}k_{3}} \tilde{V}_{\alpha, \mu, \nu} (X_{\mu}^{n_{1}} X_{\nu}^{n_{2}} X_{\lambda}^{n_{5}}) \tilde{V}_{\mu, \nu, \alpha, \lambda} \quad (56)$$

and

$$\mathbf{N}_{\alpha s}^{(Ib)} = -\frac{1}{2\sqrt{2}} t_{k_{1}k_{2}k_{3}} \tilde{V}_{\alpha, \mu, \nu} (Y_{\mu}^{k_{1}} Y_{\nu}^{k_{2}} Y_{\lambda}^{k_{3}}) \tilde{V}_{\mu, \nu, \alpha, \lambda} \quad (57)$$

Diagrammatic representations of Eqs. (56) and (57) are displayed in Figs. 6c and 7c respectively.

All the other coupling matrices with one 2NF and one 3NF are collected in Sec. A 2 of Appendix A while matrices with two interaction-irreducible 3NFs are presented in Sec. A 3 in Appendix A.

Now we introduce expressions of the interaction matrices in Eqs. (50-51), containing the $\tilde{V}_{\alpha, \beta, \gamma, \delta}$ and $W_{\alpha, \beta, \gamma, \delta, \lambda}$ matrix elements. For the two cases, we display interaction matrices appearing in both the forward-in-time and backward-in-time self-energy Goldstone diagrams of Figs. 2.

The interaction matrix that connects 2ph ISCs through a particle-particle (pp) interaction is

$$\mathbf{C}_{rt}^{pp} = \frac{1}{2} \lambda_{\mu}^{n_{1}} \lambda_{\nu}^{n_{2}} \tilde{V}_{\mu, \nu, \rho} (\lambda_{\rho}^{n_{4}} \lambda_{\sigma}^{n_{5}}) \delta_{k_{2}k_{3}} \quad (58)$$

while the one connecting through a particle-hole (ph) interaction is

$$\mathbf{C}_{rt}^{ph} = \frac{1}{2} \lambda_{12} A_{45} (\lambda_{\mu}^{n_{1}} \lambda_{\nu}^{k_{3}} \tilde{V}_{\mu, \nu, \rho} (\lambda_{\rho}^{n_{4}} \lambda_{\sigma}^{k_{5}}) \delta_{n_{2}n_{5}}) \quad (59)$$
where the action of two permutation operators \( A_{12} \) and \( A_{45} \) is defined in Eq. (42) and produces 4 terms.

We present now the corresponding interaction matrices appearing in backward-in-time self-energy Goldstone diagrams, namely those that are linked to propagators of hole-particle kind in diagrams.

We start by the interaction matrix that connects \( 2h1p \) ISCs through a hole-hole (hh) interaction, that is

\[
D_{hh}^{ss'} = -\frac{1}{2} (\nu^{k_1} \nu^{k_2})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \delta_{n, n'} ,
\]

(60)

while the one connecting through a hole-particle (hp) interaction is

\[
D_{hp}^{ss'} = -\frac{1}{2} A_{12} A_{45} \left( (\nu^{k_1} \nu^{k_2})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \lambda_{n, n'} \right) ,
\]

(61)

where permutation operators acting on hole states are defined in the same way as the one acting on particle states for the matrix \( D_{hh} \) in Eq. (59).

The only interaction matrix that connects \( 2p1h \) ISCs through a 3NF is

\[
C_{rr'}^{3N} = -\frac{1}{2} (\nu^{k_1} \nu^{k_2} \nu^{k_3})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \delta_{n, n'} ,
\]

(62)

which is explicitly antisymmetric in particle indexes, while the one connecting two \( 2h1p \) ISCs through a 3NF is

\[
D_{ss'}^{3N} = -\frac{1}{2} (\nu^{k_1} \nu^{k_2} \nu^{k_3})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} ,
\]

(63)

which is also explicitly antisymmetric in particle indexes.

2. \( \text{ADC}(3) \) matrices for selected Feynman diagrams in Fig. 5

Coupling matrices presented in this Section are obtained from the four Feynman diagrams in the first column of Fig. 5. Most of these matrices are linked to \( 3p2h \) and \( 3h2p \) ISCs, with few exceptions derived from Goldstone diagrams where ISCs are of \( 2p1h \) and \( 2h1p \) type. This subset of coupling matrices required to build the \( \text{ADC}(3) \) approximation is given by

\[
M_{j\alpha}^{(1d)} = M_{q\alpha}^{(1d)} + M_{r\alpha}^{(1d)} + M_{q\alpha}^{(1h)} + M_{r\alpha}^{(1h)} + M_{q\alpha}^{(1d)} + M_{r\alpha}^{(1o)} ,
\]

(64)

\[
N_{\alpha k}^{(1d)} = N_{\alpha k}^{(1d)} + N_{\alpha k}^{(1d)} + N_{\alpha k}^{(1h)} + N_{\alpha k}^{(1h)} + N_{\alpha k}^{(1h)} + N_{\alpha k}^{(1o)} ,
\]

(65)

We present first matrices containing two effective 2NFs. As before, we display both matrices obtained from forward-in-time and backward-in-time Goldstone diagrams, denoted with the notation \( M_{j\alpha} \) and \( N_{\alpha k} \) respectively.

In Goldstone diagrams of the term in Fig. 5d we have,

\[
M_{q\alpha}^{(1d)} = \frac{\sqrt{3}}{6} A_{45} P_{123} \left( (\nu^{k_1} \nu^{k_2} \nu^{k_3})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \delta_{n, n'} \right) ,
\]

(66)

where the combination of permutation operators in the first line performs the antisymmetrization of the indexes \( (k_1, k_2, k_3) \) and \( (n_1, n_2, n_3) \), according to definitions in Eqs. 42 [13].

We turn now to coupling matrices containing one effective 2NF and one interaction-irreducible 3NF. In the Goldstone diagrams of the term in Fig. 5d we have also,

\[
M_{r\alpha}^{(1d)} = -\frac{\sqrt{2}}{4} A_{12} \left( (\nu^{k_1} \nu^{k_2} \nu^{k_3})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) W_{\mu,\lambda,\rho} ,
\]

(67)

(68)

In the Goldstone diagrams of the term in Fig. 5h we have,

\[
M_{q\alpha}^{(1b)} = -\frac{\sqrt{3}}{6} A_{45} P_{123} \left( (\nu^{k_1} \nu^{k_2} \nu^{k_3})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) ,
\]

(69)

while in the Goldstone diagrams of the term in Fig. 5l we find,

\[
M_{q\alpha}^{(1b)} = \frac{\sqrt{3}}{6} A_{45} P_{123} \left( (\nu^{k_1} \nu^{k_2} \nu^{k_3})^* \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) W_{\mu,\lambda,\rho} ,
\]

(70)

For backward-in-time Goldstone diagrams, we can single out from the term in Fig. 5d the coupling matrix,

\[
N_{\alpha u}^{(1d)} = \frac{\sqrt{3}}{6} \nu_{\alpha u} \nu_{\mu,\nu} \nu_{\alpha u} A_{45} P_{123} \left( \nu_{\mu,\lambda,\rho} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) ,
\]

(71)

and also the following coupling matrix depending on 2N and 3N interactions, i.e.

\[
N_{\alpha u}^{(1d)} = \frac{\sqrt{7}}{4} W_{\alpha u} \nu_{\mu,\nu} \nu_{\alpha u} A_{12} \left( \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{\mu,\nu} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) .
\]

(72)

For backward-in-time Goldstone diagrams, we can single out from the term in Fig. 5l the coupling matrix,

\[
N_{\alpha u}^{(1b)} = -\nu_{\alpha u} \nu_{\mu,\nu} \nu_{\alpha u} A_{45} P_{123} \left( \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{\mu,\nu} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) ,
\]

(73)

while in Fig. 5l we find the coupling matrix,

\[
N_{\alpha u}^{(1l)} = \frac{\sqrt{3}}{12} W_{\alpha u} \nu_{\mu,\nu} \nu_{\alpha u} A_{12} \left( \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{\mu,\nu} \nu^{k_1} \nu^{k_2} \nu^{k_3} \lambda_{n, n'} \right) .
\]
Finally we introduce coupling matrices containing two interaction-irreducible 3NFs. In Goldstone diagrams of the term in Fig. 5h we have,

$$M_{\gamma\alpha}^{(Ih)} = -\sqrt{2} \frac{\lambda_{2}}{8} A_{12} \left( t_{b_{k} b_{k_{5}}} \left( \gamma^{k_{6}} \gamma^{k_{7}} \right)^{*} \gamma_{\lambda}^{k_{8}} \left( \lambda_{\eta}^{k_{9}} \lambda_{\eta_{p}}^{k_{10}} \right)^{*} \right) \right) W_{\mu_{\lambda}, \alpha_{\eta_{p}}},$$

(74)

while in Goldstone diagrams of the term in Fig. 5o we have,

$$M_{\gamma\alpha}^{(Io)} = -\sqrt{3} \frac{\lambda_{2}}{36} \left( t_{b_{k} b_{k_{5}}} \left( \gamma^{k_{6}} \gamma^{k_{7}} \right)^{*} \gamma_{\lambda}^{k_{8}} \left( \lambda_{\eta}^{k_{9}} \lambda_{\eta_{p}}^{k_{10}} \right)^{*} \right) \right) \right) \right) W_{\mu_{\lambda}, \alpha_{\eta_{p}}},$$

(75)

that is antisymmetric in the indexes $n_{1}$, $n_{2}$, $n_{3}$ and $k_{4}$,$k_{5}$.

For backward-in-time Goldstone diagrams, we can single out from the term in Fig. 5h the coupling matrix

$$N_{\alpha\gamma}^{(Ih)} = -\sqrt{2} \frac{\lambda_{2}}{8} A_{12} \left( \left( \gamma^{k_{6}} \gamma^{k_{7}} \lambda_{\eta}^{k_{8}} \lambda_{\eta_{p}}^{k_{10}} \right)^{*} \right) \right) \right) \right) \right) W_{\mu_{\lambda}, \alpha_{\eta_{p}}},$$

(76)

while the matrix

$$N_{\alpha\gamma}^{(Io)} = \sqrt{3} \frac{\lambda_{2}}{36} A_{12} \left( \left( \gamma^{k_{6}} \gamma^{k_{7}} \lambda_{\eta}^{k_{8}} \lambda_{\eta_{p}}^{k_{10}} \right)^{*} \right) \right) \right) \right) \right) W_{\mu_{\lambda}, \alpha_{\eta_{p}}},$$

(77)

appears in the Goldstone diagrams relative to Fig. 5o and it is antisymmetric in the indexes $k_{1}$, $k_{2}$, $k_{3}$ and $n_{4}$, $n_{5}$.

IV. CONCLUSIONS

We have calculated all possible Feynman diagrams for the self-energy up to third order, for an Hamiltonian including up to three-body interactions. Using these, we have then derived the complete set of working equations that are needed to calculate the self-energy non-perturbatively in the ADC(n) approach at orders $n=2$ and 3. While the expansion of the self-energy is considered perturbatively by including diagrams featuring up to three interactions, the ADC(3) formalism expands automatically certain classes of diagrams to infinite order. In particular, one resums series of ladders, rings and interaction-irreducible 3NFs diagrams. As for the usual ADC(n) computations, the Dyson equation for the 1B propagator can be implemented as a large but energy independent eigenvalue problem. However, in presence of 3NFs, intermediate state configurations of 3p2h and 3h2p type contribute already at ADC(2) and ADC(3) levels, while they would appear at ADC(4) and ADC(5) for NN-only interactions.

In showing expressions for both coupling and interaction matrices, we have organized the equations according to their importance, using criteria based on the number of excitations implied by ISCs and the natural hierarchy of many-nucleon forces. We started by revisiting the most relevant correlations in terms of 2p1h and 2h1p ISCs, with one particle-hole excitation on the reference propagator. This sector contains the well-known ADC(3) equations for the original and effective NN interactions.

A new contribution arises from the Feynman diagram of Fig. 2c and involves interaction-irreducible 3NF (that is, which cannot be expressed as simpler normal ordered forces). This last term is argued to be less relevant in virtue of the hierarchy of nuclear forces. Then, we have worked out the subset of ADC(3) coupling and interaction matrices that link to the 3p2h and 3h2p sector of ISCs. While this hierarchy suggests that 3p2h and 3h2p ISCs may be necessary only for future generations of ab initio approaches, the diagram of Fig. 2c may already have implication for present nuclear Hamiltonians. However, these conjectures have not yet been checked and knowing the importance of diagram 2c would give guidance for the inclusion of further correlations.

