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**Multi-Reference Normal Ordering  
for 3N Interactions**

Master Thesis

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# Chapter 1

## Introduction

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The goal of theoretical nuclear physics is the consistent description of the properties of atomic nuclei and the understanding of the interaction between the constituents starting from the fundamental theory of the strong interaction, which is quantum chromodynamics (QCD). A nucleus represents a finite, complex and fermionic many-body quantum system. In principle, there are two key challenges:

1. How to construct a nuclear interaction based on QCD?
2. How to solve the nuclear many-body problem?

The construction of the interaction is not unique. There are different approaches which can be roughly classified into phenomenological and QCD-motivated realistic interactions. It is desirable to derive the nuclear interaction from QCD, which contains quarks and gluons as fundamental degrees of freedom. QCD exhibits a non-perturbative character in the low-energy regime, which is relevant for nuclear physics. Therefore, an effective description of the nucleus is used, where nucleons and pions, instead of quarks and gluons, are the effective degrees of freedom. The interaction between the nucleons and pions is described consistently with respect to the symmetries of QCD in the framework of the chiral effective field theory ( $\chi$ EFT) (see [section 2.1](#)).

In order to understand the structure of nuclei, not only the nucleon-nucleon (NN) interaction but at least the 3N interaction has to be taken into account. This result is not astonishing since the nucleon is not a point-like particle. An experimental proof that the nucleon features a substructure is the existence of excited states, e.g. the delta-resonance  $\Delta(1232)$ , which can be seen at an excitation energy of about 300 MeV.

From a theoretical point of view, even interactions with higher particle rank, e.g. four-body interactions, are possible. But it is assumed that the importance of these interactions is reduced with increasing particle rank [Wei90]. Additionally, the computational cost rises tremendously when using higher-particle-rank interactions. Therefore, only the NN and 3N interactions from  $\chi$ EFT are applied in this work.

In order to solve the many-body problem with finite computational resources, the calcu-

lation is restricted to a finite subspace of the infinite-dimensional antisymmetric many-body Hilbert space, called model space. This model space is spanned by a set of energetically low-lying basis states, in order to give an adequate description for the ground and a few low-lying excited states of the nucleus. An improvement of the description is reached via a transformation of the Hamiltonian by means of the similarity renormalization group (SRG) (see [section 2.2](#)). Furthermore, the convergence behaviour of no-core shell-model (NCSM) calculations is improved with respect to the model-space size (see [section 2.3](#)). This reduction of the computational cost still does not allow to investigate heavy nuclei by using 3N interactions. Consequently, further approximations are necessary.

It has been shown that normal ordering with respect to a single-reference state provides a helpful tool to derive an approximate lower-particle-rank form of any 3N interaction. This approximation, however, is limited to closed-shell nuclei [[Rot+12](#)]. The main task of this work is to extend the normal-ordering approximation to open-shell systems using a multi-reference state, i.e. a linear combination of single Slater determinants (see [chapters 3](#) and [4](#)).

For the first time, spectra for p-shell nuclei, e.g.  ${}^6\text{Li}$ ,  ${}^{10}\text{B}$  and  ${}^{12}\text{C}$ , calculated in importance-truncated no-core shell model (IT-NCSM) using chiral 3N interactions in normal-ordering approximation with respect to a multi-reference state are presented. These results are compared to calculations using full 3N interactions (see [chapter 5](#)).

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# Chapter 2

## Basics

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### 2.1. Chiral Effective Field Theory

Quantum chromodynamics (QCD) is the fundamental theory of the strong interaction which contains quarks and gluons as internal degrees of freedom. Up to now, it is not possible to deduce the nuclear interaction which is a residual interaction of the strong interaction starting from QCD. It is well known that QCD exhibits a non-perturbative character in the low-energy regime, which is relevant for nuclear physics. Therefore, an effective description of the nucleus is used, where nucleons and pions, instead of quarks and gluons, are the effective degrees of freedom. The interaction between the nucleons and pions is described consistently with respect to the symmetries of QCD in the framework of the chiral effective field theory ( $\chi$ EFT) [Wei90].

The main idea of  $\chi$ EFT is based on the scale separation of the hadron mass spectrum and systematic expansion of the nuclear interaction in powers of  $Q/\Lambda_\chi$ , called power counting [Wei90]. Here,  $Q$  is the generic momenta in the nuclear process at the order of the pion mass  $m_\pi = 140$  MeV, and  $\Lambda_\chi$  is the break-down scale at the order of  $\rho$ -meson mass  $m_\rho = 770$  MeV. Details at short distances are not resolved by small momentum  $Q \ll \Lambda_\chi$ , which is fulfilled for nuclear physics. Thus, they are absorbed in so called contact interactions. Since  $Q/\Lambda_\chi$  is small compared to one, convergence of this expansion is expected. The resulting terms up to  $(Q/\Lambda_\chi)^4$  obtained from the expansion are depicted in figure 2.1.

At leading order (LO), meaning  $(Q/\Lambda_\chi)^0$ , and next-to-leading order (NLO), meaning  $(Q/\Lambda_\chi)^2$ , only two-nucleon interactions emerge to the nuclear interaction. The order  $(Q/\Lambda_\chi)^1$  is forbidden because of parity and time-reversal symmetry [EM03]. Three-nucleon interactions start emerging at next-to-next-to-leading order (N<sup>2</sup>LO), meaning  $(Q/\Lambda_\chi)^3$ . The corresponding diagrams—from left to right—describe a two-pion exchange term, a one-pion exchange combined with a two-nucleon contact term, and a three-nucleon contact term. Furthermore, the four-nucleon interactions begin emerging at N<sup>3</sup>LO. Hence,  $\chi$ EFT clarifies the hierarchy of nuclear interactions, namely two-nucleon interactions are more important than three-nucleon interactions due to their appearance at lower order of  $Q/\Lambda_\chi$ . The same is true

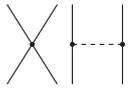
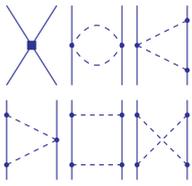
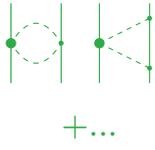
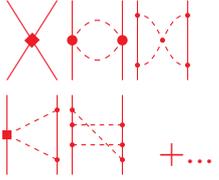
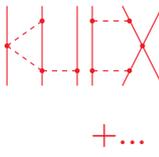
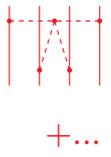
	two-nucleon interactions	three-nucleon interactions	four-nucleon interactions
LO $(Q/\Lambda_\chi)^0$			
NLO $(Q/\Lambda_\chi)^2$			
N <sup>2</sup> LO $(Q/\Lambda_\chi)^3$			
N <sup>3</sup> LO $(Q/\Lambda_\chi)^4$			

Figure 2.1.: Hierarchy of nuclear interactions in  $\chi$ EFT. The interaction terms up to the N<sup>3</sup>LO are dedicated to the particle number of the interaction. The dashed lines represent pions and the solid lines nucleons. The small dots, large solid dots, solid squares and solid diamond denote different vertices. For more details see [Mac09].

for the three-nucleon interactions compared to four-nucleon interactions.

In this work, the two-nucleon interaction at N<sup>3</sup>LO from Entem and Machleidt [EM03] and the three-nucleon interaction at N<sup>3</sup>LO in local form from Navrátil [Nav07] will be used. The low-energy constants have been fitted to the ground-state energy and  $\beta$ -decay half-life of three-nucleon systems [GQN09].

## 2.2. Similarity Renormalization Group Transformation

The similarity renormalization group (SRG) transformation is a method to soften an interaction, i.e. to pre-diagonalize its matrix representation. The basic idea is to apply an unitary transformation to the considered initial Hamiltonian such that its matrix representation changes into band- or block-diagonal form regarding a specific basis. As a consequence, convergence behaviour of many-body calculations, e.g. no-core shell-model (NCSM), is improved with respect to the model-space size. Since a unitary transformation does not change the eigenvalues of an operator, the solution of the many-body problem with the transformed Hamiltonian is equivalent to the solution of the initial eigenvalue problem.

## Mathematical Formulation

Let  $U_\alpha$  be a unitary operator depending continuously on the flow parameter  $\alpha$ . Hence, the SRG transformation on the initial Hamiltonian  $H_0$  is given by

$$H_\alpha := U_\alpha^\dagger H_0 U_\alpha, \quad (2.1)$$

where  $H_\alpha$  is called the SRG-transformed or evolved Hamiltonian. Taking the total derivative of that expression with respect to  $\alpha$  leads to

$$\frac{dH_\alpha}{d\alpha} = \frac{dU_\alpha^\dagger}{d\alpha} H_0 U_\alpha + U_\alpha^\dagger H_0 \frac{dU_\alpha}{d\alpha}. \quad (2.2)$$

Since the transformation operator  $U_\alpha$  is unitary, i.e.  $U_\alpha U_\alpha^\dagger = \mathbb{1}$ , it follows by derivation

$$\frac{dU_\alpha^\dagger}{d\alpha} = -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} U_\alpha^\dagger. \quad (2.3)$$

Making use of (2.3) and the unitarity of  $U_\alpha$ , one can simplify (2.2) to

$$\begin{aligned} \frac{dH_\alpha}{d\alpha} &= -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} U_\alpha^\dagger H_0 U_\alpha + U_\alpha^\dagger H_0 U_\alpha U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} \\ &= -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} H_\alpha + H_\alpha U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} \\ &= \left( -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} \right) H_\alpha - H_\alpha \left( -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} \right) \\ &= \left[ -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha}, H_\alpha \right], \end{aligned} \quad (2.4)$$

where a commutator has been used in the last step. Hence, one has to solve an initial value problem with the initial condition  $H_{\alpha=0} = H_0$  in order to find the evolved Hamiltonian  $H_\alpha$ . Furthermore, the generator of the transformation is defined as

$$\eta_\alpha := -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha}. \quad (2.5)$$

Using this definition, the flow equation for the evolved Hamiltonian  $H_\alpha$  is given by

$$\frac{dH_\alpha}{d\alpha} = [\eta_\alpha, H_\alpha]. \quad (2.6)$$

Since

$$\eta_\alpha + \eta_\alpha^\dagger = -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} - \frac{dU_\alpha^\dagger}{d\alpha} U_\alpha = -\frac{d(U_\alpha^\dagger U_\alpha)}{d\alpha} = -\frac{d\mathbb{1}}{d\alpha} = 0,$$

the generator of the transformation  $\eta_\alpha$  is antihermitian, i.e.  $\eta_\alpha^\dagger = -\eta_\alpha$ .

There are many possibilities for the choice of the generator  $\eta_\alpha$  discussed in the literature [Weg94]. Typically, the generator is chosen as a commutator of a hermitian operator and the evolved Hamiltonian  $H_\alpha$ , because that ensures the anti-hermiticity of the generator.

In this work, the generator of the SRG transformation is chosen as the commutator of the intrinsic kinetic energy  $T_{\text{int}}$  and the evolved Hamiltonian  $H_\alpha$ , i.e.

$$\eta_\alpha := m_N^2 [T_{\text{int}}, H_\alpha], \quad (2.7)$$

where  $m_N$  is the nucleon mass, and the intrinsic kinetic energy is defined as

$$T_{\text{int}} := T - T_{\text{cm}}. \quad (2.8)$$

Here,  $T$  and  $T_{\text{cm}}$  denote the total and the center-of-mass kinetic energy, respectively. This generator drives the Hamiltonian towards a diagonal form in a basis of eigenstates of the intrinsic kinetic energy, i.e. momentum eigenstates. For this specific choice of the generator, a dimensional analysis of the units yields that the flow parameter  $\alpha$  has the dimension of length to the power of four.

The SRG transformation of any  $i$ -body operator within a  $A$ -body system induces irreducible many-body operators up to the  $A$ -body level, e.g. for the kinetic energy operator  $T$  that is an one-body operator

$$U_\alpha^\dagger T U_\alpha = T_\alpha^{[1]} + T_\alpha^{[2]} + \dots + T_\alpha^{[A]}. \quad (2.9)$$

The number within the brackets denotes the particle-rank. Especially for the one-body operator, one observes that the transformed one-body operator  $T_\alpha^{[1]}$  does not change through the SRG transformation, that can be checked by explicitly carrying out the commutator in (2.6) using the operators in second quantization. For higher-particle-rank operators, this is not true, e.g. the SRG transformation of the two-nucleon interaction  $V_{\text{NN}}$  leads to

$$U_\alpha^\dagger V_{\text{NN}} U_\alpha = V_{\text{NN},\alpha}^{[2]} + V_{\text{NN},\alpha}^{[3]} + \dots + V_{\text{NN},\alpha}^{[A]}, \quad (2.10)$$

where  $V_{\text{NN},\alpha}^{[2]}$  is the transformed two-body operator being different from the initial operator  $V_{\text{NN}}$ .

Starting with an Hamiltonian  $H$  containing an intrinsic kinetic energy  $T_{\text{int}}$ , a two- and three-nucleon interaction  $V_{\text{NN}}$  and  $V_{3\text{N}}$ , the SRG transformation results in

$$U_\alpha^\dagger H U_\alpha = U_\alpha^\dagger (T_{\text{int}} + V_{\text{NN}} + V_{3\text{N}}) U_\alpha \quad (2.11)$$

$$= (T_{\text{int},\alpha}^{[2]} + V_{\text{NN},\alpha}^{[2]}) + (T_{\text{int},\alpha}^{[3]} + V_{\text{NN},\alpha}^{[3]} + V_{3\text{N},\alpha}^{[3]}) + \dots + (T_{\text{int},\alpha}^{[A]} + V_{\text{NN},\alpha}^{[A]} + V_{3\text{N},\alpha}^{[A]}). \quad (2.12)$$

Note that there is no one-body term because the kinetic energy operator is a two-body operator. Formally, only if all the induced terms up to the  $A$ -body level are kept, the SRG transformation is unitary and the spectrum of the Hamiltonian in an exact  $A$ -body calculation is preserved and independent of the flow parameter  $\alpha$ . In practice, the SRG transformation has to be truncated at a particle rank  $m < A$ , which formally violates the unitarity of the

SRG transformation. Hence, the flow parameter  $\alpha$  is used as a diagnostic tool to quantify the relevance of omitted beyond- $m$ -body terms.

In this work, two types of SRG-transformed Hamiltonians will be considered: The NN+3N-induced Hamiltonian omits the chiral 3N interaction from the initial Hamiltonian, but keeps all induced 3N terms throughout the transformation, i.e.

$$H_{\alpha}^{\text{NN+3N-ind.}} := \left( T_{\text{int},\alpha}^{[2]} + V_{\text{NN},\alpha}^{[2]} \right) + \left( T_{\text{int},\alpha}^{[3]} + V_{\text{NN},\alpha}^{[3]} \right); \quad (2.13)$$

the NN+3N-full Hamiltonian starts with the initial chiral NN+3N Hamiltonian and retains all terms up to the 3-body level in the SRG transformation, i.e.

$$H_{\alpha}^{\text{NN+3N-full.}} := \left( T_{\text{int},\alpha}^{[2]} + V_{\text{NN},\alpha}^{[2]} \right) + \left( T_{\text{int},\alpha}^{[3]} + V_{\text{NN},\alpha}^{[3]} + V_{\text{3N},\alpha}^{[3]} \right). \quad (2.14)$$

### 2.3. (Importance-Truncated) No-Core Shell Model

In this section, the no-core shell model (NCSM) which is a powerful method to solve the many-body problem given by the stationary Schrödinger equation

$$H |\Phi_{\nu}\rangle = E_{\nu} |\Phi_{\nu}\rangle, \quad (2.15)$$

in an *ab-initio* manner, meaning from first principles without approximation, will be presented. Here,  $E_{\nu}$  is the eigenvalue of the eigenstate  $|\Phi_{\nu}\rangle$  of the Hamiltonian  $H$ . Afterwards, the importance-truncated NCSM (IT-NCSM) will be briefly described.

#### No-Core Shell Model

In NCSM, one considers a quantum system made of  $A$  point-like and non-relativistic nucleons whose Hamiltonian contains the intrinsic kinetic energy, two-, three- or higher-particle-rank interactions. In contrast to typical shell-model calculations, in NCSM all nucleons are considered as “active”, i.e. all nucleons appear in the state and contribute to observables.

The strategy of NCSM to solve the many-body problem (2.15) is described in the following:

1. First of all, a model space  $\mathcal{M}$  spanned by particular Slater determinants is constructed. Each Slater determinant  $|\phi_i\rangle$  is an anti-symmetrized product state of single-particle harmonic-oscillator states.
2. Only those Slater determinants fulfilling the so called truncation condition will be considered.
3. Subsequently, the many-body problem can be rewritten in a matrix-eigenvalue problem using the truncated harmonic-oscillator Slater determinants.
4. Finally, the matrix-eigenvalue problem is solved for a few low-lying states, and the eigenvalues and -states of the Hamiltonian are obtained.

The truncation condition is given by the inequality

$$\sum_i^A (2n_i + l_i) \leq N_{\max}, \quad (2.16)$$

which is called the  $N_{\max}\hbar\Omega$ -truncation. Here,  $n_i$  is the radial quantum number,  $l_i$  the angular momentum, and  $N_{\max}$  the maximum number of harmonic-oscillator excitation quanta. That means that all Slater determinants within the NCSM model space have unperturbed excitation energies up to  $N_{\max}\hbar\Omega$ .

Since intrinsic properties of a self-bound nucleus are independent of the center-of-mass degree of freedom, the state of the nucleus has to separate into a state depending only on the center-of-mass coordinates, and a state depending only on relative coordinates. One can show mathematically that the harmonic-oscillator states as basis fulfill this requirement if and only if the  $N_{\max}\hbar\Omega$ -truncation condition is used. Hence, spurious center-of-mass contaminations of the eigenstates are absent. Of course, there could be another basis with a proper truncation fulfilling this requirement.

It is assumed that  $|\Phi_\nu\rangle$  is included in the NCSM model space  $\mathcal{M}$ . Thus,  $|\Phi_\nu\rangle$  can be expressed as a linear combination of the basis states, i.e.

$$|\Phi_\nu\rangle = \sum_j^N c_j^{(\nu)} |\phi_j\rangle, \quad (2.17)$$

where the number of basis state  $N$  depends explicitly on  $N_{\max}$ . Inserting this into to the many-body problem (2.15), and multiplying by  $\langle\phi_i|$  from the left side, one obtains

$$\sum_j^N \langle\phi_i| H |\phi_j\rangle c_j^{(\nu)} = E_\nu c_i^{(\nu)}, \quad (2.18)$$

which is an eigenvalue problem for the matrix representation of the Hamiltonian in a harmonic-oscillator basis  $H_{ij} := \langle\phi_i| H |\phi_j\rangle$ . Here, one uses that the harmonic-oscillator states  $\{|\phi_i\rangle\}$  build an orthonormal basis. For the solution of the matrix eigenvalue problem, one often applies Lanczos-type algorithms [Saa92].

NCSM calculations are limited by the dimension of the model space  $\mathcal{M}$  that grows factorially with increasing the number of nucleons  $A$ , and the model-space size  $N_{\max}$  that needs to be increased in order to reach convergence. Nowadays, linear dimensions of  $10^{10}$  are the upper limit of tractable matrices during the computations, such that NCSM calculations for  $^{16}\text{O}$  can practically be performed only in relatively small model spaces ( $N_{\max} \leq 8$ ) where convergence has not yet reached [Rot09].

In the next step, the importance-truncated NCSM (IT-NCSM), in which the NCSM model space can be reduced with guidance of the multi-configuration many-body perturbation theory, will be introduced.

## Importance-Truncated No-Core Shell Modell

The importance-truncated NCSM (IT-NCSM) reduces the NCSM model space to a tractable size while decreasing the computational cost compared to an NCSM calculation. The starting point is an NCSM model space  $\mathcal{M}$  and a so called reference state  $|\Phi'\rangle \in \mathcal{M}' \subseteq \mathcal{M}$ . It is required that  $|\Phi'\rangle$ , which is an approximation of the target state that will be calculated later, to have the correct angular momentum. To ensure this requirement,  $|\Phi'\rangle$  is determined in NCSM-type calculation in  $\mathcal{M}'$ .

In order to quantify the importance of the basis states which are included in  $\mathcal{M}$ , but excluded from  $\mathcal{M}'$ , the first perturbative correction of  $|\Phi'\rangle$

$$|\Phi'^{(1)}\rangle = - \sum_{|\phi_i\rangle \notin \mathcal{M}'} \frac{\langle \phi_i | H | \Phi' \rangle}{\epsilon_i - \epsilon'} |\phi_i\rangle \quad (2.19)$$

is considered, where  $\epsilon_i$  is the unperturbed energy of the basis states  $|\phi_i\rangle \notin \mathcal{M}'$  and  $\epsilon'$  is the expectation value regarding  $|\Phi'\rangle$  of the Hamiltonian  $H$ .

Afterwards, the coefficient

$$\kappa_i := - \frac{\langle \phi_i | H | \Phi' \rangle}{\epsilon_i - \epsilon'} \quad (2.20)$$

is used as an a priori importance measure of the basis state  $|\phi_i\rangle \notin \mathcal{M}'$ . Only basis states with an importance measure  $|\kappa_i|$  above a threshold  $\kappa_{\min}$  are retained in the model space. Hence, diagonalization of the matrix can be carried out in this smaller space. A variation of the threshold  $\kappa_{\min}$  allows an *a posteriori* extrapolation of  $\kappa_{\min}$  towards zero to recover the contribution of the discarded basis states.

The procedure for the importance truncation of the model space described in the following can be extended to an iterative method: One basically starts with a particular model space and a reference state calculated in NCSM-tractable model space, and reduces the model space by means of the importance measure (2.20). By diagonalizing the matrix of the Hamiltonian within the importance-truncated model space, an eigenstate is obtained that can be used for the next larger model space. This procedure is iterated while progressing to larger model spaces.

The reduction of the model space facilitates calculations in ranges that are not manageable in NCSM. For instance, calculations for  $^{16}\text{O}$  in the model space  $N_{\max} = 10$ —not tractable in the framework of NCSM—are computationally possible in IT-NCSM because of the tremendous reduction of the model-space size. Even calculations within a model space up to  $N_{\max} = 22$  and beyond are tractable in IT-NCSM—for Hamiltonians containing only an NN interaction— while this limit is set by the available two-body matrix elements and not by the IT-NCSM calculation itself [Rot09].



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# Chapter 3

## Normal Ordering and Wick's Theorem

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In [section 3.1](#) an overview of the important symbols used in this chapter will be given. Furthermore, in [section 3.2](#) the index antisymmetrizer, which is helpful to write equations in a compact form, will be introduced. Finally, normal ordering and Wick's theorem which are the main issue of this chapter will be discussed in [sections 3.3–3.5](#).