In order to provide the ADC formalism in its most general form, we have released the assumption of a fully self-consistent expansion and considered also all the additional non-skeleton diagrams that appear in this case. The resulting corrections are important (at least conceptually) when calculations are based on standard reference propagators of mean-field type. New sets of diagrams appear for both the static and dynamic self-energy and have been derived together with the corresponding contributions in the ADC framework. In total, 4 additional Feynman diagrams must be considered in the ADC(3) dynamic self-energy when one is working with uncorrelated propagators, while the 1B effective interaction defining the energy-independent self-energy is decomposed into 16 Feynman diagrams of different topologies. Hence, the complete ADC(3) formalism with 3NFs is now available for the self-energy, either self-consistent (with only skeleton diagrams) or based on an uncorrelated reference state.

The formalism presented in this work sets the basis for future advancements of the SCGF approach, especially useful for studies of nuclear structure where the full inclusion of realistic three-nucleon interactions is required. The numerical implementation of the 3p2h and 3h2p sector is a long-term project that might rely on the availability of future supercomputing computing resources. At the same time, the case for such improvements in the many-body truncation will also depend on the performance and accuracy of next-generation realistic nuclear interactions. On the other hand, calculating the diagram of Fig. 2c involves only 2p1h and 2h1p ISCs and will not require resources beyond present day computer power. Thus, we plan a follow-up study to implement this term.

Appendix A: ADC equations for self-energy at third order
In this Appendix we complete the list of the expressions of coupling and interaction matrices, found in Goldstone diagrams at third order in the expansion of the self-energy. The complete list of all terms required to build the ADC(3) formalism is

\[ M_{j\alpha}^{(ADC(3))} = M_{j\alpha}^{(ADC(2))} + M_{j\alpha}^{(IIa)} + M_{j\alpha}^{(IIb)} + M_{j\alpha}^{(IIc)} + M_{j\alpha}^{(IId)} + M_{j\alpha}^{(III)} + M_{j\alpha}^{(IIe)} + M_{j\alpha}^{(IIf)} + M_{j\alpha}^{(IIg)} + M_{j\alpha}^{(IIh)} + M_{j\alpha}^{(IIi)} + M_{j\alpha}^{(IIj)} + M_{j\alpha}^{(IIk)} + M_{j\alpha}^{(IIl)} + M_{j\alpha}^{(IIm)} + M_{j\alpha}^{(IIn)} + M_{j\alpha}^{(IIo)} + M_{j\alpha}^{(IIp)} + M_{j\alpha}^{(IIq)} \]

and

\[ N_{\alpha k}^{(ADC(3))} = N_{\alpha k}^{(ADC(2))} + N_{\alpha k}^{(IIa)} + N_{\alpha k}^{(IIb)} + N_{\alpha k}^{(IIc)} + N_{\alpha k}^{(IId)} + N_{\alpha k}^{(IIe)} + N_{\alpha k}^{(IIf)} + N_{\alpha k}^{(IIg)} + N_{\alpha k}^{(IIh)} + N_{\alpha k}^{(IIi)} + N_{\alpha k}^{(IIj)} + N_{\alpha k}^{(IIk)} + N_{\alpha k}^{(IIl)} + N_{\alpha k}^{(IIm)} + N_{\alpha k}^{(IIn)} + N_{\alpha k}^{(IIo)} + N_{\alpha k}^{(IIp)} + N_{\alpha k}^{(IIq)} \]

For the coupling matrices, these terms are denoted with superscripts ranging from (IIa) to (IIq). Their explicit expressions will be given in Eqs. (A21-A25, A31-A35) (Eqs. (A26-A30, A36-A40)). Finally, for the interaction matrices, these terms are denoted with superscripts ranging from (IId) to (IIo). Their explicit expressions will be given in Appendix C.2.

Interaction matrices appear at third order in the ADC, as listed in Eqs. (A3, A4). The first three terms thereof connecting to 2p1h and 2h1p configurations, are given in Eqs. (52, 53, 54, 55, 56, 57) for forward-in-time interactions and in Eqs. (66, 68, 69, 70, 71, 72, 73, 74, 75) for backward-in-time ones. Other matrices required to link 3p2h or 3h2p ISCs are denoted by C_{ppp}, ..., C_{qqq}, (D_{ppp}, ..., D_{qqq}). They will be given below in Eqs. (A21-A25, A31-A35) (Eqs. (A26-A30, A36-A40)). Finally, additional four interaction matrices introduced in Appendix C.2 for the non-skeleton expansion are specified in Eqs. (A3-A4) through the superscript \( \tilde{U} \).

1. Coupling matrices with two effective 2NFs

In Fig. 5c we find the following coupling matrices,

\[ M_{q\alpha}^{(IIc)} = -\frac{\sqrt{3}}{6} \tilde{V}_{\alpha,\mu,\lambda} P_{13} (\gamma_{k_{3}k_{6}}^{\gamma_{1}n_{3}} \gamma_{\mu_{1}}^{\gamma_{1}} \gamma_{\nu_{2}}^{\gamma_{2}} (\lambda_{k_{0}}^{\gamma_{n_{6}}})^{*} \tilde{V}_{\nu_{\mu},\lambda,\alpha}) \]

and

\[ N_{\alpha k}^{(IIc)} = -\frac{\sqrt{3}}{6} \tilde{V}_{\alpha,\mu,\lambda} P_{13} (\gamma_{k_{3}k_{6}}^{\gamma_{1}n_{3}} \gamma_{\mu_{1}}^{\gamma_{1}} \gamma_{\nu_{2}}^{\gamma_{2}} (\lambda_{k_{0}}^{\gamma_{n_{6}}})^{*} \tilde{V}_{\nu_{\mu},\lambda,\alpha}) \]

for the forward-in-time and backward-in-time Goldstone diagrams, respectively.

2. Coupling matrices with one effective 2NF and one interaction-irreducible 3NF

Diagrams in Fig. 5c contains also an interaction-irreducible 3NF, therefore another coupling matrix can be obtained from the corresponding Goldstone diagrams. For the forward-in-time and backward-in-time parts we have,

\[ M_{q\alpha}^{(IIc')} = \frac{\sqrt{3}}{6} \tilde{V}_{\alpha,\mu,\lambda} P_{13} (\gamma_{k_{3}k_{6}}^{\gamma_{1}n_{3}} \gamma_{\mu_{1}}^{\gamma_{1}} \gamma_{\nu_{2}}^{\gamma_{2}} (\lambda_{k_{0}}^{\gamma_{n_{6}}})^{*} W_{\mu,\lambda,\alpha}^{n_{3}n_{5}}) \]

and

\[ N_{\alpha k}^{(IIc')} = \frac{\sqrt{3}}{6} \tilde{V}_{\alpha,\mu,\lambda} P_{13} (\gamma_{k_{3}k_{6}}^{\gamma_{1}n_{3}} \gamma_{\mu_{1}}^{\gamma_{1}} \gamma_{\nu_{2}}^{\gamma_{2}} (\lambda_{k_{0}}^{\gamma_{n_{6}}})^{*} W_{\mu,\lambda,\alpha}^{n_{3}n_{5}}) \]

respectively.

Also diagrams in the second and third row of Fig. 5c feature coupling matrices with 2NFs and interaction-irreducible 3NFs. We list them below considering both forward- and backward-in-time contributions. In the Goldstone diagrams of the term in Fig. 5c we have,

\[ M_{q\alpha}^{(III)} = \frac{\sqrt{3}}{12} A_{45} (\gamma_{k_{3}k_{6}}^{\gamma_{1}n_{3}} \gamma_{\mu_{1}}^{\gamma_{1}} \gamma_{\nu_{2}}^{\gamma_{2}} (\lambda_{k_{0}}^{\gamma_{n_{6}}})^{*} \tilde{V}_{\nu_{\mu},\lambda,\alpha}) \]

and

\[ N_{\alpha k}^{(III)} = \frac{\sqrt{3}}{12} A_{45} (\gamma_{k_{3}k_{6}}^{\gamma_{1}n_{3}} \gamma_{\mu_{1}}^{\gamma_{1}} \gamma_{\nu_{2}}^{\gamma_{2}} (\lambda_{k_{0}}^{\gamma_{n_{6}}})^{*} \tilde{V}_{\nu_{\mu},\lambda,\alpha}) \]
In the Goldstone diagrams of the term in Fig. 5m we can single out the coupling matrices,

\[ M^{(1m)}_{q \alpha} \equiv \frac{\sqrt{3}}{4} A_{145} P_{123} \left( \ell_{k_1k_4}^{n_1n_6} (\gamma_{\mu}^{k_7})^* \lambda^{n_2} \lambda^{n_3} \right) \gamma^{n_4}_\eta (\lambda^{n_6}_\rho)^* W_{\mu\nu,\lambda,\alpha\rho} \),

(A11)

and

\[ N^{(1m)}_{\alpha u} \equiv \frac{\sqrt{3}}{4} A_{k_4k_2} P_{123} \left( W_{\alpha_Q,\mu,\nu}(\gamma_{\mu}^{k_7})^* \lambda^{n_2} \lambda^{n_3} \right) (\lambda^{n_6}_\rho)^* \gamma^{k_3\eta} \gamma^{k_4n_5n_6}_\mu k_{k_1k_7} \),

(A12)

Finally, in the Goldstone diagrams of the term in Fig. 5n, we have,

\[ M^{(1n)}_{q \alpha} \equiv \frac{\sqrt{3}}{12} k_{k_1k_5} \gamma^{n_1} \lambda^{n_2} \lambda^{n_3} (\lambda^{n_6}_\rho)^* W_{\mu\nu,\lambda,\alpha\rho} \),

(A13)

and

\[ N^{(1n)}_{\alpha u} \equiv \frac{\sqrt{3}}{12} W_{\alpha_Q,\mu,\nu,\lambda}(\gamma^{k_7})^* \lambda^{n_2} \lambda^{n_3} \gamma^{k_3\eta} \gamma^{k_4n_5n_6}_\mu k_{k_1k_7} \),

(A14)

that are both antisymmetric in their particle and hole indexes.

3. Coupling matrices with two interaction-irreducible 3NFs

All the Feynman diagrams in Fig. 5 but the ones in the first row, can contain coupling matrices with two interaction-irreducible 3NFs. Again, for each different topology we list the expressions for forward-in-time contributions first, followed by the backward-in-time ones.

In the Goldstone diagrams of the term in Fig. 5o, we have,

\[ M^{(Ii')}_{r \alpha} \equiv \frac{\sqrt{3}}{12} k_{k_3k_1k_7} \left( \gamma^{k_5} \lambda^{n_1} \lambda^{n_2} \lambda^{n_3} \right) \gamma^{k_3} \gamma^{n_4}_\eta W_{\mu\nu,\lambda,\alpha\rho} \),

(A15)

that is antisymmetric in the indexes \( n_1 \) and \( n_2 \), and

\[ N^{(Ii')}_{s \alpha} \equiv \frac{\sqrt{3}}{12} W_{\alpha_Q,\mu,\nu,\lambda}(\gamma^{k_7})^* \lambda^{n_3} \lambda^{n_4} \lambda^{n_5} \lambda^{n_6} (\lambda^{n_6}_\rho)^* \gamma^{n_4}_\eta W_{\mu\nu,\lambda,\alpha\rho} \),

(A16)

that is antisymmetric in the indexes \( k_1 \) and \( k_2 \).