### 3.1. Notations and Definitions

This section gives an overview of the symbols used in the following chapter. To simplify the notation fermionic creation- and annihilation operators are written as

$$a^p := a_p^\dagger, \quad (3.1)$$

$$a_q := a_q. \quad (3.2)$$

Furthermore, the tensor notation for an  $n$ -body operator

$$a_{q_1 q_2 \dots q_n}^{p_1 p_2 \dots p_n} := a^{p_1} a^{p_2} \dots a^{p_n} a_{q_n} a_{q_{n-1}} \dots a_{q_1} \quad (3.3)$$

is used. Hence, one-, two- and three-body operators in tensor notation are

$$a_q^p = a^p a_q, \quad (3.4)$$

$$a_{qs}^{pr} = a^p a^r a_s a_q, \quad (3.5)$$

$$a_{qsu}^{prt} = a^p a^r a^t a_u a_s a_q. \quad (3.6)$$

The  $n$ -particle density matrix element with respect to a state  $|\Psi\rangle$  is given by

$$\gamma_{q_1 q_2 \dots q_n}^{p_1 p_2 \dots p_n} := \langle \Psi | a_{q_1 q_2 \dots q_n}^{p_1 p_2 \dots p_n} | \Psi \rangle, \quad (3.7)$$

Relevant for this work are one-, two- and three-body density matrix elements

$$\gamma_q^p = \langle \Psi | a_q^p | \Psi \rangle, \quad (3.8)$$

$$\gamma_{qs}^{pr} = \langle \Psi | a_{qs}^{pr} | \Psi \rangle, \quad (3.9)$$

$$\gamma_{qsu}^{prt} = \langle \Psi | a_{qsu}^{prt} | \Psi \rangle. \quad (3.10)$$

For the whole chapter, let  $A_1, A_2, \dots, A_n$  be pairwise distinct fermionic operators each of them representing either a creation operator  $a^p$  or an annihilation operator  $a_q$ .

A contraction with respect to the vacuum  $|0\rangle$  between the operators  $A_1$  and  $A_2$  is symbolized by

$$\overline{A_1 A_2}. \quad (3.11)$$

A contraction with respect to a single Slater determinant  $|\phi\rangle$  between the operators  $A_1$  and  $A_2$  is symbolized by

$$\overline{\overline{A_1 A_2}}. \quad (3.12)$$

In the multi-reference Wick's theorem, there are  $l$ -tuple contractions defined as contractions between  $l$  operators

$$\overline{\overline{\overline{A_1 A_2 \dots A_l}}}. \quad (3.13)$$

Finally, the residual  $l$ -particle density matrix element will be denoted as

$$\lambda_{q_1 q_2 \dots q_l}^{p_1 p_2 \dots p_l}. \quad (3.14)$$

These symbols will be defined in the following sections in detail. This section serves just as a summary.

## 3.2. Index Antisymmetrizer

In this section, the index antisymmetrizer  $\mathbb{A}$  is introduced. A mathematically rigorous definition can be found in [KNM10]. In this work, the index antisymmetrizer  $\mathbb{A}$  will be used to write equations in a compact form and is defined as follows:

**Definition 3.1.** Acting with  $\mathbb{A}$  on a multiply-indexed object  $f = f_{q_1 \dots q_n}^{p_1 \dots p_n}$ , it generates all forms by permuting the upper indices and permuting the lower indices in all possible ways, such that  $\mathbb{A}f$  is antisymmetric with respect to a transposition of any two indices among the upper indices or among the lower indices. Each unique permutation form appears with a coefficient unity. The sign for any permuted form is determined by the parity of the permutation, which brings the indices of the permuted form into the original index pairing order.

This definition will be clarified by some examples. Let  $f$  be a multiply-indexed object with  $n$  upper and  $n$  lower indices, i.e.  $f = f_{q_1 \dots q_n}^{p_1 \dots p_n}$ . For all  $i$  and  $j$ , it holds

$$\mathbb{A}f_{\dots q_i \dots q_j \dots}^{p_i \dots p_j \dots} = -\mathbb{A}f_{\dots q_j \dots q_i \dots}^{p_j \dots p_i \dots} = -\mathbb{A}f_{\dots q_j \dots q_i \dots}^{p_i \dots p_j \dots}. \quad (3.15)$$

Per definition, the index antisymmetrizer  $\mathbb{A}$  is linear

$$\mathbb{A}(\lambda f + g) = \lambda \mathbb{A}f + \mathbb{A}g, \quad (3.16)$$

and idempotent

$$\mathbb{A}^2 f = \mathbb{A}(\mathbb{A}f) = \mathbb{A}f, \quad (3.17)$$

where  $g$  has the same indices as  $f$ , and  $\lambda$  represents a complex number. Furthermore, for any multiply-indexed objects  $f$  and  $g$  it is

$$\mathbb{A}(fg) = \mathbb{A}(gf). \quad (3.18)$$

The action of  $\mathbb{A}$  will be demonstrated on some relevant examples.

Firstly, the simplest (non-trivial) example is given by a multiply-indexed object  $f = f_{qs}^{pr}$  with two upper and two lower indices. It is assumed that  $f$  is not antisymmetric either with respect to the upper nor with respect to the lower indices. Hence, the action of  $\mathbb{A}$  on  $f$  generates  $2! \cdot 2! = 4$  different terms given by

$$\mathbb{A}(f_{qs}^{pr}) = f_{qs}^{pr} + f_{sq}^{rp} - f_{sq}^{pr} - f_{qs}^{rp}. \quad (3.19)$$

One can easily check the antisymmetry of  $\mathbb{A}f$ .

In general, the equality of two multiply-indexed objects is defined as:

**Definition 3.2.** Two multiply-indexed objects  $g = g_{q_1 \dots q_n}^{p_1 \dots p_n}$  and  $h = h_{q_1 \dots q_m}^{p_1 \dots p_m}$  are equal ( $g \equiv h$ ), if and only if they have the same number of upper and lower indices ( $n = m$ ), and if for all  $p_1, \dots, p_m$  and  $q_1, \dots, q_m$

$$g_{q_1 \dots q_n}^{p_1 \dots p_n} = h_{q_1 \dots q_m}^{p_1 \dots p_m}. \quad (3.20)$$

Let  $g$  and  $h$  be multiply-indexed objects each of them with one upper and one lower index. Two cases, namely  $g \equiv h$  and  $g \not\equiv h$ , have to be distinguished.

If  $g \not\equiv h$ , then with the aid of (3.19) the action of  $\mathbb{A}$  on  $gh$  results in

$$\mathbb{A}(g_q^p h_s^r) = g_q^p h_s^r + g_s^r h_q^p - g_s^p h_q^r - g_q^r h_s^p, \quad (3.21)$$

i.e. the multiply-indexed objects  $g$  and  $h$  can be treated as one multiply-indexed object  $f_{qs}^{pr} := g_q^p h_s^r$ .

The case of  $g \equiv h$  needs to be considered carefully. Inserting  $g$  for  $h$  into the right hand side

of (3.21), one obtains

$$2(g_q^p g_s^r - g_s^p g_q^r). \quad (3.22)$$

Since per definition 3.1, each unique permuted form appears with a coefficient unity, it follows

$$\mathbb{A}(g_q^p g_s^r) = g_q^p g_s^r - g_s^p g_q^r. \quad (3.23)$$

Secondly, let  $f = f_{qsu}^{prt}$  be a multiply-indexed object with three upper and three lower indices. If  $f$  is not antisymmetric either with respect to the upper nor with respect to the lower indices then acting with  $\mathbb{A}$  on  $f$  generates  $36 = 3! \cdot 3!$  terms which will not be written out explicitly, because only the following examples are of interest.

Consider the action of  $\mathbb{A}$  on the multiply-indexed objects  $h, g$  and  $j$ , each with one upper and one lower index. If  $h, g$  and  $j$  are pairwise distinct, then  $\mathbb{A}(h_q^p g_s^r j_u^t)$  consists of 36 different terms which will not be written out explicitly, either.

Assuming  $g \equiv j$  and  $g \not\equiv h$ , the number of different terms is halved

$$\begin{aligned} \mathbb{A}(h_q^p g_s^r g_u^t) = & + h_q^p (g_s^r g_u^t - g_u^r g_s^t) - h_s^p (g_q^r g_u^t - g_u^r g_q^t) - h_u^p (g_s^r g_q^t - g_q^r g_s^t) \\ & - h_q^r (g_s^p g_u^t - g_u^p g_s^t) + h_s^r (g_q^p g_u^t - g_u^p g_q^t) - h_u^r (g_q^p g_s^t - g_s^p g_q^t) \\ & - h_q^t (g_u^p g_s^r - g_s^p g_u^r) - h_s^t (g_q^p g_u^r - g_u^p g_q^r) + h_u^t (g_q^p g_s^r - g_s^p g_q^r). \end{aligned} \quad (3.24)$$

If one assumes  $g \equiv j \equiv h$ , the remaining terms are

$$\begin{aligned} \mathbb{A}(g_q^p g_s^r g_u^t) = & + g_q^p g_s^r g_u^t + g_u^p g_q^r g_s^t + g_s^p g_u^r g_q^t \\ & - g_u^p g_s^r g_q^t - g_s^p g_q^r g_u^t - g_q^p g_u^r g_s^t. \end{aligned} \quad (3.25)$$

Another group of special cases is given by the action of  $\mathbb{A}$  on the multiply-indexed objects  $h = h_u^t$  and  $g = g_{qs}^{pr}$  being antisymmetric with respect to transposition of the upper, respectively lower, indices. Using (3.24) and taking care that every term within the bracket represents one term due to antisymmetry of  $g$ , it follows

$$\begin{aligned} \mathbb{A}(h_q^p g_{su}^{rt}) = & + h_q^p g_{su}^{rt} - h_s^p g_{qu}^{rt} - h_u^p g_{sq}^{rt} \\ & - h_q^r g_{su}^{pt} + h_s^r g_{qu}^{pt} - h_u^r g_{qs}^{pt} \\ & - h_q^t g_{us}^{pr} - h_s^t g_{qu}^{pr} + h_u^t g_{qs}^{pr}, \end{aligned} \quad (3.26)$$

where additionally the antisymmetry of  $g$  has been used to write this result in a convenient form. The results obtained in (3.26) can be used for  $g_u^t$  and  $g_{qs}^{pr}$  because they are not equal to each other in the sense of definition 3.1 because of the different number of indices. Using relation (3.18), it is clear that

$$\mathbb{A}(g_{qs}^{pr} h_u^t) = \mathbb{A}(h_q^p g_{su}^{rt}). \quad (3.27)$$

Finally, a summary of the results obtained in this section which will be helpful to write equations in a compact form in the following sections are presented assuming  $g \neq h$  and  $g_{su}^{rt}$  is antisymmetric with respect to transposition of the upper and lower indices, respectively:

$$\mathbb{A}(g_q^p h_s^r) = + g_q^p h_s^r + g_s^r h_q^p - g_s^p h_q^r - g_q^r h_s^p, \quad (3.28)$$

$$\mathbb{A}(g_q^p g_s^r) = + g_q^p g_s^r - g_s^p g_q^r, \quad (3.29)$$

$$\begin{aligned} \mathbb{A}(h_q^p g_s^r g_u^t) = & + h_q^p (g_s^r g_u^t - g_u^r g_s^t) - h_s^p (g_q^r g_u^t - g_u^r g_q^t) - h_u^p (g_s^r g_q^t - g_q^r g_s^t) \\ & - h_q^r (g_s^p g_u^t - g_u^p g_s^t) + h_s^r (g_q^p g_u^t - g_u^p g_q^t) - h_u^r (g_q^p g_s^t - g_s^p g_q^t) \\ & - h_q^t (g_u^p g_s^r - g_s^p g_u^r) - h_s^t (g_q^p g_u^r - g_u^p g_q^r) + h_u^t (g_q^p g_s^r - g_s^p g_q^r), \end{aligned} \quad (3.30)$$

$$\mathbb{A}(g_q^p g_s^r h_u^t) = \mathbb{A}(h_q^p g_s^r g_u^t), \quad (3.31)$$

$$\begin{aligned} \mathbb{A}(g_q^p g_s^r g_u^t) = & + g_q^p g_s^r g_u^t + g_u^p g_q^r g_s^t + g_s^p g_u^r g_q^t \\ & - g_u^p g_s^r g_q^t - g_s^p g_q^r g_u^t - g_q^p g_u^r g_s^t, \end{aligned} \quad (3.32)$$

$$\begin{aligned} \mathbb{A}(h_q^p g_{su}^{rt}) = & + h_q^p g_{su}^{rt} - h_s^p g_{qu}^{rt} - h_u^p g_{sq}^{rt} \\ & - h_q^r g_{su}^{pt} + h_s^r g_{qu}^{pt} - h_u^r g_{qs}^{pt} \\ & - h_q^t g_{us}^{pr} - h_s^t g_{qu}^{pr} + h_u^t g_{qs}^{pr}, \end{aligned} \quad (3.33)$$

$$\mathbb{A}(g_{qs}^{pr} h_u^t) = \mathbb{A}(h_q^p g_{su}^{rt}). \quad (3.34)$$

### 3.3. Normal Ordering und Wick's Theorem with respect to the Vacuum

In this section, the concept of normal ordering and the statement of Wick's Theorem with respect to the vacuum will be introduced.

#### 3.3.1. Normal Ordering with respect to the Vacuum

The starting point is the following definition:

**Definition 3.3.** A product of fermionic operators is in normal order with respect to the vacuum  $|0\rangle$ , briefly an operator in V-NO, if all creation operators are to the left of all annihilation operators.

Obviously, any single creation operator  $a^p = a_p^\dagger$ , and annihilation operator  $a_q$  is an operator in V-NO. To give more examples, the one-, two- and three-body operators  $a_q^p, a_{qs}^{pr}, a_{qsu}^{prt}$  are operators in V-NO, too. The tensor notation has been used as a simplification. For the mathematical description, an operator  $N$  is defined which brings a product of operators in V-NO taking into account a sign factor.

As a reminder,  $A_1, A_2, \dots, A_n$  are pairwise distinct fermionic operators each of them representing either a creation operator  $a^p$  or an annihilation operator  $a_q$ . Using this requirement, the definition of the normal-ordering operator  $N$  reads as follows:

**Definition 3.4.** The normal-ordering operator  $N$  is defined by

$$N\{A_1 A_2 \dots A_n\} := \text{sgn}(\pi) A_{\pi(1)} A_{\pi(2)} \dots A_{\pi(n)}, \quad (3.35)$$

where  $\text{sgn}(\pi)$  is the sign of the permutation

$$\pi = \begin{pmatrix} 1 & 2 & \dots & n \\ \pi(1) & \pi(2) & \dots & \pi(n) \end{pmatrix} \quad (3.36)$$

needed to bring the product  $A_1 A_2 \dots A_n$  into normal order with respect to the vacuum, i.e. the product  $A_{\pi(1)} A_{\pi(2)} \dots A_{\pi(n)}$  is an operator in V-NO. Generally, this depiction is not unique, because two different creation- and annihilation operators anticommute. Additionally, it is required that the normal-ordering operator is linear and maps the identity operator of the antisymmetric Fock space  $\hat{1}$  on itself. Linearity means, that for a complex number  $\lambda$  and, two operators  $C$  and  $D$ , it holds

$$\begin{aligned} N\{A_1 A_2 \dots A_j (\lambda C + D) A_{j+1} \dots A_n\} &= \lambda N\{A_1 A_2 \dots A_j C A_{j+1} \dots A_n\} \\ &+ N\{A_1 A_2 \dots A_j D A_{j+1} \dots A_n\}. \end{aligned} \quad (3.37)$$

Per definition, the normal-ordering operator is antisymmetric under transposition of any

two operators, i.e. for  $i \neq j$

$$N\{A_1 A_2 \dots A_i \dots A_j \dots A_n\} = -N\{A_1 A_2 \dots A_j \dots A_i \dots A_n\}. \quad (3.38)$$

This can be proven with the aid of the signum function's property

$$\text{sgn}(\pi\pi') = \text{sgn}(\pi)\text{sgn}(\pi'), \quad (3.39)$$

where  $\pi$  and  $\pi'$  denote two arbitrary permutations. Moreover, the sign of any transposition, which is a special permutation, is always negativ. From the linearity and requirement, that  $\hat{1}$  is mapped on itself, one obtains

$$N\{\lambda\hat{1}\} = \lambda N\{\hat{1}\} = \lambda\hat{1}, \quad (3.40)$$

using a short notation  $N\{\lambda\} = \lambda$ . A very important property of an operator in V-NO is that its vacuum expectation value vanishes, i.e.

$$\langle 0 | N\{A_1 A_2 \dots A_n\} | 0 \rangle = 0. \quad (3.41)$$

The action of the normal-ordering operator  $N$  is illustrated on simple examples:

$$N\{a_q a^p\} = -N\{a^p a_q\} = -a^p a_q, \quad (3.42)$$

$$N\{a_q a^p a_s a^r\} = +a^p a^r a_s a_q = -a^r a^p a_s a_q, \quad (3.43)$$

$$N\{a_q a_s a^p\} = (-1)^2 a^p a_q a_s. \quad (3.44)$$

These simple examples demonstrate that, in general, acting with the normal-ordering operator  $N$  on a given product of operators, generates a different operator compared to the initial one, i.e.

$$A_1 A_2 \dots A_n \neq N\{A_1 A_2 \dots A_n\}. \quad (3.45)$$

The arising question is how to transform a product of operator into normal order with respect to the vacuum, while claiming that the given product remains unchanged. This procedure will be called normal-ordering transformation.

The straight-forward way is to put creation operators to the left of all annihilation operators using the anticommutation relations, given by

$$[a_q, a_p] = [a^q, a^p] = 0, \quad (3.46)$$

$$[a_q, a^p] = \delta_q^p, \quad (3.47)$$

where the brackets  $[]$  are defined as  $[A_1, A_2] := A_1 A_2 + A_2 A_1$ . By means of the anticommu-

tation relations, e.g. the product of  $a_q a_s a^p$  can be transformed to

$$a_q a_s a^p \longrightarrow a_q a_s a^p = a^p a_q a_s + \delta_s^p a_q - \delta_q^p a_s. \quad (3.48)$$

The first term in (3.48) can be identified with the term obtained in (3.44), namely  $N\{a_q a_s a^p\}$ , and the two additional terms are operators in V-NO, too. Hence, the given product is expressed as a sum of operators in V-NO. Since only equivalent transformation has been used, (3.48) is an operator identity.

The normal-ordering transformation can be very exhausting especially if the number of operators is large. It is convenient to make use of Wick's theorem which is the standard approach to this problem. The normal-ordering operator  $N$  plays an important role in Wick's theorem, which will be illustrated in the next subsection.

### 3.3.2. Wick's Theorem with respect to the Vacuum

According to the statement of Wick's theorem with respect to the vacuum (V-WT), a product of  $n$  operators  $A_1, A_2, \dots, A_n$  can be expressed as a sum of operators in V-NO including all (possible) contractions with respect to the vacuum [Wic50; KM97], i.e. in a notation using the normal-ordering operator

$$A_1 A_2 \dots A_n = N\{A_1 A_2 \dots A_n\} + \sum_{\text{all contractions}} N\{A_1 A_2 \dots A_n\}. \quad (3.49)$$

A contraction with respect to the vacuum between  $A_1$  and  $A_2$  is symbolized by a dot

$$\dot{A}_1 \dot{A}_2, \quad (3.50)$$

and denotes a complex number if and only if the operators  $A_1$  and  $A_2$  are adjacent. If more contractions are involved in an expression, then one, two and more dots are used for distinction, e.g. a contraction between  $A_1$  and  $A_2$  respectively  $A_3$  and  $A_4$  is written as

$$\dot{A}_1 \dot{A}_2 \ddot{A}_3 \ddot{A}_4. \quad (3.51)$$

Normal ordering with a contraction between the operators  $A_i$  and  $A_j$  with  $i < j$

$$N\{A_1 A_2 \dots A_{i-1} \dot{A}_i A_{i+1} \dots A_{j-1} \dot{A}_j A_{j+1} \dots A_n\} \quad (3.52)$$

is defined to be evaluated in the following way: If the operators which should be contracted are already adjacent make use of the linearity of the normal-ordering operator (3.37). Otherwise, first make use of the antisymmetry of the normal-ordering operator (3.38) to bring the operators  $A_i$  and  $A_j$  adjacent with the additional condition that the original order of  $A_i$

and  $A_j$  is conserved, namely

$$\begin{aligned} & N\{A_1 A_2 \dots A_{i-1} \dot{A}_i A_{i+1} \dots A_{j-1} \dot{A}_j A_{j+1} \dots A_n\} \\ & := \text{sgn}(\pi) N\{A_1 A_2 \dots A_{i-1} \dot{A}_i \dot{A}_j A_{i+1} \dots A_{j-1} A_{j+1} \dots A_n\}, \end{aligned} \quad (3.53)$$

where  $\pi$  is a permutation that brings the operators  $A_i$  and  $A_j$  adjacent. Finally, making use of the linearity of the normal-ordering operator (3.37) one obtains

$$\begin{aligned} & N\{A_1 A_2 \dots A_{i-1} \dot{A}_i A_{i+1} \dots A_{j-1} \dot{A}_j A_{j+1} \dots A_n\} \\ & = \text{sgn}(\pi) \dot{A}_i \dot{A}_j N\{A_1 A_2 \dots A_{i-1} A_{i+1} \dots A_{j-1} A_{j+1} \dots A_n\}. \end{aligned} \quad (3.54)$$

This complicated definition is necessary because the contraction  $\dot{A}_i \dot{A}_j$  is in general not equal to  $\dot{A}_j \dot{A}_i$ .

A formula to calculate the contraction with respect to the vacuum appearing in Wick's theorem (3.49) will be derived. For that purpose, Wick's theorem (3.49) is applied to the product of two operators  $A_1$  and  $A_2$ , leading to

$$A_1 A_2 = N\{A_1 A_2\} + N\{\dot{A}_1 \dot{A}_2\} = N\{A_1 A_2\} + \dot{A}_1 \dot{A}_2. \quad (3.55)$$

Taking the vacuum expectation value and making use of (3.41), a formula for the contraction can be derived

$$\dot{A}_1 \dot{A}_2 = \langle 0 | A_1 A_2 | 0 \rangle. \quad (3.56)$$

Since the vacuum expectation value of the product of the operators  $A_1$  and  $A_2$  is in general neither symmetric nor antisymmetric under permutation of  $A_1$  and  $A_2$ , the contraction  $\dot{A}_1 \dot{A}_2$  is in general not proportional to  $\dot{A}_2 \dot{A}_1$ . This observation justifies the complicated definition (3.53).