In the Goldstone diagrams of the term in Fig. 5p, we have,

\[ M^{(Ii')}_{q \alpha} \equiv \frac{\sqrt{3}}{12} A_{145} P_{123} \left( \ell_{k_1k_4}^{n_1n_6} (\gamma_{\mu}^{k_7})^* \lambda^{n_2} \lambda^{n_3} \right) \gamma^{n_4}_\eta (\lambda^{n_6}_\rho)^* W_{\mu\nu,\lambda,\alpha\rho} \),

(A17)

and

\[ N^{(Ii')}_{\alpha u} \equiv \frac{\sqrt{3}}{12} W_{\alpha_Q,\mu,\nu,\lambda}(\gamma^{k_7})^* \lambda^{n_2} \lambda^{n_3} \gamma^{k_3\eta} \gamma^{k_4n_5n_6}_\mu k_{k_1k_7} \),

(A18)

In the Goldstone diagrams of the term in Fig. 5q, we can also single out the following coupling matrices,

\[ M^{(Iq)}_{q \alpha} \equiv -\frac{\sqrt{3}}{12} P_{123} \left( \ell_{k_1k_4}^{n_1n_6} (\gamma_{\mu}^{k_7})^* \lambda^{n_2} \lambda^{n_3} \right) \gamma^{n_4}_\eta (\lambda^{n_6}_\rho)^* W_{\mu\nu,\lambda,\alpha\rho} \),

(A19)

and

\[ N^{(Iq)}_{\alpha u} \equiv \frac{\sqrt{3}}{12} W_{\alpha_Q,\mu,\nu,\lambda}(\gamma^{k_7})^* \lambda^{n_2} \lambda^{n_3} \gamma^{k_3\eta} \gamma^{k_4n_5n_6}_\mu k_{k_1k_7} \),

(A20)

4. Formulas for 2NF interaction matrices with \( 3p2h \) and \( 3h2p \) configurations

The interaction matrices that we have introduced in Sec. 3.1.3 do not exhaust the list of all possible terms required for the ADC(3). A more complicated pattern in terms of ISCs is present in interaction matrices connecting \( 2p1h \) and \( 3p2h \) ISCs, as for the forward-in-time terms in the diagrams of Figs. 5d-5g.

In the Feynman diagram of Fig. 5d one can find,

\[ C_{pq}^{pp} = \frac{\sqrt{6}}{12} \delta_{n_1n_6} \delta_{k_3k_9} \),

(A21)

while its complex conjugate term is contained in the diagram of Fig. 5i.

An interaction matrix connecting the same ISCs as the one in Eq. (A21) is

\[ C_{pq}^{ph} = -\frac{\sqrt{6}}{12} \delta_{n_1n_6} \delta_{k_3k_9} \),

(A22)

which is contained in the diagram of Fig. 5e while the diagram in Fig. 5g contains the complex conjugate of Eq. (A22).

In the self-energy diagrams represented in Figs. 5k and 5m when two \( 3p2h \) propagators are connected via ISCs containing a 2NF, we find interaction matrices of the following form,

\[ C_{pq}^{pp} = \frac{1}{12} A_{145} P_{123} P_{678} \left( \lambda^{n_1} \lambda^{n_2} \gamma^{k_3\eta} \gamma^{k_4n_5n_6}_\mu k_{k_1k_7} \right) \),

(A23)

which is composed by 18 terms when all the permutations indicated are taken, and the ones with a particle-hole 2NF connecting two \( 3p2h \) propagators, i.e.

\[ C_{pq}^{pp} = \frac{1}{12} A_{145} A_{910} A_{123} A_{678} \left( \lambda^{n_1} \lambda^{k_3\eta} \gamma^{k_4n_5n_6}_\mu k_{k_1k_7} \right) \),

(A24)
that contains 72 terms when the explicit antisymmetrization with respect to single-particle indexes is performed. The interaction matrices in Eqs. (A23) and (A24) are found in the diagrams in Figs. 5j and 5k respectively.

A forward-in-time interaction matrix connecting two 3p2h ISCs through a hole-hole 2NF is found in the self-energy diagram in Fig. 5n. This has the following expression,

\[ C_{qq'}^{hh} = \frac{1}{12} A_{123} \left( (\gamma_{\mu}^{\nu})^k \gamma_{\nu}^{k_{10}} V_{\mu,\lambda,\rho} (\gamma_{\lambda}^{\rho})^{k_5} \right) \delta_{n_1 n_6} \delta_{n_2 n_7} \delta_{n_3 n_8}. \]  

(A25)

We present now the corresponding interaction matrices appearing in backward-in-time self-energy Goldstone diagrams. We remind that these interaction matrices are the ones connecting propagators of hole-particle type in self-energy diagrams.

We consider first terms contained in Figs. 5d, 5g, namely those connecting the 2h1p propagator to the 3h2p propagator. We find,

\[ D_{uu}^{hh} \equiv \frac{\sqrt{6}}{12} A_{123} A_{910} P_{678} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} \gamma_{\rho}^{k_7} \right) \delta_{k_1 k_2} \delta_{n_3 n_9}. \]  

(A26)

that must be combined with another interaction matrix,

\[ D_{uu}^{sp} \equiv - \frac{\sqrt{6}}{12} A_{678} \left( (\gamma_{\mu}^{\nu})^k \gamma_{\mu}^{k_{10}} V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} (\gamma_{\lambda}^{\rho})^{k_7} \right) \delta_{k_1 k_2} \delta_{k_3 k_4}. \]  

(A27)

Interaction matrices in Eqs. (A26) and (A26) are found in the self-energy diagrams of Figs. 5d and 5g respectively, while their complex conjugates are contained in the diagrams of Figs. 5d and 5g.

When two 3h2p propagators in a self-energy diagram are connected via ISCs linked to 2NFs, as in diagrams of Figs. 5j, 5m, we have an interaction matrix of the following form,

\[ D_{uu}^{hh} \equiv - \frac{1}{12} A_{45} P_{123} P_{678} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} (\gamma_{\lambda}^{\rho})^{k_7} \right) \delta_{k_3 k_6} \delta_{n_4 n_9} \delta_{n_5 n_{10}}. \]  

(A28)

contained in the diagram of Fig. 5j, and another one found when a particle-hole 2NF connects two 3h2p ISCs, i.e.

\[ D_{uu}^{sp} \equiv - \frac{1}{12} A_{45} A_{910} A_{123} A_{678} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} (\gamma_{\lambda}^{\rho})^{k_7} \right) \delta_{k_3 k_6} \delta_{k_4 k_7} \delta_{n_5 n_{10}}. \]  

(A29)

which appears in the Feynman diagram of Fig. 5m.

Finally, also a backward-in-time interaction matrix connecting two 3h2p ISCs through a particle-particle 2NF is found in the self-energy diagram of Fig. 5n that is

\[ D_{uu}^{sp} \equiv - \frac{1}{12} A_{123} \left( (\gamma_{\mu}^{\nu})^k \gamma_{\nu}^{k_{10}} V_{\mu,\lambda,\rho} (\gamma_{\lambda}^{\rho})^{k_5} \right) \delta_{k_1 k_2} \delta_{k_3 k_4} \delta_{n_5 n_{10}}. \]  

(A30)

5. Formulas for 3NF interaction matrices with 3p2h and 3h2p configurations

One more set of interaction matrices is required to complete the ADC(3), which is given by those terms containing the interaction-irreducible 3NF.

First we consider interaction matrices in which the 3NF connects 2p1h ISCs to 3p2h ISCs, as in the diagrams in Figs. 5l, 5k. We find in the diagram of Fig. 5k,

\[ C_{qq'}^{3NF(1)} \equiv \frac{\sqrt{6}}{12} A_{910} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} \right) \delta_{n_1 n_7}. \]  

(A31)

and a second 3NF interaction matrix connecting the 2p1h propagator to the 3p2h propagator, requiring an explicit antisymmetrization only with respect to two particle indexes. Its expression from a Goldstone diagram of Fig. 5l reads,

\[ C_{qq'}^{3NF(II)} \equiv \frac{\sqrt{6}}{12} A_{910} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} \right) \delta_{n_3 n_9}. \]  

(A32)

Complex conjugate interaction matrices corresponding to Eqs. (A31) and (A32) can be found in the Goldstone diagrams from Figs. 5j and 5k.

Two 3p2h propagators can be connected in a self-energy diagram via ISCs containing a 3NF. They are contained in the three self-energy diagrams represented in Figs. 5p, 5m. We have then an interaction matrix of the following form in Fig. 5p,

\[ C_{qq'}^{3NF(III)} \equiv \frac{1}{12} A_{45} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} (\gamma_{\lambda}^{\rho})^{k_5} \right) \delta_{k_3 k_6} \delta_{k_5 k_{10}}. \]  

(A33)

Other 3NF interaction matrices connecting two 3p2h ISCs are found in Fig. 5m

\[ C_{qq'}^{3NF(IV)} \equiv - \frac{1}{12} A_{45} A_{910} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} \right) \delta_{k_3 k_6} \delta_{n_3 n_{10}}. \]  

(A34)

and in Fig. 5n that is

\[ C_{qq'}^{3NF(V)} \equiv \frac{1}{12} A_{123} A_{678} \left( (\gamma_{\mu}^{\nu})^k (\gamma_{\nu}^{k_{10}})^* V_{\mu,\lambda,\rho} \gamma_{\lambda}^{k_5} \right) \delta_{n_1 n_7} \delta_{n_2 n_{10}}. \]  

(A35)
We can present now 3NF interaction matrices appearing in backward-in-time self-energy Goldstone diagrams. These interaction matrices connect then hole-particle ISCs in the diagrams, i.e. 2h1p and/or 3h2p propagators. As the corresponding interaction matrices for the forward-in-time part shown above, they are found in the diagrams of Figs. 5h-5k and Figs. 5o-5q.

First we have the terms,

\[
D_{su}^{(I)} = \frac{\sqrt{6}}{12} A_{678} \left( (\chi^{k_1}_e)^* \chi^{m_10}_e W_{\lambda\nu,\rho \eta} \gamma^{k_2}_\rho \gamma^{k_3}_\eta \delta_{n_4n_9} \delta_{n_5n_{10}} \right),
\]

(A36)

and

\[
D_{su}^{(II)} = -\frac{\sqrt{6}}{12} A_{910} \left( (\chi^{k_1}_e)^* \chi^{m_10}_e W_{\lambda\nu,\rho \eta} \gamma^{k_2}_\rho \gamma^{k_3}_\eta \delta_{n_4n_9} \delta_{n_5n_{10}} \right),
\]

(A37)

which are found in Figs. 5h and 5i, respectively.

Finally, 3NF interaction matrices can connect two 3h2p ISCs within a self-energy diagram, as does the interaction matrices in Eqs. (A38) and (A39).

Specifically, in Figs. 5o and 5p, we can single out the interaction matrices,

\[
D_{uu}^{(II)} = \frac{1}{12} A_{45} \left( (\chi^{k_1}_e)^* \chi^{m_10}_e W_{\lambda\nu,\rho \eta} \gamma^{k_2}_\rho \gamma^{k_3}_\eta \delta_{n_4n_9} \delta_{n_5n_{10}} \right),
\]

(A38)

and

\[
D_{uu}^{(IV)} = -\frac{1}{12} A_{45} A_{910} P_{123} P_{678} \left( (\chi^{k_1}_e)^* \chi^{m_10}_e W_{\lambda\nu,\rho \eta} \gamma^{k_2}_\rho \gamma^{k_3}_\eta \delta_{n_4n_9} \delta_{n_5n_{10}} \right),
\]

(A39)

respectively. Matrices in Eqs. (A38) and (A39) must be complemented with another backward-in-time interaction matrix that also connects two 3h2p ISCs. This is given by the expression,

\[
D_{uu}^{(IV)} = \frac{1}{12} A_{123} P_{678} \left( (\chi^{k_1}_e)^* \chi^{m_10}_e W_{\lambda\nu,\rho \eta} \gamma^{k_2}_\rho \gamma^{k_3}_\eta \delta_{n_4n_9} \delta_{n_5n_{10}} \right),
\]

(A40)

as it is singled out from the Goldstone diagram corresponding to Fig. 5p.

Appendix B: Irreducible self-energy in angular momentum coupling formalism

Most implementations in nuclear physics are based on the assumption of a spherical ground state, and exploit spherical single-particle basis and angular momentum coupling techniques. By applying these techniques, the diagonalization of Eq. (27) can be performed separately for each partial wave, and the required computational resources are significantly reduced.

In this Appendix we consider the specific case of spherical nuclei and derive the corresponding working equations for the ADC(3) formalism. In general, a spherical single-particle state with isospin function \(\chi_q\) is given by coupling the spherical harmonic \(Y_l(r)\) to \(\frac{1}{2}\), the function of the intrinsic spin of the nucleon,

\[
\phi_\beta(r, \sigma, \tau) = f_{n_\beta}(r)[|Y_{l_\beta}(r) \otimes \chi_{\frac{1}{2}}(\sigma)\rangle^\beta \chi_{q_\beta}(\tau), \]

(B1)

with \(\sigma\) and \(\tau\) being spin and isospin coordinates, respectively.