It immediately follows from (3.56)

$$\dot{a}_q \dot{a}^p = \langle 0 | a_q a^p | 0 \rangle = \delta_q^p \quad (3.57)$$

and for all other combinations

$$\dot{a}^p \dot{a}_q = \dot{a}_p \dot{a}_q = \dot{a}^p \dot{a}^q = 0. \quad (3.58)$$

In the following, these vanishing contractions will be neglected. From now on, the normal-ordering transformation can be performed by means of Wick's theorem in a sophisticated and systematic way. The application of Wick's theorem on the same example as in (3.48)

leads to

$$\begin{aligned} a_q a_s a^p &= N\{a_q a_s a^p\} + N\{a_q \dot{a}_s \dot{a}^p\} + N\{\dot{a}_q a_s \dot{a}^p\} \\ &= a^p a_q a_s + \delta_s^p a_q - \delta_q^p a_s, \end{aligned} \quad (3.59)$$

which is equal to the result in (3.48).

It should be noted that the vacuum expectation value of a product of operators  $A_1, A_2, \dots, A_n$  can be calculated by the sum of all full contractions, i.e.

$$\langle 0 | A_1 A_2 \dots A_n | 0 \rangle = \sum_{\text{full contractions}} N\{A_1 A_2 \dots A_n\}. \quad (3.60)$$

A full contraction is a contraction where all operators are contracted among each other. For instance, the vacuum expectation of the product  $a_q a_s a^p a^r$  is given by

$$\begin{aligned} \langle 0 | a_q a_s a^p a^r | 0 \rangle &= N\{\dot{a}_q \ddot{a}_s \ddot{a}^p \dot{a}^r\} + N\{\dot{a}_q \ddot{a}_s \dot{a}^p \ddot{a}^r\} \\ &= \delta_s^p \delta_q^r - \delta_q^p \delta_s^r, \end{aligned} \quad (3.61)$$

because all not fully-contracted terms vanish. Formula (3.60) can be derived by means of Wick's theorem (3.49) and the property of the normal-ordering operator (3.41).

### 3.4. Normal Ordering and Wick's Theorem with respect to a Single-Reference State

In the following section, the normal-ordering concept will be extended to a single-reference (SR) state, which is a single Slater determinant. In general the state used for the normal ordering is called reference state. Up to now, the reference state was the vacuum. The basic idea is to redefine the creation and annihilation operators using the particle-hole formalism, which will be introduced in the following.

#### 3.4.1. Normal Ordering with respect to a Single-Reference State

Let  $|\phi\rangle$  be an  $A$ -body single-reference state, i.e. a single Slater determinant

$$|\phi\rangle = \prod_{i=1}^A a^i |0\rangle. \quad (3.62)$$

Furthermore, let the occupied single-particle states

$$a^i |0\rangle \quad \text{with } i = 1, 2, \dots, A \quad (3.63)$$

and the unoccupied single-particle states

$$a^b |0\rangle \quad \text{with } b > A \quad (3.64)$$

form an orthonormal basis  $\{a^p |0\rangle : p = 1, 2, \dots\}$ . Conventionally, the indices  $i, j, k, \dots$  are called hole indices, while the indices  $b, c, d, \dots$  are called particle indices. The indices  $p, q, r, \dots$  can refer to both. This is basically the particle-hole formalism.

Acting with the operator  $a^i$  on the reference state  $|\phi\rangle$ , due to Pauli exclusion principle that leads to

$$a^i |\phi\rangle = 0. \quad (3.65)$$

Per definition, it holds

$$a_b |\phi\rangle = 0. \quad (3.66)$$

Since these operators act like annihilation operator with respect to the reference state  $|\phi\rangle$ , they are redefined to quasiparticle annihilators. On the other hand, the operators  $a_i$  and  $a^b$  create a hole and a particle, relatively. Hence, they are redefined to quasiparticle creators.

Now, normal ordering with respect to a single-reference state  $|\phi\rangle$  can be defined in analogy to the vacuum case.

**Definition 3.5.** A product of operators is in normal order with respect to a single-reference state  $|\phi\rangle$ , briefly an operator in SR-NO, if all quasiparticle creators are to the left of all quasiparticle annihilators.

Thus, for the mathematical description a normal-ordering operator  $\mathcal{N}_{\text{SR}}$  with respect to a single-reference state  $|\phi\rangle$  can be defined. In order to distinguish this operator from the normal-ordering operator with respect to the vacuum from [definition 3.4](#) a different symbol is used.

As before, linearity means, that for a complex number  $\lambda$  and two operators  $C$  and  $D$ , it is

$$\begin{aligned} \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_j (\lambda C + D) A_{j+1} \dots A_n\} &= \lambda \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_j C A_{j+1} \dots A_n\} \\ &+ \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_j D A_{j+1} \dots A_n\}. \end{aligned} \quad (3.67)$$

Antisymmetry means, that for all  $i, j$  with  $i \neq j$

$$\mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_i \dots A_j \dots A_n\} = -\mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_j \dots A_i \dots A_n\}. \quad (3.68)$$

The requirement, that the identity operator of the antisymmetric Fock space  $\hat{1}$  is mapped by  $\mathcal{N}_{\text{SR}}$  on itself, is made here, too. As a consequence, the normal-ordering operator  $\mathcal{N}_{\text{SR}}$  leaves a complex number  $\lambda$  unchanged, i.e.

$$\mathcal{N}_{\text{SR}}\{\lambda\} = \lambda. \quad (3.69)$$

For any product of operators  $A_1, A_2 \dots A_n$  the expectation value regarding the reference state

$|\phi\rangle$  of an operator in SR-NO vanishes, i.e.

$$\langle\phi|\mathcal{N}_{\text{SR}}\{A_1A_2\dots A_n\}|\phi\rangle=0. \quad (3.70)$$

Some examples are listed here in order to demonstrate the action of the normal-ordering operator  $\mathcal{N}_{\text{SR}}$ :

$$\mathcal{N}_{\text{SR}}\{a^i a_j\} = -a_j a^i, \quad (3.71)$$

$$\mathcal{N}_{\text{SR}}\{a_b a^c\} = -a^c a_b, \quad (3.72)$$

$$\mathcal{N}_{\text{SR}}\{a^i a_b\} = a^i a_b, \quad (3.73)$$

$$\mathcal{N}_{\text{SR}}\{a_b a_j\} = -a_j a_b. \quad (3.74)$$

### 3.4.2. Wick's Theorem with respect to a Single-Reference State

Wick's theorem with respect to a single-reference state  $|\phi\rangle$  (SR-WT) can be formulated analogously to the vacuum case: A product of  $n$  operators  $A_1, A_2, \dots, A_n$  can be expressed as a sum of operators in SR-NO including all (possible) contractions with respect to  $|\phi\rangle$  [Muk97]

$$A_1 A_2 \dots A_n = \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_n\} + \sum_{\text{all contractions}} \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_n\}. \quad (3.75)$$

A contraction with respect to  $|\phi\rangle$  between  $A_1$  and  $A_2$  is indicated by

$$\overline{A_1 A_2}. \quad (3.76)$$

It should be noted that a different symbol is used here not to get confused with the contraction with respect to the vacuum (3.50). This contraction also denotes a complex number if and only if the operators  $A_1$  and  $A_2$  are adjacent.

Normal ordering with a contraction between the operators  $A_i$  and  $A_j$  with  $i < j$

$$\mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_{i-1} \overline{A_i A_{i+1} \dots A_{j-1} A_j} A_{j+1} \dots A_n\} \quad (3.77)$$

has to be evaluated exactly as in the vacuum case in section 3.3.1: If the operators which should be contracted are already adjacent make use of the linearity of the normal-ordering operator (3.67). Otherwise, first make use of the antisymmetry of the normal-ordering operator (3.68) to bring the operators  $A_i$  and  $A_j$  adjacent with the additional condition that the original order of  $A_i$  and  $A_j$  is conserved, namely

$$\begin{aligned} & \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_{i-1} \overline{A_i A_{i+1} \dots A_{j-1} A_j} A_{j+1} \dots A_n\} \\ & := \text{sgn}(\pi) \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_{i-1} \overline{A_i A_j} A_{i+1} \dots A_{j-1} A_{j+1} \dots A_n\}, \end{aligned} \quad (3.78)$$

where  $\pi$  is a permutation that brings the operators  $A_i$  and  $A_j$  adjacent. Finally, making use of the linearity of the normal-ordering operator (3.67) one obtains

$$\begin{aligned} & \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_{i-1} \overbrace{A_i A_{i+1} \dots A_{j-1} A_j A_{j+1} \dots A_n} \} \\ &= \text{sgn}(\pi) \overbrace{A_i A_j} \mathcal{N}_{\text{SR}}\{A_1 A_2 \dots A_{i-1} A_{i+1} \dots A_{j-1} A_{j+1} \dots A_n\}. \end{aligned} \quad (3.79)$$

### 3.4.3. Formula for the Contraction

In order to derive a formula for the contraction with respect to  $|\phi\rangle$ , the SR-WT is applied to a product of two operators  $A_1$  and  $A_2$  which leads to

$$A_1 A_2 = \mathcal{N}_{\text{SR}}\{A_1 A_2\} + \overbrace{A_1 A_2} = \mathcal{N}_{\text{SR}}\{A_1 A_2\} + \overbrace{A_1 A_2}. \quad (3.80)$$

Taking the expectation value regarding  $|\phi\rangle$  of (3.80), a formula for the contraction with respect to  $|\phi\rangle$

$$\overbrace{A_1 A_2} = \langle \phi | A_1 A_2 | \phi \rangle \quad (3.81)$$

can be derived with the aid of (3.70). One defines a hole contraction as

$$\overbrace{a^p a_q} = \langle \phi | a^p a_q | \phi \rangle =: \gamma_q^p, \quad (3.82)$$

which describes an one-particle density matrix element  $\gamma_q^p$ , and a particle contraction as

$$\overbrace{a_q a^p} = \langle \phi | a_q a^p | \phi \rangle =: \eta_q^p, \quad (3.83)$$

which describes an one-hole density matrix element  $\eta_q^p$ . All other combinations given by

$$\overbrace{a^p a^q} = \overbrace{a_p a_q} = 0 \quad (3.84)$$

vanish for all  $p$  and  $q$ . Especially for a single-reference state, the one-particle and one-hole density matrix elements can be calculated via

$$\gamma_q^p = \delta_q^p n_q, \quad (3.85)$$

$$\eta_q^p = \delta_q^p (1 - n_q) = \delta_q^p - \gamma_q^p, \quad (3.86)$$

with the occupation number

$$n_q = \begin{cases} 1, & \text{if } q \text{ occupied,} \\ 0, & \text{if } q \text{ unoccupied.} \end{cases} \quad (3.87)$$

A hole contraction has only a non-vanishing contribution if both indices  $p$  and  $q$  are hole indices ( $i, j, \dots$ ). The analogous statement holds for the particle contraction. In other

words, any mixing of particle and hole indices always leads to vanishing contraction. This justifies the naming convention of these two types of contractions.

A general relationship between a contraction with respect to  $|\phi\rangle$  and  $|0\rangle$  can be derived. Taking the expectation value of (3.55) leads to

$$\langle\phi|A_1A_2|\phi\rangle = \langle\phi|N\{A_1A_2\}|\phi\rangle + \dot{A}_1\dot{A}_2. \quad (3.88)$$

Hence, the general relationship between the contraction with respect to  $|\phi\rangle$  and  $|0\rangle$  is

$$\overline{A_1A_2} = \langle\phi|N\{A_1A_2\}|\phi\rangle + \dot{A}_1\dot{A}_2. \quad (3.89)$$

Choosing  $A_1 = a_q$  and  $A_2 = a^p$ , a general relationship between a particle and hole contraction can be found

$$\begin{aligned} \overline{a_q a^p} &= \langle\phi|N\{a_q a^p\}|\phi\rangle + \dot{a}_q \dot{a}^p \\ &= -\langle\phi|a^p a_q|\phi\rangle + \dot{a}_q \dot{a}^p \\ &= -\overline{a^p a_q} + \delta_q^p, \end{aligned} \quad (3.90)$$

which is equivalent to (3.86).

#### 3.4.4. Results for the One-, Two- and Three-Body Operators

In order to make the statement of Wick's theorem (3.75) clear some examples for the one-, two- and three-body operators will be shown. The simplest example, which is a product of two operators  $A_1$  and  $A_2$ , has already been expressed in (3.80), and leads in the special case of  $A_1 = a^p$  and  $A_2 = a_q$ , to

$$\begin{aligned} a_q^p &= a^p a_q \\ &= \mathcal{N}_{\text{SR}}\{a_q^p\} + \gamma_q^p. \end{aligned} \quad (3.91)$$

Applying Wick's theorem with respect to  $|\phi\rangle$  to a product of four operators leads to

$$\begin{aligned} A_1 A_2 A_3 A_4 &= \mathcal{N}_{\text{SR}}\{A_1 A_2 A_3 A_4\} \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \overline{A_{\pi(1)} A_{\pi(2)}} \mathcal{N}_{\text{SR}}\{A_{\pi(3)} A_{\pi(4)}\} \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \mathcal{N}_{\text{SR}}\{A_{\pi(1)} A_{\pi(2)}\} \overline{A_{\pi(3)} A_{\pi(4)}} \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \overline{A_{\pi(1)} A_{\pi(2)}} \overline{A_{\pi(3)} A_{\pi(4)}}, \end{aligned} \quad (3.92)$$

where  $\text{sgn}(\pi)$  is the sign of the permutation  $\pi$  containing in the set of permutation

$$\Pi := \left\{ \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 2 & 4 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 2 & 3 \end{pmatrix} \right\}. \quad (3.93)$$

For a special choice of  $A_1, A_2, A_3$  and  $A_4$ , one obtains

$$\begin{aligned} a_{qs}^{pr} &= a^p a^r a_s a_q \\ &= \mathcal{N}_{\text{SR}}\{a_{qs}^{pr}\} + \gamma_q^p \mathcal{N}_{\text{SR}}\{a_s^r\} + \gamma_s^r \mathcal{N}_{\text{SR}}\{a_q^p\} - \gamma_s^p \mathcal{N}_{\text{SR}}\{a_q^r\} - \gamma_q^r \mathcal{N}_{\text{SR}}\{a_s^p\} + \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r. \end{aligned} \quad (3.94)$$

All terms containing exactly one contraction can be written in the compact form using the index antisymmetrizer of [section 3.2](#), namely

$$\begin{aligned} \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_s^r\}) &= \mathcal{N}_{\text{SR}}\{\mathbb{A}(\gamma_q^p a_s^r)\} \\ &= \mathcal{N}_{\text{SR}}\{\gamma_q^p a_s^r + \gamma_s^r a_q^p - \gamma_s^p a_q^r - \gamma_q^r a_s^p\} \\ &= \gamma_q^p \mathcal{N}_{\text{SR}}\{a_s^r\} + \gamma_s^r \mathcal{N}_{\text{SR}}\{a_q^p\} - \gamma_s^p \mathcal{N}_{\text{SR}}\{a_q^r\} - \gamma_q^r \mathcal{N}_{\text{SR}}\{a_s^p\}, \end{aligned} \quad (3.95)$$

where the linearity of the index antisymmetrizer and of the normal-ordering operator have been exploited. Furthermore, the fully-contracted terms are equivalent to the two-body density matrix element regarding a single-reference state  $|\phi\rangle$  given by

$$\gamma_{qs}^{pr} := \langle \phi | a_{qs}^{pr} | \phi \rangle = \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r. \quad (3.96)$$

Hence, [\(3.94\)](#) can be simplified to

$$a_{qs}^{pr} = \mathcal{N}_{\text{SR}}\{a_{qs}^{pr}\} + \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_s^r\}) + \gamma_{qs}^{pr}. \quad (3.97)$$

The final example is a product of six operators  $A_1, A_2, \dots, A_6$ , which can be written by means of SR-WT as follows:

$$\begin{aligned} A_1 A_2 A_3 A_4 A_5 A_6 &= \mathcal{N}_{\text{SR}}\{A_1 A_2 A_3 A_4 A_5 A_6\} \\ &\quad + \mathcal{N}_{\text{SR}}\{\overbrace{A_1 A_2 A_3 A_4 A_5 A_6}^{\quad}\} + \dots \\ &\quad + \mathcal{N}_{\text{SR}}\{\overbrace{A_1 A_2 A_3 A_4 A_5 A_6}^{\quad}\} + \dots \\ &\quad + \mathcal{N}_{\text{SR}}\{\overbrace{A_1 A_2 A_3 A_4 A_5 A_6}^{\quad}\} + \dots \end{aligned} \quad (3.98)$$

The special case  $A_1 = a^p, A_2 = a^r, A_3 = a^t, A_4 = a_u, A_5 = a_s$  and  $A_6 = a_q$  is of interest for this work.

By means of the index antisymmetrizer, all terms containing only one contraction in [\(3.98\)](#)

can be written as

$$\begin{aligned}
 \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_{su}^{rt}\}) &= +\gamma_q^p \mathcal{N}_{\text{SR}}\{a_{su}^{rt}\} - \gamma_s^p \mathcal{N}_{\text{SR}}\{a_{qu}^{rt}\} - \gamma_u^p \mathcal{N}_{\text{SR}}\{a_{sq}^{rt}\} \\
 &\quad - \gamma_q^r \mathcal{N}_{\text{SR}}\{a_{su}^{pt}\} + \gamma_s^r \mathcal{N}_{\text{SR}}\{a_{qu}^{pt}\} - \gamma_u^r \mathcal{N}_{\text{SR}}\{a_{qs}^{pt}\} \\
 &\quad - \gamma_q^t \mathcal{N}_{\text{SR}}\{a_{us}^{pr}\} - \gamma_s^t \mathcal{N}_{\text{SR}}\{a_{qu}^{pr}\} + \gamma_u^t \mathcal{N}_{\text{SR}}\{a_{qs}^{pr}\}.
 \end{aligned} \tag{3.99}$$

Furthermore, all terms involving two contractions in (3.98) can be expressed with the aid of the index antisymmetrizer and the two-body density matrix element with respect to a single-reference state as follows:

$$\begin{aligned}
 \mathbb{A}(\gamma_{qs}^{pr} \mathcal{N}_{\text{SR}}\{a_u^t\}) &= +(\gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r) \mathcal{N}_{\text{SR}}\{a_u^t\} - (\gamma_q^p \gamma_u^r - \gamma_u^p \gamma_q^r) \mathcal{N}_{\text{SR}}\{a_s^t\} - (\gamma_u^p \gamma_s^r - \gamma_s^p \gamma_u^r) \mathcal{N}_{\text{SR}}\{a_q^t\} \\
 &\quad - (\gamma_q^p \gamma_s^t - \gamma_s^p \gamma_q^t) \mathcal{N}_{\text{SR}}\{a_u^r\} + (\gamma_q^p \gamma_u^t - \gamma_u^p \gamma_q^t) \mathcal{N}_{\text{SR}}\{a_s^r\} - (\gamma_s^p \gamma_u^t - \gamma_u^p \gamma_s^t) \mathcal{N}_{\text{SR}}\{a_q^r\} \\
 &\quad - (\gamma_s^r \gamma_q^t - \gamma_q^r \gamma_s^t) \mathcal{N}_{\text{SR}}\{a_u^p\} - (\gamma_q^r \gamma_u^t - \gamma_u^r \gamma_q^t) \mathcal{N}_{\text{SR}}\{a_s^p\} + (\gamma_s^r \gamma_u^t - \gamma_u^r \gamma_s^t) \mathcal{N}_{\text{SR}}\{a_q^p\}.
 \end{aligned} \tag{3.100}$$

All terms involving three contractions in (3.98) are equivalent to the three-body density matrix element with respect to a single-reference state  $|\phi\rangle$

$$\begin{aligned}
 \gamma_{qsu}^{prt} &:= \langle \phi | a_{qsu}^{prt} | \phi \rangle \\
 &= +\gamma_q^p \gamma_s^r \gamma_u^t + \gamma_u^p \gamma_q^r \gamma_s^t + \gamma_s^p \gamma_u^r \gamma_q^t - \gamma_q^p \gamma_u^r \gamma_s^t - \gamma_s^p \gamma_q^r \gamma_u^t - \gamma_u^p \gamma_s^r \gamma_q^t.
 \end{aligned} \tag{3.101}$$

Putting all intermediate results together leads to

$$a_{qsu}^{prt} = \mathcal{N}_{\text{SR}}\{a_{qsu}^{prt}\} + \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_{su}^{rt}\}) + \mathbb{A}(\gamma_{qs}^{pr} \mathcal{N}_{\text{SR}}\{a_u^t\}) + \gamma_{qsu}^{prt}. \tag{3.102}$$

Summarizing all examples, one obtains

$$a_q^p = \mathcal{N}_{\text{SR}}\{a_q^p\} + \gamma_q^p, \tag{3.103}$$

$$a_{qs}^{pr} = \mathcal{N}_{\text{SR}}\{a_{qs}^{pr}\} + \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_s^r\}) + \gamma_{qs}^{pr}, \tag{3.104}$$

$$a_{qsu}^{prt} = \mathcal{N}_{\text{SR}}\{a_{qsu}^{prt}\} + \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_{su}^{rt}\}) + \mathbb{A}(\gamma_{qs}^{pr} \mathcal{N}_{\text{SR}}\{a_u^t\}) + \gamma_{qsu}^{prt}. \tag{3.105}$$

The operators  $\mathcal{N}_{\text{SR}}\{a_q^p\}$ ,  $\mathcal{N}_{\text{SR}}\{a_{qs}^{pr}\}$  and  $\mathcal{N}_{\text{SR}}\{a_{qsu}^{prt}\}$  are defined as the one-, two- and three-body operator in SR-NO. One can easily check that the expectation value regarding  $|\phi\rangle$  of these operators vanish, i.e.

$$\langle \phi | \mathcal{N}_{\text{SR}}\{a_q^p\} | \phi \rangle = \langle \phi | (a_q^p - \gamma_q^p) | \phi \rangle = \langle \phi | a_q^p | \phi \rangle - \gamma_q^p = \gamma_q^p - \gamma_q^p = 0, \tag{3.106}$$

$$\begin{aligned}
 \langle \phi | \mathcal{N}_{\text{SR}}\{a_{qs}^{pr}\} | \phi \rangle &= \langle \phi | a_{qs}^{pr} | \phi \rangle - \langle \phi | \mathbb{A}(\gamma_q^p \mathcal{N}_{\text{SR}}\{a_s^r\}) | \phi \rangle - \gamma_{qs}^{pr} \\
 &= \gamma_{qs}^{pr} - \mathbb{A}(\gamma_q^p \langle \phi | \mathcal{N}_{\text{SR}}\{a_s^r\} | \phi \rangle) - \gamma_{qs}^{pr} = \gamma_{qs}^{pr} - 0 - \gamma_{qs}^{pr} = 0,
 \end{aligned}$$

$$\langle \phi | \mathcal{N}_{\text{SR}}\{a_{qsu}^{prt}\} | \phi \rangle = \langle \phi | a_{qsu}^{prt} | \phi \rangle - 0 - 0 - \gamma_{qsu}^{prt} = \gamma_{qsu}^{prt} - \gamma_{qsu}^{prt} = 0. \tag{3.107}$$

Equation (3.105) is basically the starting point of the normal-ordering approximation with respect to a single-reference state for any 3N interaction [Rot<sup>+</sup>12]. It allows to define systematically an approximate lower-particle-rank form of any 3N interaction by neglecting the three-body operator in SR-NO (it will be explicitly demonstrated in chapter 4). These approximations are called SR-NO $n$ B approximation, where  $n < 3$  is the highest particle rank included.