The collective index \(\beta\) denotes the set of quantum numbers \((n_\beta, \pi_\beta, j_\beta, m_\beta, q_\beta)\) where \(n_\beta\) denotes the principal quantum number, \(\pi_\beta\) is the parity corresponding to the orbital angular momentum \(l_\beta\), \(j_\beta\) and \(m_\beta\) are the total angular momentum and its projection along the z axis respectively, and \(q_\beta\) represents the isospin projection. In this basis, the creation operator \(a_\beta^\dagger\) of the single-particle basis is the \(m_\beta^0\) component of an irreducible tensor of rank \(j_\beta\), according to the definition,

\[
a_\beta^\dagger = a^\dagger_{n_\beta, \pi_\beta, j_\beta, m_\beta, q_\beta} = a^\dagger_{k, m_\beta},
\]

(B2)

where we made use of the notation \(\beta \equiv (b, m_\beta) \equiv (n_\beta, \pi_\beta, j_\beta, m_\beta, q_\beta)\), i.e.

\[
b \equiv (n_\beta, \pi_\beta, j_\beta, q_\beta).
\]

(B3)

The destruction operator is treated in the same fashion, with the form of an irreducible tensor being achieved by choosing the phase \((-1)^{j_\beta - m_\beta} a_\beta^\dagger\). For particle and hole orbits defining the states \(|\Psi_n^{A+1}\rangle\) and \(|\Psi_k^{A-1}\rangle\) of (A+1)- and (A-1)-body systems, we use again the compact notation of Eq. (B2) according to \(n \equiv (\tilde{n}, m_n)\) and \(k \equiv (\tilde{k}, m_k)\), with \(\tilde{n} \equiv (n_\pi, \pi_\beta, j_\beta, m_\beta, q_\beta)\) and \(\tilde{k} \equiv (n_\pi, \pi_\beta, j_\beta, m_\beta, q_\beta)\), respectively. According to these definitions, the set of shorthand notations in Eqs. (19-20) are assumed also for indexes not-dependent on the quantum number \(m\) and coupled to the total angular momentum, i.e., \(\tilde{r} \equiv [(\tilde{n}_1, \tilde{n}_2, \tilde{J}_1, \tilde{k}_3, J_4), \tilde{s} \equiv [(k_1, \tilde{k}_2, \tilde{J}_2, \tilde{n}_3, J_5)\), and so on.

In the following we revisit the formalism of the angular momentum coupling of the self-energy, when the g.s. state \(|\Psi_{A}^0\rangle\) in Eq. (1) has angular momentum and parity \(J^p=0^+\). For these systems, the formalism is considerably simplified because the total angular momentum of the A+1 (A-1) many-body states \(j_n\) (\(j_k\)), its projection along the z axis \(m_\pi\) \((m_\pi)\) of excited states \(|\Psi_{A+1}^0\rangle\) \((|\Psi_{A-1}^0\rangle\) are the same as the corresponding quantum numbers of creation (annihilation) single-particle tensor operators appearing in the definition of the Green’s function in Eq. (1). The total isospin is uniquely determined by isospin projections of the reference state and tensor operators. With this assumption (i.e. \(|\Psi_{A}^0\rangle\) has \(J^p=0^+\)), the irreducible self-energy in the
Dyson equation \((6)\) is diagonal in the quantum numbers \((\pi, j, m, q)\), and it is independent on \(m\), i.e.

\[
\Sigma^*_{a\beta}(\omega) = \delta^{(\pi jq)} \delta_{m_{\pi} m_{\beta}} \Sigma^*_{ab}(\omega), \tag{B4}
\]

Moreover, by applying the Wigner-Eckart theorem, the transition amplitudes in Eqs. \((5)\) acquire the form,

\[
\lambda^\alpha_{\pi, m, q} = (-1)^{2j_a} \frac{\delta^{(\pi jq)} \delta_{m_{\pi} m_{\alpha}}}{\sqrt{2j_a + 1}} \langle \Psi^{A+}_n || a^\dagger || \Psi^A_0 \rangle \equiv \lambda^\alpha_{\pi, m, q} \delta^{(\pi jq)} \delta_{m_{\pi} m_{\alpha}} \tag{B6}
\]

and

\[
\lambda^\beta_{\pi, m, q} = (-1)^{2j_b} (-1)^{j_a - m_{\alpha}} \frac{\delta^{(\pi jq)} \delta_{m_{\pi} m_{\beta}}}{\sqrt{2j_a + 1}} \langle \Psi^{A-}_k || a^\dagger || \Psi^A_0 \rangle \equiv \lambda^\beta_{\pi, m, q} (-1)^{j_a - m_{\alpha}} \delta^{(\pi jq)} \delta_{m_{\pi} m_{\beta}}, \tag{B7}
\]

defining the \(m\)-independent spectroscopic amplitudes \(\lambda^\alpha_{\pi, m, q}\) and \(\lambda^\beta_{\pi, m, q}\).

2NFs and 3NFs are coupled as \(m\)-independent matrix elements according to,

\[
\mathcal{V}_{ab, \gamma\delta}^{J} = \sum_{m_{\alpha}, m_{\beta}} \sum_{m_{\gamma}, m_{\delta}} (j_\alpha j_\beta m_{\alpha} m_{\beta} | J M \rangle (j_\gamma j_\delta m_{\gamma} m_{\delta} | J M \rangle \mathcal{V}_{\alpha\beta, \gamma\delta}^{J} \sqrt{1 + \delta_{ab} \sqrt{1 + \delta_{\gamma\delta}}}, \tag{B8}
\]

\[
\mathcal{W}_{ab, \gamma\delta}^{J_1 J_2} = \sum_{m_{\alpha}, m_{\beta}} \sum_{m_{\gamma}, m_{\delta}} (j_\alpha j_\beta m_{\alpha} m_{\beta} | J_1 M_1 \rangle (j_\gamma j_\delta m_{\gamma} m_{\delta} | J_2 M_2 \rangle (J_1 j_\lambda M_1 | J M \rangle (J_2 j_\nu M_2 | J M \rangle \mathcal{W}_{ab, \gamma\delta}^{J_1 J_2} \mathcal{W}_{\alpha\beta, \gamma\delta}^{J_1 J_2}, \tag{B9}
\]

For the recoupling of 3NF matrix elements within the self-energy Goldstone diagrams of Fig. \(2c\), it turns out to be more convenient the coupling for the particle-particle-hole interaction \(W^{(pph)}\),

\[
W_{ab, \gamma\delta}^{(pph) J_1 J_2} = \sum_{m_{\alpha}, m_{\beta}} \sum_{m_{\gamma}, m_{\delta}} (j_\alpha j_\beta m_{\alpha} m_{\beta} | J_1 M_1 \rangle (j_\gamma j_\delta m_{\gamma} m_{\delta} | J_2 M_2 \rangle (J_1 j_\lambda M_1 | J M \rangle (J_2 j_\nu M_2 | J M \rangle \mathcal{W}_{ab, \gamma\delta}^{(pph) J_1 J_2} \mathcal{W}_{\alpha\beta, \gamma\delta}^{J_1 J_2}, \tag{B10}
\]

which is based on the definition,

\[
W_{ab, \gamma\delta}^{(pph) J_1 J_2} = \mathcal{W}_{\alpha\beta, \gamma\delta}^{J_1 J_2}, \tag{B11}
\]

with the “bar” notation denoting the time-reversed state with quantum numbers \(\bar{\alpha} \equiv (a, -m_{\alpha})\). In order to transform coupled matrix elements of \(W^{(pph)}\) into matrix elements of \(\bar{W}\), we make use of the Pandya relation \((30)\), that is

\[
W_{ab, \gamma\delta}^{(pph) J_1 J_2} = (-1)^J \sum_{J'} (2J' + 1) \left\{ \begin{array}{c} J_1, J_\lambda, J, J_2, J_\nu, J' \\ J_2, J_\nu, J' \\ J_1, J_\lambda, J, J_2, J_\nu, J' \end{array} \right\} W_{ab, \gamma\delta}^{J_1 J_2}, \tag{B12}
\]

1. General J-coupling conventions for ISCs

In order to express \(\Sigma^*_{ab}(\omega)\) of Eq. \((B4)\) in terms of the coupling and interaction matrices within the angular momentum coupling formalism, we have adopted specific choices in the way we couple different ISCs. Since we are going to present Feynman diagrams of Fig. \(2\) we need to specify the couplings for 2p1h and 2h1p ISCs. While the final form of the irreducible self-energy is independent from conventional phases, we specify here working equations based on the following angular couplings.

For 2p1h coupling matrices we defined the coupled \(M_{ra}\) as,

\[
\sum_{m_{n_1}, m_{n_2}} (j_{n_1} j_{n_2} m_{n_1} m_{n_2} | J_1 M_1 \rangle (J_1 j_{k_3} M_{12} m_{k_3} | J_e M_e \rangle \mathcal{M}_{ra} \equiv \delta^{(\pi jq)} \delta_{m_{\pi} m_{\alpha}} \mathcal{M}_{ra}, \tag{B13}
\]
with the parity \( \pi_r = (-1)^{l_1+l_2+l_3} \), the charge \( q_r = q_1 + q_2 - q_3 \) and the total angular momentum \( J_r \) of the 2p1h ISC \( \tilde{s} \equiv [(\tilde{n}_1, \tilde{n}_2, J_{12}, \tilde{n}_3), J_r] \). For backward-in-time 2h1p coupling matrices \( N_{\alpha s} \), we define the coupling,

\[
\sum_{m_{k_1} m_{k_2}} (j_{k_1} j_{k_2} m_{k_1} m_{k_2} | J_12 M_{12} ) (j_{j_1} j_{j_2} m_{j_1} m_{j_2} | J_s M_s ) N_{\alpha s} \equiv \delta^{(\pi q)}_a \delta_{m_a-M_r} N_{\alpha \tilde{s}} , \tag{B14}
\]

with the charge \( q_r = -q_1 - q_2 + q_3 \) and the total angular momentum \( J_s \) of the 2h1p ISC \( \tilde{s} \equiv [(\tilde{k}_1, \tilde{k}_2, J_{12}, \tilde{n}_3), J_s] \).

Concerning interaction matrices, we couple \( C_{j j'} \) and \( D_{kk'} \) matrix elements in the following way. For 2p1h interaction matrices \( C_{rr'} \) we write the coupling,

\[
\sum_{m_{k_1} m_{k_2}} \sum_{m_{n_1} m_{n_2}} (j_{n_1} j_{n_2} m_{n_1} m_{n_2} | J_{12} M_{12} ) (j_{j_1} j_{j_2} m_{j_1} m_{j_2} | J_{r} M_{r} ) (j_{j_{12}} j_{j_{12}} m_{j_{12}} m_{j_{12}} | J_{45} M_{45} ) (j_{j_{45}} j_{j_{45}} m_{j_{45}} m_{j_{45}} | J_{r'} M_{r'} ) C_{rr'} ,
\]

We use also the analogous coupling for 2h1p interaction matrices \( D_{ss'} \), that is

\[
\sum_{m_{k_1} m_{k_2}} \sum_{m_{n_1} m_{n_2}} (j_{n_1} j_{n_2} m_{n_1} m_{n_2} | J_{12} M_{12} ) (j_{j_1} j_{j_2} m_{j_1} m_{j_2} | J_{s} M_{s} ) (j_{j_{12}} j_{j_{12}} m_{j_{12}} m_{j_{12}} | J_{45} M_{45} ) (j_{j_{45}} j_{j_{45}} m_{j_{45}} m_{j_{45}} | J_{s'} M_{s'} ) D_{ss'}
\]

Eqs. (B15) and (B16) define the coupled \( C_{rr'} \) and \( D_{ss'} \) that are independent of \( M_r \) and \( M_s \), respectively. For a more compact notation we define also,

\[
E_{r'} \equiv \text{diag}\{\varepsilon^+_{n_1}, \varepsilon^+_{n_2}, \varepsilon^+_{n_3}\}, \tag{B17}
\]

and similar expressions for different configurations energies.

Once again, we stress the fact that phases appearing in previous Eqs. (B13) and (B16) result from a specific choice in performing the coupling within each interaction and coupling matrix, with other possible choices being equally legitimate. Their combined contribution gives the overall phase of the self-energy term.

With the body of definitions and choices of the coupling specified above, we can now present the angular momentum coupled form of the self-energy \( \Sigma^*_{\alpha \beta}(\omega) \) in Eq. (B1). In this Appendix we display only the working equations for 2p1h and 2h1p ISCs, that describe completely the diagrams depicted in Fig. 2. For each diagram of Fig. 2 we will introduce coupling and interaction matrices entering in the corresponding Goldstone diagram, bearing in mind that the same type of coupling or interaction matrix can enter in diagrams with different topologies and order, as specified below. By starting from Eq. (B18) we get,

\[
\Sigma^*_{\alpha \beta}(\omega) = \sum_{rr'} M^*_{\alpha r} \omega - (E_r C_{rr'} + D_{rr'}) + i\eta M^*_{\alpha r'} - \sum_{ss'} N_{s s'} \omega - (E_s D_{s s'} + D_{s s'}) - i\eta N^*_{s s'}
\]

which proves Eq. (B14) and defines the \( m \)-independent irreducible self-energy \( \Sigma^*_{\alpha \beta}(\omega) \).

2. Angular momentum coupling of ADC(3) matrices for the diagrams in Fig. 2

We are now in the position to give expressions for coupling and interaction matrices entering in the diagrams depicted in Fig. 2 presented according to the angular momentum coupling formalism.
Coupling matrices with 2p1h ISCs

The coupling matrix $M_{ra}^{(1a)}$ of Eq. (33) and $M_{ra}^{(1b)}$ of Eq. (52) are coupled according to Eq. (B13). The coupling matrix in Eq. (33) has the following representation in the angular momentum coupling,

$$M_{ra}^{(1a)} = \Delta(j_{n_1}, j_{n_2}, J_{12}) \Delta(j_{k_3}, J_{12}, J_r)(-1)^{j_{n_1}+j_{k_3}-J_{12}} \tilde{j}_{12} \sum_{j_\alpha \leq j_\beta}^{J_{12}} \sum_{\gamma = m} X_{m}^{n_1} \chi_{m}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \sqrt{1 + \delta_{m} \sqrt{1 + \delta_{j_{k_3}}} - \delta_{j_{k_3}}},$$

with the “hat factor” defined as,

$$\hat{j} = \sqrt{2j + 1},$$

and the triangular condition $\Delta(j, j', J)$ defined as usual,

$$|j - j'| \leq J \leq j + j'.$$

The coupling matrix in Eq. (52) becomes

$$M_{ra}^{(1b)} = \Delta(j_{n_1}, j_{n_2}, J_{12}) \Delta(j_{k_3}, J_{12}, J_r)(-1)^{j_{n_1}+j_{k_3}-J_{12}} \tilde{j}_{12} \sum_{j_\alpha \leq j_\beta}^{J_{12}} \sum_{\gamma = m} X_{m}^{n_1} \chi_{m}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \sqrt{1 + \delta_{m} \sqrt{1 + \delta_{j_{k_3}}} - \delta_{j_{k_3}}},$$

containing the angular momentum coupled version of the term in Eq. (40), i.e.

$$\tilde{j}_{k_4, J_{12}}^{n_1 n_2} = \sum_{m \leq \gamma \leq s} \sum_{r \leq \delta} X_{m}^{n_1} \chi_{m}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \sqrt{1 + \delta_{m} \sqrt{1 + \delta_{j_{k_3}}} - \delta_{j_{k_3}}},$$

that is coupled according to the following convention,

$$\sum_{m \leq \gamma \leq s} \sum_{r \leq \delta} \delta_{m} \delta_{r} \delta_{\gamma} \delta_{\delta} \delta_{j_{k_3}} \chi_{m}^{n_1} \chi_{m}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \sqrt{1 + \delta_{m} \sqrt{1 + \delta_{j_{k_3}}} - \delta_{j_{k_3}}},$$

$$= \Delta(j_{n_1}, j_{n_2}, J) \Delta(j_{k_3}, J) \tilde{j}_{k_4, J_{12}}^{n_1 n_2}.$$

The $M_{ra}^{(1b)}$ of Eq. (53) in the angular momentum coupling representation is given by

$$M_{ra}^{(1b)} = \Delta(j_{n_1}, j_{n_2}, J_{12}) \Delta(j_{k_3}, J_{12}, J_r)(-1)^{j_{n_1}+j_{k_3}-J_{12}} \tilde{j}_{12} \sum_{j_\alpha \leq j_\beta}^{J_{12}} \sum_{\gamma = m} X_{m}^{n_1} \chi_{m}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \sqrt{1 + \delta_{m} \sqrt{1 + \delta_{j_{k_3}}} - \delta_{j_{k_3}}},$$

which is explicitly antisymmetrized with respect to the $n_1, n_2$ indices. Also the coupling matrix could be expressed through the term of Eq. (40), but more conveniently coupled according to this choice,

$$\sum_{m \leq \gamma \leq s} \sum_{r \leq \delta} \delta_{m} \delta_{r} \delta_{\gamma} \delta_{\delta} \delta_{j_{k_3}} \chi_{m}^{n_1} \chi_{m}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \tilde{\chi}_{m}^{n_1} \chi_{\gamma}^{n_2} \sqrt{1 + \delta_{m} \sqrt{1 + \delta_{j_{k_3}}} - \delta_{j_{k_3}}},$$

$$= \Delta(j_{n_1}, j_{n_2}, J) \Delta(j_{k_3}, J) \tilde{j}_{k_4, J_{12}}^{n_1 n_2}.$$
The coupling matrix \( M_{\alpha}^{(1c)} \) of Eq. (56), which is found in the diagram of Fig. 2c and contains an interaction-reducible 3NF, has the following form in the angular momentum coupling representation,

\[
M_{\alpha}^{(1c)} = \sum_{J_{\alpha} \Delta J_{\alpha}} \sum_{I_{\alpha} \Delta I_{\alpha}} \sum_{k_{5} \leq k_{5}} \sum_{n_{4}} \sum_{v \leq m} \Delta(J_{n_{1}}, J_{n_{2}}, J_{12}) \Delta(J_{k_{5}}, J_{k_{6}}, J_{56}) \Delta(J_{n_{4}}, J_{56}, J_{\alpha}) \Delta(J_{12}, J_{k_{3}}, J_{n_{4}})(-1)^{J_{n_{4}}+J_{56}-J_{n_{4}}} \frac{j_{56}}{j_{\alpha}} \\
(2J' + 1) \left\{ \begin{array}{c} J_{15} \, J_{n_{4}} \, J_{0} \\ J_{12} \, J_{k_{3}} \, J' \end{array} \right\} \left( \frac{Y^{k_{5}} m_{k_{5}} - (-1)^{J_{k_{5}}+J_{k_{6}}-J_{56}} Y^{k_{6}} y_{m}}{\sqrt{1 + \delta_{l} m_{v} \sqrt{1 + \delta_{k_{5}} k_{6}}} \, (\lambda_{l}^{*})^{*}} \right) \right.
\]

and it contains the angular momentum coupled version of the term in Eq. (47) with the interaction-reducible 3NF, i.e.

\[
j_{\tilde{a}} n_{4}, J_{12} J' = \sum_{g \leq d} \sum_{l \leq p} \left( \begin{array}{c} \lambda_{g}^{n_{1}} \lambda_{l}^{n_{2}} \, (-1)^{J_{n_{1}}+J_{n_{2}}-J_{12}} \lambda_{l}^{n_{1}} \, \lambda_{r}^{n_{4}} \, \lambda_{l}^{*} \, \lambda_{r}^{*} \, \lambda_{l}^{*} \, \lambda_{r}^{*} \\ \frac{V_{J_{12}J_{56}J'}^{l_{n_{4}} \Delta J_{l}}}{(1 + \delta_{l} g m_{d} \sqrt{1 + \delta_{l} h_{l} n_{2}})} \right) \right.
\]

\[\left. \left( \begin{array}{c} Y_{l}^{k_{5}} y_{m}^{k_{6}} \, (-1)^{J_{k_{5}}+J_{k_{6}}-J_{56}} Y_{l}^{k_{6}} y_{m}^{k_{5}} \, \delta_{l}^{(\pi_{n} q _{j})} \, \delta_{l}^{(\pi_{n} q _{j})} \, \delta_{l}^{(\pi_{n} q _{j})} \, \delta_{l}^{(\pi_{n} q _{j})} \, \delta_{l}^{(\pi_{n} q _{j})} \, \delta_{l}^{(\pi_{n} q _{j})} \\ \frac{V_{J_{12}J_{56}J'}^{l_{n_{4}} \Delta J_{l}}}{(1 + \delta_{l} g m_{d} \sqrt{1 + \delta_{l} h_{l} n_{2}})} \right) \right. \]

(b. Coupling matrices with 2h1p ISC)

For backward-in-time contributions to the self-energy, we have the angular momentum representation of the coupling matrix in Eq. (34), i.e.

\[
N_{\alpha \bar{a}}^{(1a)} = \Delta(J_{k_{1}}, J_{k_{2}}, J_{12}) \Delta(J_{n_{3}}, J_{12}, J_{s}) \frac{j_{12}}{j_{\alpha}} (-1)^{J_{n_{3}}+J_{12}} \frac{1}{\sqrt{1 + \delta_{l} m_{v} \sqrt{1 + \delta_{k_{1}} k_{2}}} (\lambda_{l}^{*})^{*}} \right.
\]

which is coupled with the coupling matrix of Eq. (54).

\[
N_{\alpha \bar{a}}^{(1a)} = \Delta(J_{k_{1}}, J_{k_{2}}, J_{12}) \Delta(J_{n_{3}}, J_{12}, J_{s}) \frac{j_{12}}{j_{\alpha}} (-1)^{J_{n_{3}}+J_{12}} \frac{1}{\sqrt{1 + \delta_{l} m_{v} \sqrt{1 + \delta_{k_{1}} k_{2}}} (\lambda_{l}^{*})^{*}} \right.
\]

The backward-in-time coupling matrix of Eq. (55) is

\[
N_{\alpha \bar{a}}^{(1b)} = \Delta(j_{k_{1}}, j_{k_{2}}, J_{12}) \Delta(j_{n_{3}}, J_{12}, J_{s}) \frac{j_{12}}{j_{\alpha}} (-1)^{J_{n_{3}}+J_{12}} \frac{1}{\sqrt{1 + \delta_{l} m_{v} \sqrt{1 + \delta_{k_{1}} k_{2}}} (\lambda_{l}^{*})^{*}} \right.
\]

which is explicitly antisymmetrized with respect to the \( \tilde{k}_{1}, \tilde{k}_{2} \) indices.
Finally, the coupling matrix $N^{(1c)}_{ac}$ of Eq. (57), which is found in the backward-in-time diagram of Fig. 2c and contains a 3NF, has the following form in the angular momentum coupling representation,

$$
N^{(1c)}_{ac} \equiv \sum_{J_{45}, J_{k6}} \sum_{n_{4}, n_{5}, v_{4}, m_{4}} \Delta(j_{k1}, j_{k2}, J_{12}) \Delta(j_{n4}, j_{n5}, J_{45}) \Delta(j_{12}, j_{n3}, J_{a}) \Delta(j_{45}, j_{k6}, J_{a}) (-1)^{j_{a} - m_{a}} (-1)^{j_{a} + j_{k6} + J_{45}} \frac{j_{12}}{j_{a}} 
\nonumber
$$

$$
(2J' + 1) \left\{ J_{12} j_{n3} j_{a} \right\} \left\{ J_{45} j_{k6} J' \right\} \left( \begin{array}{c} \tilde{n}_{4} \tilde{n}_{5} \tilde{n}_{3}, J_{45} J' \end{array} \right) \ast \left( \begin{array}{c} \tilde{n}_{4} \tilde{n}_{5} \tilde{n}_{v}, J_{45} J' \end{array} \right) 
\frac{\left( \chi^{n_{4}}_{m} \chi^{n_{5}}_{v} - (-1)^{j_{n4} + j_{n5} - J_{45}} \chi^{n_{4}}_{m} \chi^{n_{5}}_{v} \right)}{\sqrt{1 + \delta_{m v} \sqrt{1 + \delta_{n4} n_{5}}}} V_{J_{45} J_{k6}}^{J_{12} J_{12}}. 
\right) 
$$

(B32)

c. Interaction matrices with 2p1h and 2h1p ISCs

The interaction matrix $C_{\tilde{p} \tilde{p}'}$ can connect 2p1h propagators through particle-particle, particle-hole and 3NFs, according to,

$$
C_{\tilde{p} \tilde{p}'} \equiv C_{\tilde{p} \tilde{p}'}^{pp} + C_{\tilde{p} \tilde{p}'}^{ph} + C_{\tilde{p} \tilde{p}'}^{3N}, 
$$

(B33)

that have been introduced in Eqs. (58), (59) and (62), respectively.