In analogy to the vacuum case, the expectation value regarding a single-reference state  $|\phi\rangle$  of a product of operators  $A_1, A_2, \dots, A_n$  can be calculated by the sum of all full contractions with respect to  $|\phi\rangle$ , i.e.

$$\langle\phi|A_1A_2\dots A_n|\phi\rangle = \sum_{\substack{\text{full contractions} \\ \text{w.r.t. } |\phi\rangle}} \mathcal{N}_{\text{SR}}\{A_1A_2\dots A_n\}. \quad (3.108)$$

This formula can be derived by means of Wick's theorem (3.75) and the property of the normal-ordering operator (3.70).

### 3.5. Normal Ordering and Wick's Theorem with respect to a Multi-Reference State

The normal-ordering concept provides a convenient tool to derive approximations of any 3N interaction. Since the normal ordering with respect to a single-reference state is limited to closed-shell nuclei, it is desirable to extend the normal-ordering concept to open-shell systems using a multi-reference state, i.e. a linear combination of single Slater determinants. This is the aim of this section.

In the whole section the following requirements are made: Let  $\mathcal{H}_n$  be a finite-dimensional subspace of the  $A$ -body Hilbert space  $\mathcal{H}$ , and  $\{|\phi_i\rangle : i = 1, \dots, n\}$  be a complete orthonormal basis of  $\mathcal{H}_n$ . Furthermore, let  $|\Psi\rangle \in \mathcal{H}_n$  be a normalized  $A$ -body state

$$|\Psi\rangle := \sum_{i=1}^n c_i |\phi_i\rangle, \quad (3.109)$$

with  $c_i \in \mathbb{C}$  and single Slater determinants  $|\phi_i\rangle$ .

As a reminder,  $A_1, A_2, \dots, A_n$  are pairwise distinct fermionic operators each of them representing either a creation operator  $a^p$  or an annihilation operator  $a_q$ .

#### 3.5.1. Problem and Guiding Principle

The “traditional” definition of normal ordering says, that a product of operators is in normal order with respect to a reference state, if all (quasiparticle) creation operators are to the left of all (quasiparticle) annihilation operators. This statement is no longer useful for a multi-reference state  $|\Psi\rangle$ . The reason is, that in general for all  $i$  and  $j \neq i$  there is a single-particle state  $p$  occupied in the  $i$ -th single Slater determinant and unoccupied in the  $j$ -th single Slater

determinant, i.e.

$$a^p |\phi_i\rangle = 0, \quad (3.110)$$

$$a^p |\phi_j\rangle \neq 0. \quad (3.111)$$

Consequently, the operator  $a^p$  is a (quasiparticle) annihilation operator with respect to  $|\phi_i\rangle$  and (quasiparticle) creation operator with respect to  $|\phi_j\rangle$ . Hence, it is not obvious how to define normal ordering with respect to  $|\Psi\rangle$ . This simple observation implies that one has to give up the “traditional” definition of normal-ordering. Normal ordering has to be understood as an abstract process (defined in following [section 3.5.2](#)), and normal-ordering transformation is defined only in the framework of a Wick-like theorem.

For the generalization of Wick's theorem with respect to a multi-reference state  $|\Psi\rangle$  some requirements have to be fulfilled:

- (I) If an operator  $X \neq \hat{1}$  is in normal order with respect to  $|\Psi\rangle$ , briefly an operator in MR-NO, then the expectation value regarding  $|\Psi\rangle$  of  $X$

$$\langle \Psi | X | \Psi \rangle = 0 \quad (3.112)$$

has to vanish. The opposite direction of this statement is in general wrong.

- (II) In the special case of  $|\Psi\rangle$  consisting of a single Slater determinant, the well-known normal-ordering with respect to a single-reference state must reappear.

A generalization fulfilling both requirements was proposed and proven by Mukherjee and Kutzelnigg [[Muk97](#); [KM97](#); [KNM10](#)], and formulated in form of a Wick-like theorem with respect to a multi-reference state (MR-WT). The statement will be formulated in [section 3.5.3](#).

### 3.5.2. Introduction of the Normal-Ordering Operator

For the mathematical formulation of the normal ordering with respect to a multi-reference state  $|\Psi\rangle$  a normal-ordering operator  $\mathcal{N}$  is introduced. In order not to be confused with the normal-ordering operator with respect to the vacuum and single-reference state, a different symbol is used. This definition is more abstract, i.e. it does not correspond to reordering by transferring creation operators to the left of all annihilation operators. But the normal-ordering operator  $\mathcal{N}$  is required to be linear, antisymmetric and maps the identity operator  $\hat{1}$  on itself:

Let  $\lambda$  be a complex number,  $C$  and  $D$  be operators. Linearity states

$$\begin{aligned} \mathcal{N}\{A_1 A_2 \dots A_j (\lambda C + D) A_{j+1} \dots A_n\} &= \lambda \mathcal{N}\{A_1 A_2 \dots A_j C A_{j+1} \dots A_n\} \\ &+ \mathcal{N}\{A_1 A_2 \dots A_j D A_{j+1} \dots A_n\}. \end{aligned} \quad (3.113)$$

Antisymmetry means, that for all  $i, j$  with  $i \neq j$

$$\mathcal{N}\{A_1 A_2 \dots A_i \dots A_j \dots A_n\} = -\mathcal{N}\{A_1 A_2 \dots A_j \dots A_i \dots A_n\} \quad (3.114)$$

holds. The requirement, that the identity operator of the antisymmetric Fock space  $\hat{1}$  is mapped by  $\mathcal{N}$  on itself, is made here, too. As a consequence, the normal-ordering operator  $\mathcal{N}$  leaves a complex number  $\lambda$  unchanged, i.e.

$$\mathcal{N}\{\lambda\} = \lambda. \quad (3.115)$$

To emphasize the abstract definition of the normal-ordering operator  $\mathcal{N}$ , its action on the one-, two- and three-body operator will be denoted as

$$\tilde{a}_q^p := \mathcal{N}\{a_q^p\}, \quad (3.116)$$

$$\tilde{a}_{qs}^{pr} := \mathcal{N}\{a_{qs}^{pr}\}, \quad (3.117)$$

$$\tilde{a}_{qsu}^{prt} := \mathcal{N}\{a_{qsu}^{prt}\}, \quad (3.118)$$

and are called the one-, two- and three-body operators in MR-NO. The goal is to express the one-, two- and three-body operators as sums of the one-, two- and three-body operators in MR-NO. For that purpose, the MR-WT will be formulated and used in the next subsection.

### 3.5.3. Wick's Theorem with respect to a Multi-Reference State

According to the statement of Wick's theorem with respect to a multi-reference state  $|\Psi\rangle$  (MR-WT), a product of  $n$  operators  $A_1, A_2, \dots, A_n$  can be expressed as a sum of operators in MR-NO including all (possible) contractions with respect to  $|\Psi\rangle$  [KM97; Muk97]

$$A_1 A_2 \dots A_n = \mathcal{N}\{A_1 A_2 \dots A_n\} + \sum_{\text{all contractions}} \mathcal{N}\{A_1 A_2 \dots A_n\}. \quad (3.119)$$

A contraction with respect to  $|\Psi\rangle$  between  $A_1$  and  $A_2$  is denoted by

$$\overline{A_1 A_2}. \quad (3.120)$$

It should be noted that a different symbol is used here not to be confused with the contraction with respect to the vacuum (3.50) and a single-reference state (3.76). This contraction also yields a complex number if and only if the operators  $A_1$  and  $A_2$  are adjacent.

The new key statement of the MR-WT is that a contraction between  $l$  operators, called  $l$ -tuple contraction, is also possible, which is denoted as

$$\overline{A_1 A_2 \dots A_l}, \quad (3.121)$$

where  $l$  is positive natural number less or equal than  $n$ . This  $l$ -tuple contraction is also just a complex number if and only if all operators, which are contracted, are adjacent.

On the one hand, normal ordering with an  $l$ -tuple contraction ( $l > 2$ ) can be directly calculated making use of the antisymmetry and linearity of the normal-ordering operator. On the other hand, normal ordering with a 2-tuple contraction has to be defined carefully. Normal ordering with a contraction between two operators  $A_i$  and  $A_j$  ( $i < j$ )

$$\mathcal{N}\{A_1 A_2 \dots A_{i-1} \overline{A_i} A_{i+1} \dots A_{j-1} \overline{A_j} A_{j+1} \dots A_n\} \quad (3.122)$$

has to be evaluated exactly as in the vacuum case of [section 3.3.1](#) and single-reference case in [section 3.4.1](#): If the operators which should be contracted are already adjacent make use of the linearity of the normal-ordering operator [\(3.113\)](#). Otherwise, first make use of the antisymmetry of the normal-ordering operator [\(3.114\)](#) to bring the operators  $A_i$  and  $A_j$  adjacent with the additional condition that the original order of  $A_i$  and  $A_j$  is conserved, namely

$$\begin{aligned} & \mathcal{N}\{A_1 A_2 \dots A_{i-1} \overline{A_i} A_{i+1} \dots A_{j-1} \overline{A_j} A_{j+1} \dots A_n\} \\ & := \text{sgn}(\pi) \mathcal{N}\{A_1 A_2 \dots A_{i-1} \overline{A_i} \overline{A_j} A_{i+1} \dots A_{j-1} A_{j+1} \dots A_n\}, \end{aligned} \quad (3.123)$$

where  $\pi$  is a permutation that brings the operators  $A_i$  and  $A_j$  adjacent. Finally, using the linearity of the normal-ordering operator [\(3.113\)](#) one obtains

$$\begin{aligned} & \mathcal{N}\{A_1 A_2 \dots A_{i-1} \overline{A_i} A_{i+1} \dots A_{j-1} \overline{A_j} A_{j+1} \dots A_n\} \\ & = \text{sgn}(\pi) \overline{A_i} \overline{A_j} \mathcal{N}\{A_1 A_2 \dots A_{i-1} A_{i+1} \dots A_{j-1} A_{j+1} \dots A_n\}. \end{aligned} \quad (3.124)$$

It should be noted that the expectation value regarding a multi-reference state  $|\Psi\rangle$  of a product of operators  $A_1, A_2, \dots, A_n$  can be calculated by the sum of all full contractions with respect to  $|\Psi\rangle$ , i.e.

$$\langle \Psi | A_1 A_2 \dots A_n | \Psi \rangle = \sum_{\substack{\text{full contractions} \\ \text{w.r.t. } |\Psi\rangle}} \mathcal{N}\{A_1 A_2 \dots A_n\}. \quad (3.125)$$

This formula can be derived by means of Wick's theorem [\(3.119\)](#) and the property of the normal-ordering operator [\(3.112\)](#).

In order to make use of the MR-WT, one needs to derive formulas for these  $l$ -tuple contractions. Since the number of possible contractions is very large, properties of the  $l$ -tuple contraction will be analyzed in the next section before deriving formulas for the relevant cases in [section 3.5.5](#).