The particle-particle interaction matrix coupled as in Eq. (B15) and resulting from the diagram in Fig. 2a reads,

$$
C_{\tilde{p} \tilde{p}'}^{pp} \equiv \Delta(j_{n1}, j_{n2}, J_{12}) \Delta(j_{k3}, J_{12}, J_{r}) \Delta(j_{n4}, j_{n5}, J_{12}) \Delta(j_{k6}, J_{12}, J_{r}') \sum_{g \leq d} \sum_{t \leq p} (\chi^{n_{4}}_{g} \chi^{n_{5}}_{p} - (-1)^{j_{n4} + j_{n5} - J_{12}} \chi^{n_{4}}_{g} \chi^{n_{5}}_{p}) \ast \left( \begin{array}{c} \tilde{p} \tilde{p} \end{array} \right) \delta_{n1} n_{1} \delta_{n2} n_{2} \delta_{v} \pi jq \delta_{p3} p3 \delta_{k3} k3 \delta_{k6} k6. 
$$

(B34)

while $C_{\tilde{p} \tilde{p}'}^{ph}$ results from the ring diagram in Fig. 2b, which contains four different matrices owing to the antisymmetrization specified in Eq. (59),

$$
C_{\tilde{p} \tilde{p}'}^{ph} \equiv -\frac{1}{2} \Delta(j_{n1}, j_{n2}, J_{12}) \Delta(j_{k3}, J_{12}, J_{r}) \Delta(j_{n4}, j_{n5}, J_{12}) \Delta(j_{k6}, J_{12}, J_{r}') \sum_{g \leq d} \sum_{t \leq p} (-1)^{2J} (2J + 1) \times \left( \begin{array}{c} J_{k3} j_{n3} J_{r} \ J_{k5} j_{n5} J_{r} \ J_{k6} j_{n6} J_{r} \ J_{k1} j_{n1} J_{r} \end{array} \right) \left( \chi^{n_{4}}_{g} \chi^{n_{5}}_{p} \chi^{n_{6}}_{q} \chi^{n_{3}}_{r} \ast \delta_{n1} n_{1} \delta_{n2} n_{2} \delta_{v} \pi jq \delta_{p3} p3 \delta_{k3} k3 \delta_{k6} k6. 
$$

(B35)
The 3NF interaction matrix in Eq. (B33) reads,

\[
C^{3N}_{rr} = \delta_{J_r J_r} \Delta(j_{n_1}, j_{n_2}, J_{r}) \Delta(j_{k_1}, j_{k_2}, J_{r}) \Delta(j_{n_4}, j_{n_5}, J_{45}) \Delta(j_{k_4}, j_{k_5}, J_{45}) \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]

\[
\frac{\lambda_{g}^{n_1} \lambda_{d}^{n_2}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{gd})}} \frac{\lambda_{g}^{n_3} \lambda_{d}^{n_4}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{tp})}} \frac{\lambda_{g}^{n_5} \lambda_{d}^{n_6}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{tp})}} W_{gda,typ} J_r \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]

The backward-in-time interaction matrix \( \tilde{D}_{ss'} \) can connect the 2h1p propagators through hole-hole, hole-particle and backward-in-time 3NFs, according to,

\[
D_{ss'}^{hh} = D_{ss'}^{pp} + D_{ss'}^{3N},
\]

with the three matrices on the r.h.s. introduced in Eqs. (60), (61) and (63), respectively.

The hole-hole interaction matrix resulting from the diagram in Fig. 2a reads,

\[
D_{ss'}^{hh} = \sum_{g \leq d \leq t} \Delta(j_{k_1}, j_{k_2}, J_{r}) \Delta(j_{n_3}, J_{12} J_{ss'}) \Delta(j_{k_4}, j_{k_5}, J_{12} J_{12} J_{12}) \Delta(j_{n_4}, j_{n_5}, J_{45} J_{45} J_{45} J_{45}) \Delta(j_{k_4}, j_{k_5}, J_{45} J_{45} J_{45} J_{45}) \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]

\[
\frac{\lambda_{g}^{n_1} \lambda_{d}^{n_2}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{gd})}} \frac{\lambda_{g}^{n_3} \lambda_{d}^{n_4}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{tp})}} \frac{\lambda_{g}^{n_5} \lambda_{d}^{n_6}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{tp})}} W_{gda,typ} J_r \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]

while \( D_{ss'}^{hp} \) results from the ring diagram in Fig. 2b which contains four different terms owing to the antisymmetrization specified in Eq. (61),

\[
D_{ss'}^{hp} = \frac{1}{2} \Delta(j_{k_1}, j_{k_2}, J_{r}) \Delta(j_{n_3}, J_{12} J_{s}) \Delta(j_{k_4}, j_{k_5}, J_{45}) \Delta(j_{n_4}, J_{45} J_{45} J_{45} J_{s}) \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]

Finally, the backward-in-time 3NF interaction matrix in Eq. (B34) is given by

\[
D_{ss'}^{3N} = -\delta_{J_r J_r} \Delta(j_{k_1}, j_{k_2}, J_{r}) \Delta(j_{k_4}, j_{k_5}, J_{45}) \Delta(j_{n_3}, J_{12}, J_{s}) \Delta(j_{n_4}, J_{45}, J_{s'}) \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]

\[
\frac{\lambda_{g}^{n_1} \lambda_{d}^{n_2}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{gd})}} \frac{\lambda_{g}^{n_3} \lambda_{d}^{n_4}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{tp})}} \frac{\lambda_{g}^{n_5} \lambda_{d}^{n_6}}{\sqrt{1 + \delta_{k_1 k_6} (1 + \delta_{tp})}} W_{gda,typ} J_r \sum_{g \leq d \leq t} \sum_{i \leq p} (2J' + 1) \left\{ \begin{array}{c}
J_{12} j_{k_3} J_r \\
J_{45} j_{k_6} J_r
\end{array} \right\}
\]
Appendix C: Self-energy without renormalization of the propagators

In this Appendix we discuss how the diagrammatic content of the self-energy is modified when one works with uncorrelated (bare) propagators. This is the case when the self-energy is built as a non-skeleton expansion. Correlations which are re-summed within the skeleton expansion correspond to those self-energy diagrams, which can be inserted into a fermion line by cutting it twice at any two different points. Such an insertion must have the form of a 1B operator, therefore the new set of non-skeleton diagrams to be included can be obtained from an expansion of the 1B effective interaction \( \tilde{U} \). The consequences of this expansion for the static self-energy are shown in Appendix C2, where as many as 16 new self-energy non-skeleton diagrams are introduced up to third order. However, their number can be reduced by choosing the spectrum of the 1B Hamiltonian \( \tilde{H}_0 \) as the model space of the calculation, as it is the case in the Hartree-Fock approximation. For the dynamic self-energy, four third-order diagrams are derived in Section C2: they are obtained by inserting the first-order term of the 1B effective interaction \( \tilde{U} \) according to the framework of the ADC truncated case of diagrams in the skeleton expansion, they can be recast according to the form of a 1B operator, therefore the new set of non-skeleton diagrams to be included can be obtained from an expansion of the 1B effective interaction \( \tilde{U} \). The consequences of this expansion for the static self-energy are shown in Appendix C1, where as many as 16 new self-energy non-skeleton diagrams are introduced up to third order. However, their number can be reduced by choosing the spectrum of the 1B Hamiltonian \( \tilde{H}_0 \) as the model space of the calculation, as it is the case in the Hartree-Fock approximation. For the dynamic self-energy, four third-order diagrams are derived in Section C2: they are obtained by inserting the first-order term of the 1B operator expansion in the uncorrelated fermionic lines of dynamic self-energy diagrams at second order. As for the case of diagrams in the skeleton expansion, they can be recast according to the framework of the ADC truncated at third order.

Since we are now working with bare propagators, we need to redefine the transition amplitudes for uncorrelated states of the \( A(A \pm 1) \)-body system, denoted by \( |\phi^{A(A \pm 1)}\rangle \). These definitions are,

\[
Z_n^{i,n,k} = \begin{cases} 
(X^{(n)})^* = \langle \phi_0^A | a^\alpha_n | \phi_0^{A+1} \rangle \\
Y_n^{k} = \langle \phi_0^{A+1} | a_{\alpha}^\dagger | \phi_0^A \rangle.
\end{cases}
\]  

(C1)

1. Static Self-energy

It is apparent from Eq. (12) that the 1B effective interaction is defined through correlated propagators, i.e. for the skeleton expansion: for this reason, it is required in practical calculations an iterative procedure in order to “dress” the propagator and evaluate self-consistently the first-order static irreducible self-energy. As an alternative to the renormalization of propagators, one can consider explicitly the expansion of \( \Sigma_{\alpha \beta} \) expressed through uncorrelated propagators. In turn, this is achieved by formally expanding the effective interaction \( \tilde{U} \) according to,

\[
\tilde{U} = \sum_{\alpha \beta} \left( \tilde{U}^{(1)}_{\alpha \beta} + \tilde{U}^{(2)}_{\alpha \beta} + \tilde{U}^{(3)}_{\alpha \beta} + \ldots \right) a^\dagger_{\alpha} a_{\beta} .
\]  

(C2)

In a similar fashion, one can consider the expansion (up to second order) of \( \tilde{V} \), that is

\[
\tilde{V} = \sum_{\alpha \beta \gamma \delta} \left( \tilde{V}^{(1)}_{\alpha \gamma, \beta \delta} + \tilde{V}^{(2)}_{\alpha \gamma, \beta \delta} + \ldots \right) a^\dagger_{\alpha} a^\dagger_{\gamma} a_{\delta} a_{\beta} .
\]  

(C3)

The first-order term in Eq. (C2) is given by the expression in Eq. (12) once correlated propagators are substituted with bare ones. It is composed by three terms represented in Fig. 8 and can be written in terms of one-body and two-body reduced density matrices, \( \rho^{(0)} \) and \( \Gamma^{(0)} \), which are uncorrelated versions of the densities in Eqs. (15) and (16) respectively. With these definitions, we have

\[
\tilde{U}^{(1)}_{\alpha \beta} = -U_{\alpha \beta} + \sum_{\gamma \delta} V_{\alpha \gamma, \beta \delta} \rho^{(0)}_{\gamma \delta} + \frac{1}{4} \sum_{\delta \eta} W_{\alpha \gamma \epsilon, \beta \delta \eta} \Gamma^{(0)}_{\delta \epsilon \gamma \eta} .
\]  

(C4)

\[
\tilde{V}^{(1)}_{\alpha \gamma, \beta \delta} = -V_{\alpha \gamma, \beta \delta} + \sum_{\epsilon \eta} W_{\alpha \gamma \epsilon, \beta \delta \eta} \rho^{(0)}_{\epsilon \eta} + \frac{1}{4} \sum_{\delta \gamma} W_{\alpha \gamma \epsilon, \beta \delta \eta} \Gamma^{(0)}_{\delta \gamma \epsilon \eta} .
\]  

(C5)

FIG. 8. Diagrammatic representation of the first-order term \( \tilde{U}^{(1)} \) (zigzag line) in the expansion (C2) of the effective 1B interaction of Eq. (12). Fermionic lines denote here uncorrelated propagators. Dotted lines denote the 1B potential \( U_{\alpha \beta} \), while short (long) dashed lines denote 2N (3N) interactions.

FIG. 9. Diagrammatic representation of the first-order term \( \tilde{V}^{(1)} \) in the expansion (C3) of the effective 2N interaction of Eq. (14).

The first-order term in Eq. (C2) is given by the expression in Eq. (12) once correlated propagators are substituted with bare ones. It is composed by three terms represented in Fig. 8 and can be written in terms of one-body and two-body reduced density matrices, \( \rho^{(0)} \) and \( \Gamma^{(0)} \), which are uncorrelated versions of the densities in Eqs. (15) and (16) respectively. With these definitions, we have

\[
\tilde{U}^{(1)}_{\alpha \beta} = -U_{\alpha \beta} + \sum_{\gamma \delta} V_{\alpha \gamma, \beta \delta} \rho^{(0)}_{\gamma \delta} + \frac{1}{4} \sum_{\delta \eta} W_{\alpha \gamma \epsilon, \beta \delta \eta} \Gamma^{(0)}_{\delta \epsilon \gamma \eta} .
\]  

(C4)

Again, the explicit expression for the matrix element \( \tilde{V}^{(1)}_{\alpha \gamma, \beta \delta} \), depicted in Fig. 9, can be directly read from Eq. (14), once the correlated fermionic loop is substituted with a loop obtained from an uncorrelated propagator, i.e. \( g^{(0)}_{\eta \epsilon} (t - t^+). \)
The amplitudes of Eq. (C1) becomes diagonal in the two indexes $i$ and $\alpha$. Each term containing a matrix element $U_{\alpha\beta}$ vanishes because in this case the auxiliary 1B potential is non zero only in the hole-hole space; moreover, the effective interactions obtained by contracting at least one pair of fermion legs in 2NFs or 3NFs vanish, because they contain 1B densities in the particle-hole space.

We have then,

$$
\tilde{U}^{(2)}_{\alpha\beta} = -i\hbar \int \frac{d\omega}{2\pi} \sum_{\eta\gamma} \left[ V_{\alpha\gamma,\beta\delta} + \sum_{\epsilon \eta} W_{\alpha\gamma\epsilon,\beta\delta\eta} \rho^{(0)}_{\eta\epsilon} \right] g^{(0)}_{\delta\epsilon}(\omega) g^{(0)}_{\gamma\eta}(\omega) \tilde{U}^{(1)}_{\epsilon\eta}
$$

$$
+ \frac{(i\hbar)^3}{4} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \int \frac{d\omega_3}{2\pi} \sum_{\epsilon \eta \rho \lambda \mu \nu} W_{\alpha\gamma\epsilon,\beta\delta\eta} g^{(0)}_{\delta\epsilon}(\omega_1) g^{(0)}_{\delta\rho}(\omega_2) g^{(0)}_{\lambda\mu}(\omega_3) g^{(0)}_{\eta\nu}(\omega_1 + \omega_3 - \omega_2) \left[ V_{\rho\mu,\nu\lambda} + \sum_{\epsilon \eta} W_{\rho\mu\nu\lambda\eta} \rho^{(0)}_{\eta\epsilon} \right],
$$

(C5)

with the corresponding representation in terms of Feynman diagrams displayed in Fig. 10.

The terms in Eq. (C5) can be further reduced by using the effective 2NF at the first order,

$$
\tilde{U}^{(2)}_{\alpha\beta} = -i\hbar \int \frac{d\omega}{2\pi} \sum_{\eta\gamma} \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} g^{(0)}_{\delta\epsilon}(\omega) g^{(0)}_{\gamma\eta}(\omega) \tilde{U}^{(1)}_{\epsilon\eta}
$$

$$
+ \frac{(i\hbar)^3}{4} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \int \frac{d\omega_3}{2\pi} \sum_{\epsilon \eta \rho \lambda \mu \nu} W_{\alpha\gamma\epsilon,\beta\delta\eta} g^{(0)}_{\delta\epsilon}(\omega_1) g^{(0)}_{\delta\rho}(\omega_2) g^{(0)}_{\lambda\mu}(\omega_3) g^{(0)}_{\eta\nu}(\omega_1 + \omega_3 - \omega_2) \tilde{V}^{(1)}_{\rho\mu,\nu\lambda},
$$

(C6)

as depicted in Fig. 11.

When the integrations over the frequencies are performed, the second order term $\tilde{U}^{(2)}$ becomes

$$
\tilde{U}^{(2)}_{\alpha\beta} = \sum_{\gamma \delta} \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} \tilde{U}^{(1)}_{\gamma\delta} \left( \sum_{n_1 n_2 k_1 k_2} \frac{Y^{n_1}_{\delta\gamma} Y^{n_2}_{\gamma\eta} Y^{k_1}_{\gamma\eta} Y^{k_2}_{\eta\gamma}}{-\varepsilon_{n_1}^{k_1} - \varepsilon_{k_2}^{n_2} + i\eta} - \sum_{k_1 n_2} \frac{Y^{k_1}_{\delta\gamma} (Y^{k_1}_{\gamma\eta})^* Y^{n_2}_{\gamma\eta} (Y^{n_2}_{\eta\gamma})^*}{-\varepsilon_{k_1}^{n_2} - \varepsilon_{n_2}^{k_1} - i\eta} \right)
$$

$$
+ \frac{1}{4} \sum_{\epsilon \eta \rho \lambda \mu \nu} W_{\alpha\gamma\epsilon,\beta\delta\eta} \left( \sum_{n_1 n_2 k_1 k_2} \frac{X^{n_1}_{\epsilon\gamma} X^{n_2}_{\gamma\eta} X^{k_1}_{\gamma\eta} X^{k_2}_{\eta\gamma}}{-\varepsilon_{n_1}^{k_1} + \varepsilon_{n_2}^{k_2} - \varepsilon_{k_1}^{n_1} - \varepsilon_{k_2}^{n_2} + i\eta} - \sum_{k_1 k_2 n_1 n_2} \frac{Y^{k_1}_{\mu\nu} Y^{k_2}_{\lambda\rho} X^{n_1}_{\gamma\eta} X^{n_2}_{\gamma\eta} X^{k_1}_{\gamma\eta} X^{k_2}_{\eta\gamma}}{-\varepsilon_{k_1}^{n_1} + \varepsilon_{k_2}^{n_2} - \varepsilon_{k_1}^{n_1} - \varepsilon_{k_2}^{n_2} - i\eta} \right) \tilde{V}^{(1)}_{\rho\mu,\nu\lambda}.
$$

(C7)

A possible choice is to take the single-particle spectrum of the unperturbed Hamiltonian $\tilde{H}_0$ as the model space in the calculation, for instance when the 1B potential in $\tilde{H}_0$ is an Hartree-Fock potential. With this choice the transition amplitudes of Eq. (C1) becomes diagonal in the two indexes $i$ and $\alpha$. Each term containing a matrix element $U_{\alpha\beta}$ vanish because in this case the auxiliary 1B potential is non zero only in the hole-hole space; moreover, the effective interactions obtained by contracting at least one pair of fermion legs in 2NFs or 3NFs vanish, because they contain 1B densities in the particle-hole space.
As a specific example of this choice of the model space, we see that only the third diagram of the second-order potential \( \tilde{V}^{(2)} \) in Fig. 10 does not vanish. Its expression is

\[
\tilde{V}^{(2)}_{\alpha\beta,\gamma\delta} = \frac{1}{4} \sum_{\epsilon\rho\sigma, \gamma\lambda\mu} W_{\alpha\epsilon, \beta\rho, \gamma\delta} \delta_{\nu\gamma} \delta_{\rho\delta} \delta_{\lambda\epsilon} \delta_{\mu\eta} \\
\left( \sum_{n_1n_2} \frac{\delta_{n_1\nu} \delta_{n_2\lambda} \delta_{k_3\delta} \delta_{k_4\mu}}{(\epsilon_{n_1} + \epsilon_{n_2} - \epsilon_{k_3} - \epsilon_{k_4} + i\eta)} + i\eta \sum_{k_1k_2} \frac{\delta_{k_1\nu} \delta_{k_2\lambda} \delta_{n_3\delta} \delta_{n_4\mu}}{(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{n_3} - \epsilon_{n_4})} \right) \tilde{U}_{\nu\mu,\sigma\lambda},
\]

where the first-order effective 2NF reduces to the original (not contracted) 2NF.

For the second-order term \( \tilde{V}^{(2)}_{\alpha\beta,\gamma\delta} \) in the expansion of Eq. (C3), the three diagrams on the r.h.s. of Fig. 12 have the following expressions,

\[
\tilde{V}^{(2)}_{\alpha\beta,\gamma\delta} = i\hbar \int \frac{d\omega}{2\pi} \sum_{\epsilon\rho\sigma, \gamma\lambda\mu} W_{\alpha\epsilon, \beta\rho, \gamma\delta} g_{\mu\epsilon}^{(0)}(\omega) g_{\eta\rho}^{(0)}(\omega) U_{\nu\mu} - i\hbar \int \frac{d\omega}{2\pi} \sum_{\epsilon\rho\sigma, \gamma\lambda\mu} W_{\alpha\epsilon, \beta\rho, \gamma\delta} g_{\mu\epsilon}^{(0)}(\omega) g_{\eta\rho}^{(0)}(\omega) \rho_{\lambda\rho}^{(0)} V_{\nu\mu, \sigma\lambda} \\
- \frac{i\hbar}{2} \int \frac{d\omega}{2\pi} \sum_{\epsilon\rho\sigma, \gamma\lambda\mu} W_{\alpha\epsilon, \beta\rho, \gamma\delta} g_{\mu\epsilon}^{(0)}(\omega) g_{\eta\rho}^{(0)}(\omega) W_{\nu\lambda\sigma, \mu\rho\tau} \rho_{\rho\lambda}^{(0)} \rho_{\tau\sigma}^{(0)} \\
= -i\hbar \int \frac{d\omega}{2\pi} \sum_{\epsilon\rho\sigma, \gamma\lambda\mu} W_{\alpha\epsilon, \beta\rho, \gamma\delta} g_{\mu\epsilon}^{(0)}(\omega) g_{\eta\rho}^{(0)}(\omega) \tilde{U}_{\nu\mu}^{(1)},
\]

where in the last equality we have written a more compact expression for \( \tilde{V}^{(2)} \) by using the first term in the expansion of \( \tilde{U} \). The integration over the frequency in Eq. (C9) gives the expression of \( \tilde{V}^{(2)} \) in terms of the uncorrelated transition amplitudes, expressed here with Einstein’s summing convention,

\[
\tilde{V}^{(2)}_{\alpha\beta,\gamma\delta} = W_{\alpha\beta,\gamma\delta} \left( \sum_{n_1k_2} \frac{X^{n_1}_{\mu} X_{\epsilon}^{n_1} Y^{k_2}_{\epsilon} (Y^{k_2}_{\epsilon})^{*}}{(\epsilon_{n_1} - \epsilon_{k_2}) + i\eta} - \sum_{k_1n_2} \frac{Y^{k_1}_{\epsilon} (Y^{k_1}_{\epsilon})^{*} X_{\epsilon}^{n_2} X_{\epsilon}^{n_2}}{(\epsilon_{k_1} + \epsilon_{n_2}) - i\eta} \right) \tilde{U}_{\nu\mu}^{(1)},
\]

which vanishes in the case in which the spectrum of the unperturbed 1B Hamiltonian provides the single-particle model space.

The expansion of \( \tilde{U} \) in Eq. (C2) contains also the term \( \tilde{U}^{(3)}_{\alpha\beta} \) composed by the 11 contributions shown in Fig. 13. By using the same Feynman rules applied for the terms at second and third order (see Appendix A of Ref. [20]), one can derive the expressions for those eleven diagrams. Here we give the working equations suitable to be implemented numerically, after integrals over the frequencies have been performed. Using the compact notation of Eqs. (45-47)
and Einstein’s summing convention, they are listed below according to the order of appearance in Fig. 13

$$\tilde{U}^{(3)}_{\alpha\beta} \overset{(13a)}{=} \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} (X^{n_1\gamma} X^{n_2\eta} X^{n_3\delta})^* - \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} (Y^{k_2} X^{n_3\delta})^*$$

\[\begin{align*}
+ \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} \tilde{U}^{(1)}_{\epsilon\eta} \tilde{U}^{(1)}_{\mu\nu} \left( \frac{X^{n_1\eta} X^{n_2\eta} X^{n_3\delta}}{(-\varepsilon_{k_1} - \varepsilon_{k_2} + \varepsilon_{k_3} + \varepsilon_{k_4})} - \frac{Y^{k_1} X^{n_3\delta}}{(-\varepsilon_{k_1} - \varepsilon_{k_2} + \varepsilon_{k_3} + \varepsilon_{k_4})} \right) \\
+ \frac{(X^{n_1\eta} X^{n_2\eta} X^{n_3\delta})^* X^{n_1\eta} X^{n_2\eta} X^{n_3\delta}}{(-\varepsilon_{k_1} + \varepsilon_{k_2} + \varepsilon_{k_3} + \varepsilon_{k_4})} - \frac{(Y^{k_1} X^{n_3\delta})^* Y^{k_1} X^{n_3\delta}}{(-\varepsilon_{k_1} + \varepsilon_{k_2} + \varepsilon_{k_3} + \varepsilon_{k_4})}\end{align*}\]

\[\begin{align*}
\tilde{U}^{(3)}_{\alpha\beta} \overset{(13b)}{=} \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} \left( (X^{n_1\gamma} X^{n_2\eta} X^{n_3\delta})^* t_{n_1}^{k_1} \right) ;
\end{align*}\]

\[\begin{align*}
\tilde{U}^{(3)}_{\alpha\beta} \overset{(13c)}{=} -\frac{1}{2} \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} \left( (X^{n_2\eta} X^{n_3\delta})^* t_{n_2}^{k_2} \right) + \frac{1}{2} \tilde{V}^{(1)}_{\alpha\gamma,\beta\delta} \left( (X^{n_2\eta} X^{n_3\delta})^* t_{n_2}^{k_2} \right) \right);
\end{align*}\]
\[ \vec{U}_{\alpha\beta}^{(3)} \]
\[ U_{\alpha \beta}^{(1)} = \frac{1}{2} W_{\alpha \gamma, \beta \delta} \left( (X_{\delta}^\dagger Y_{\gamma}^k) X_{\epsilon} Y_{\eta} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n + (Y_{\epsilon} Y_{\eta}) Y_{\eta} X_{\gamma} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n) + \right. \\
\left. + \frac{1}{2} W_{\alpha \gamma, \beta \delta} \bar{V}_{\mu \lambda, \nu \rho} \left( (X_{\delta}^\dagger Y_{\gamma}^k) X_{\epsilon} Y_{\eta} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n) + (Y_{\epsilon} Y_{\eta}) Y_{\eta} X_{\gamma} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n) \right) \right) ; \]

\[ U_{\alpha \beta}^{(2)} = \frac{1}{4} W_{\alpha \gamma, \beta \delta} \left( (X_{\delta}^\dagger Y_{\gamma}^k) X_{\epsilon} Y_{\eta} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n + (Y_{\epsilon} Y_{\eta}) Y_{\eta} X_{\gamma} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n) \right) \]

\[ U_{\alpha \beta}^{(3)} = \frac{1}{12} W_{\alpha \gamma, \beta \delta} \left( (X_{\delta}^\dagger Y_{\gamma}^k) X_{\epsilon} Y_{\eta} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n + (Y_{\epsilon} Y_{\eta}) Y_{\eta} X_{\gamma} (t_{k_{\delta \gamma}^n}^n t_{k_{\epsilon \eta}^n}^n) \right) \]

Again, one can simplify Eqs. (C11) (C20) for the case in which the transition amplitudes are diagonal in the model space indexes, when the 1B interaction matrix element vanishes. The vanishing terms are the diagrams of Figs. 13a 13c 13f and 13g, while the final expressions for the non-vanishing diagrams can be derived straightforwardly and we omit them for brevity.

2. Dynamic Self-energy

The self-consistent procedure, through which the propagator is renormalized, includes the nuclear medium correlations already at the level of the reference propagator. In the general case, when the ADC(n) is built on a reference state which is not renormalized according to the skeleton expansion, a new set of non-skeleton diagrams must be considered also for the energy-dependent part of the self-energy. The lack of correlations in the reference propagator, must be taken into account by considering explicitly the insertions of the diagrams of the expansion (C2) into all the fermionic lines of the self-energy.

Specifically, when fermionic lines represent propagators with respect to the reference state (Eq. (7)), one-particle irreducible and interaction-irreducible diagrams
These terms listed in Eqs. (A3-A4) are:

- For the interaction matrices, the non-skeleton expansion is enriched by additional coupling matrices. The second-order diagrams of Fig. 1 are obtained by inserting the first-order 1B effective interaction in each diagram. Diagrammatically, they are obtained by inserting the first-order 1B effective interaction of Eq. (1) into the second-order diagrams of Fig. 1.

In this case, the ADC(3) expansion of the self-energy matrix in Eq. (27) is enriched with additional coupling matrices, already listed in Eq. (A1) and (A2) for the forward-in-time and backward-in-time diagrams respectively, and repeated here for sake of completeness,

\[ M_{ja}^{(II)} = M_{ra}^{(II)} + M_{qa}^{(II)} + M_{qα}^{(II)} + M_{qα}^{(II)} , \]  
\[ N_{αk}^{(II)} = N_{αs}^{(II)} + N_{αs}^{(II)} + N_{αu}^{(II)} + N_{αu}^{(II)} . \]  

Also for the interaction matrices, the non-skeleton expansion is enriched by additional coupling matrices. These terms listed in Eqs. (A3-A4) are:

\[ C_{jj'} = C_{rr'}^{(II)} + C_{rr'}^{(II)} + C_{qq'}^{(II)} + C_{qq'}^{(II)} , \]  
\[ D_{kk'} = D_{ss'}^{(II)} + D_{ss'}^{(II)} + D_{uu'}^{(II)} + D_{uu'}^{(II)} . \]  

a. ADC(3) terms with 2p1h and 2h1p ISCs

By following the same procedure used to find the expressions of the coupling matrices containing 2NFs and/or 3NFs, we can derive the analogous expressions of \( M_{ja} \) and \( N_{αk} \) containing one \( \tilde{U} \) insertion, and expressed in terms of the uncorrelated transition amplitudes of Eq. (C1).

From the Goldstone-Feynman diagrams in Figs. 14r and 14s we find,

\[ M_{ra}^{(II)} = \frac{1}{\sqrt{2}} \tilde{U}_{γδ}^{(1)} V_{γα,αγ} A_{12} X_{μ1}^{μ1} Y_{μ1}^{μ1} Y_{δ1}^{μ1} \frac{ε_{n1} - ε_{k4}}{ε_{n4} - ε_{k3}} , \]

and

\[ M_{ra}^{(II)} = \frac{1}{\sqrt{2}} \tilde{U}_{γδ}^{(1)} V_{γα,αγ} X_{μ1}^{μ1} Y_{μ1}^{μ1} X_{μ2}^{μ2} \frac{ε_{n1} - ε_{k4}}{ε_{n4} - ε_{k3}} , \]

respectively.

The 2p1h interaction matrices in Eq. (C23) are

\[ C_{rr'}^{(II)} = \frac{1}{2} \tilde{U}_{γδ}^{(1)} V_{γα,αγ} A_{12} X_{μ1}^{μ1} X_{μ2}^{μ2} \frac{ε_{n1} - ε_{k4}}{ε_{n4} - ε_{k3}} , \]

and

\[ C_{rr'}^{(II)} = \frac{1}{2} \tilde{U}_{γδ}^{(1)} V_{γα,αγ} A_{12} X_{μ1}^{μ1} X_{μ2}^{μ2} X_{μ3}^{μ3} X_{μ4}^{μ4} \frac{ε_{n1} - ε_{k4}}{ε_{n4} - ε_{k3}} , \]

The backward-in-time Goldstone diagrams of Figs. 14t and 14u find, connecting 2h1p ISCs, are

\[ D_{ss'}^{(II)} = \frac{1}{2} \tilde{U}_{γδ}^{(1)} V_{γα,αγ} A_{12} X_{μ1}^{μ1} X_{μ2}^{μ2} \frac{ε_{n1} - ε_{k4}}{ε_{n4} - ε_{k3}} , \]

and

\[ D_{ss'}^{(II)} = \frac{1}{2} \tilde{U}_{γδ}^{(1)} V_{γα,αγ} A_{12} X_{μ1}^{μ1} X_{μ2}^{μ2} X_{μ3}^{μ3} X_{μ4}^{μ4} \frac{ε_{n1} - ε_{k4}}{ε_{n4} - ε_{k3}} . \]

b. ADC(3) terms with 3p2h and 3h2p ISCs

The Goldstone-Feynman diagrams of Figs. 14r and 14s involve 3p2h and 3h2p ISCs. They contain the coupling matrices that complete the expressions for \( M_{ja} \) and \( N_{αk} \), when the reference state adopted has not be calculated self-consistently.
The working equations for the forward-in-time coupling matrices are,

\[ M_{qa}^{(\text{It})} = \frac{1}{\sqrt{12}} U_{\gamma d}^{(1)} W_{\mu \nu \rho, \alpha \lambda \eta} A_{45} X_{\gamma \delta}^{n_5} Y_{\delta}^{k_5} X_{\mu}^{n_1} X_{\nu}^{n_2} X_{\rho}^{n_3} X_{\lambda}^{k_4} (X_{\eta}^{n_4})^* \varepsilon_{k_5}^+ - \varepsilon_{n_5}^- , \]  
\( (C33) \)

and

\[ M_{qa}^{(\text{Hu})} = \frac{1}{\sqrt{12}} U_{\gamma d}^{(1)} W_{\mu \nu \rho, \alpha \lambda \eta} P_{123}^{(c)} X_{\mu}^{n_1} Y_{\mu}^{k_1} (Y_{\nu}^{k_2} Y_{\nu}^{k_3} X_{\nu}^{n_4})^* \varepsilon_{n_1}^+ - \varepsilon_{n_4}^- , \]  
\( (C34) \)

while the interaction matrices in Eq. (C23) connecting two 3p2h ISCs are,

\[ C_{qq'}^{\tilde{U}pp} = \frac{1}{12} U_{\mu \nu}^{(1)} A_{45} A_{123} A_{678} X_{\mu}^{n_1} (X_{\nu}^{n_4})^* \delta_{n_2 n_5} \delta_{n_3 n_6} \delta_{k_4 k_9} \delta_{k_5 k_{10}} , \]  
\( (C35) \)

and

\[ C_{qq'}^{\tilde{U}hh} = -\frac{1}{12} U_{\mu \nu}^{(1)} A_{45} A_{910} A_{123} (Y_{\mu}^{k_4})^* Y_{\nu}^{k_2} Y_{\nu}^{k_3} \delta_{n_1 n_4} \delta_{n_2 n_5} \delta_{n_3 n_6} \delta_{k_4 k_9} , \]  
\( (C36) \)

Expressions for the backward-in-time coupling matrices, containing one effective 1B interaction and one interaction-irreducible 3NF insertions, are,

\[ N_{\alpha \mu}^{(\text{It})} = \frac{1}{\sqrt{12}} U_{\gamma d}^{(1)} W_{\mu \nu \rho, \alpha \lambda \eta} A_{45} (Y_{\mu}^{k_1})^* (X_{\nu}^{n_4})^* (Y_{\nu}^{k_2} Y_{\nu}^{k_3} X_{\nu}^{n_4})^* Y_{\lambda}^{n_5} \varepsilon_{k_1}^+ - \varepsilon_{n_5}^- , \]  
\( (C37) \)

and

\[ N_{\alpha \mu}^{(\text{Hu})} = \frac{1}{\sqrt{12}} U_{\gamma d}^{(1)} W_{\mu \nu \rho, \alpha \lambda \eta} P_{123}^{(c)} (Y_{\mu}^{k_1})^* (X_{\nu}^{n_4})^* X_{\nu}^{n_6} (Y_{\nu}^{k_2} Y_{\nu}^{k_3} X_{\nu}^{n_4} X_{\eta}^{n_5})^* \varepsilon_{k_1}^+ - \varepsilon_{n_6}^- , \]  
\( (C38) \)

while the interaction matrices in Eq. (C24) connecting two 3h2p ISCs are

\[ D_{uu'}^{\tilde{U}pp} = -\frac{1}{12} U_{\mu \nu}^{(1)} A_{45} A_{910} A_{123} X_{\mu}^{n_5} (X_{\nu}^{n_1})^* \delta_{k_1 k_4} \delta_{k_2 k_5} \delta_{k_3 k_9} \delta_{n_1 n_4} \]  
\( (C39) \)

and

\[ D_{uu'}^{\tilde{U}hh} = \frac{1}{12} U_{\mu \nu}^{(1)} A_{45} A_{910} A_{123} A_{678} (Y_{\mu}^{k_4})^* Y_{\nu}^{k_2} X_{\nu}^{n_4} \delta_{n_5 n_9} \delta_{n_6 n_{10}} . \]  
\( (C40) \)


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<td>[34]</td>
<td>F. Raimondi and C. Barbieri, in preparation.</td>
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