### 3.5.4. Particle-Number Non-Conserving $l$ -Tuple Contractions

Before analyzing the properties of the  $l$ -tuple contractions, some important definitions have to be made [\[Muk97\]](#).

**Definition 3.6.** The effective creation rank of a product of operators  $A_1, A_2, \dots, A_l$  is defined as the number of creation operators minus the number of annihilation operators and will be

denoted as

$$\text{ecr}(A_1 A_2 \dots A_l). \quad (3.126)$$

**Definition 3.7.** A product of operators  $A_1, A_2, \dots, A_l$  is called a particle-number conserving operator if

$$\text{ecr}(A_1 A_2 \dots A_l) = 0, \quad (3.127)$$

i.e. the product contains the same number of creation and annihilation operators. Otherwise, it is called particle-number non-conserving.

**Definition 3.8.** An  $l$ -tuple contraction  $\overline{A_1 A_2 \dots A_l}$  is called to be particle-number conserving if

$$\text{ecr}(A_1 A_2 \dots A_l) = 0, \quad (3.128)$$

otherwise particle-number non-conserving.

**Proposition 3.1.** *If a product of operators  $A_1, A_2, \dots, A_l$  is particle-number non-conserving, then the  $l$ -tuple contraction vanishes, i.e.*

$$\text{ecr}(A_1 A_2 \dots A_l) \neq 0 \implies \overline{A_1 A_2 \dots A_l} = 0. \quad (3.129)$$

*Proof.* The proof is separated into two parts. First, assume that  $l$  is odd, and prove [proposition 3.1](#) inductively. It is started by the basis step for a product of  $l = 3$  operators: According to MR-WT, one obtains

$$\begin{aligned} A_1 A_2 A_3 &= \mathcal{N}\{A_1 A_2 A_3\} + \mathcal{N}\{\overline{A_1 A_2} A_3\} + \mathcal{N}\{\overline{A_1 A_2} \overline{A_3}\} + \mathcal{N}\{A_1 \overline{A_2 A_3}\} + \mathcal{N}\{\overline{A_1 A_2} \overline{A_3}\} \\ &= \mathcal{N}\{A_1 A_2 A_3\} + \overline{A_1 A_2} \mathcal{N}\{A_3\} - \overline{A_1 A_3} \mathcal{N}\{A_2\} + \overline{A_2 A_3} \mathcal{N}\{A_1\} + \overline{A_1 A_2} \overline{A_3}. \end{aligned} \quad (3.130)$$

Taking the expectation regarding  $|\Psi\rangle$  of [\(3.130\)](#) and using requirement [\(3.112\)](#), it follows

$$\langle \Psi | A_1 A_2 A_3 | \Psi \rangle = \overline{A_1 A_2 A_3}.$$

Since  $|\Psi\rangle$  has a well-defined particle number, the expectation value regarding  $|\Psi\rangle$  of a product of three operators vanishes. Hence, the 3-tuple contraction results in

$$\overline{A_1 A_2 A_3} = 0.$$

In the inductive step, one needs to prove that [proposition 3.1](#) is true for the odd number  $l + 2$ , while assuming it is valid for all odd numbers  $l' < l + 2$ : According to [\(3.125\)](#), the expectation value regarding  $|\Psi\rangle$  of the product of  $l + 2$  operators can be expressed as a sum

of all fully-contracted terms with respect to  $|\Psi\rangle$

$$\langle \Psi | A_1 A_2 \dots A_{l+2} | \Psi \rangle = \sum_{\substack{\text{full contractions} \\ \text{w.r.t. } |\Psi\rangle}} \mathcal{N}\{A_1 A_2 \dots A_{l+2}\}. \quad (3.131)$$

The left side of (3.131) vanishes trivially. All terms on the right hand side of (3.131), except for the  $l+2$ -tuple contraction, contain at least one  $l'$ -tuple contraction while  $l'$  is an odd number less than  $l+2$ . Due to induction hypothesis, those terms disappear. Putting both results together, proposition 3.1 is proven for the case that  $l$  is odd.

Second, assume that  $l$  is even and  $\text{ecr}(A_1 A_2 \dots A_l) \neq 0$ . The proof will be carried out inductively, too. According to MR-WT, the product of two operators  $A_1$  and  $A_2$  can be expressed as

$$A_1 A_2 = \mathcal{N}\{A_1 A_2\} + \overline{A_1 A_2}, \quad (3.132)$$

where  $A_1$  and  $A_2$  are both either creation operators or annihilation operators because the product of  $A_1$  and  $A_2$  is particle-number non-conserving. Taking the expectation value and making use of requirement (3.112), leads to

$$\langle \Psi | A_1 A_2 | \Psi \rangle = \overline{A_1 A_2}. \quad (3.133)$$

Since  $|\Psi\rangle$  has a well-defined particle number and the product of  $A_1$  and  $A_2$  is particle-number non-conserving, the expectation value regarding  $|\Psi\rangle$  of  $A_1$  and  $A_2$  has to vanish. Hence, the basis step is shown. In the inductive step, it is assumed that all particle-number non-conserving  $l$ -tuple contractions with an even number  $l$  vanish. It should be shown that a particle-number non-conserving  $l+2$ -tuple contraction vanish, too. Furthermore, due to (3.125) the expectation value regarding  $|\Psi\rangle$  of the product of  $l+2$  operators can be written as

$$\langle \Psi | A_1 A_2 \dots A_{l+2} | \Psi \rangle = \sum_{\substack{\text{full contractions} \\ \text{w.r.t. } |\Psi\rangle}} \mathcal{N}\{A_1 A_2 \dots A_{l+2}\}. \quad (3.134)$$

Since  $|\Psi\rangle$  has a well-defined particle number and the product of  $A_1, A_2, \dots, A_{l+2}$  is particle-number non-conserving, the left side of (3.134) has to vanish. On the right side, one only needs to consider  $l'$ -tuple contractions with an even number  $l' \leq l+2$ , because all  $l''$ -tuple contractions with an odd number  $l''$  vanish as proven in the first step. Hence, every fully-contracted term, except for the  $l+2$  contraction, on the right hand side of (3.134) contains at least one particle-number non-conserving  $\tilde{l}$ -tuple contraction with an even number  $\tilde{l} < l+2$ . Due to induction hypothesis, those terms vanish. That leads to

$$\overline{A_1 A_2 \dots A_{l+2}} = 0. \quad (3.135)$$

□

In the following subsection, formulas for the 2-, 4- and 6-tuple contractions will be derived and it will be proven that these  $l$ -tuple contractions for  $l > 2$  are antisymmetric under permutation of two arbitrarily chosen operators.

### 3.5.5. Formulas for the 2-, 4-, 6-Tuple Contractions

In the previous [section 3.5.4](#), it was proven that the  $l$ -tuple contraction vanishes if the product of operators, that is contracted, is particle-number non-conserving. Since the one-, two- and three-body operators are of interest, one consequently needs to consider only particle-number conserving 2-, 4- and 6-tuple contractions.

In order to derive formulas for the  $l$ -tuple contractions, one needs to apply the MR-WT at a product of  $l$  operators and take the expectation value regarding  $|\Psi\rangle$  of the given product. Due to [\(3.125\)](#), only fully-contracted terms do not vanish. Additionally, exactly one term including the  $l$ -tuple contractions remains. By activating this equation towards the  $l$ -tuple contraction, a formula for the  $l$ -tuple contraction is generated as a function of all  $l'$ -tuple contractions with  $l' < l$ . This means, one has to start with  $l = 2$  and generates all higher-tuple contractions iteratively.

Furthermore, it will be shown that these  $l$ -tuple contractions for  $l > 2$  are antisymmetric under permutation of two arbitrarily chosen operators  $A_i$  and  $A_j$ , i.e.

$$\overline{A_1 A_2 \dots A_i \dots A_j \dots A_l} = -\overline{A_1 A_2 \dots A_j \dots A_i \dots A_l} \quad (3.136)$$

To prove this statement, one needs to apply the V-WT on the product of  $l$  operators and compare the results obtained using the MR-WT as aforementioned. This kind of proof can be very exhausting. Thus, it will be explicitly carried out only for the 4-tuple contraction.

One needs to consider a particular choice of the particle-number conserving 4- and 6-tuple contractions, namely

$$\overline{a^p a^r a_s a_q}, \quad (3.137)$$

$$\overline{a^p a^r a^t a_u a_s a_q}. \quad (3.138)$$

All other 4- and 6-tuple contractions can be generated by making use of the antisymmetry of the 4- and 6-tuple contractions.

In order to derive a formula for the 2-tuple contraction with respect to  $|\Psi\rangle$ , the MR-WT is applied to a product of two operators  $A_1$  and  $A_2$ , leading to

$$A_1 A_2 = \mathcal{N}\{A_1 A_2\} + \overline{A_1 A_2}. \quad (3.139)$$

Taking the expectation value regarding  $|\Psi\rangle$  of [\(3.139\)](#), a formula for the 2-tuple contraction with respect to  $|\Psi\rangle$

$$\overline{A_1 A_2} = \langle \Psi | A_1 A_2 | \Psi \rangle, \quad (3.140)$$

can be derived with the aid of requirement (3.112). One defines a hole contraction as follows

$$\overline{a^p a_q} = \langle \Psi | a^p a_q | \Psi \rangle =: \gamma_q^p, \quad (3.141)$$

which describes an one-particle density matrix element with respect to  $|\Psi\rangle$ , denoted as  $\gamma_q^p$ , and a particle contraction

$$\overline{a_q a^p} = \langle \Psi | a_q a^p | \Psi \rangle =: \eta_q^p, \quad (3.142)$$

which describes an one-hole density matrix element with respect to  $|\Psi\rangle$ , denoted as  $\eta_q^p$ . Notice that for the one-hole and one-particle density matrix element with respect to  $|\Psi\rangle$  has been used the same symbol as for the density matrix element with respect to a single-reference state  $|\phi\rangle$  (see section 3.4). In contrast to the single-reference case, the one-hole and one-particle density matrix element cannot be simplified anymore. All other combinations given by

$$\overline{a^p a^q} = \overline{a_p a_q} = 0 \quad (3.143)$$

vanish for all  $p$  and  $q$ , because they are particle-number non-conserving.

A general relationship between the 2-tuple contraction with respect to  $|\Psi\rangle$  and the contraction with respect to the vacuum  $|0\rangle$  can be derived, which will be necessary to prove the antisymmetry of the  $l$ -tuple contraction for  $l > 2$ . Taking the expectation value regarding  $|\Psi\rangle$  of (3.55) leads to

$$\langle \Psi | A_1 A_2 | \Psi \rangle = \langle \Psi | N\{A_1 A_2\} | \Psi \rangle + \dot{A}_1 \dot{A}_2, \quad (3.144)$$

where  $N$  is the normal-ordering operator with respect to the vacuum from definition 3.4. Hence, the general relationship between the contraction with respect to  $|\Psi\rangle$  and  $|0\rangle$  is

$$\overline{A_1 A_2} = \langle \Psi | N\{A_1 A_2\} | \Psi \rangle + \dot{A}_1 \dot{A}_2. \quad (3.145)$$

Choosing  $A_1 = a_q$  and  $A_2 = a^p$ , a general relationship between a particle and hole contraction can be found

$$\begin{aligned} \overline{a_q a^p} &= \langle \Psi | N\{a_q a^p\} | \Psi \rangle + \dot{a}_q \dot{a}^p \\ &= -\langle \Psi | a^p a_q | \Psi \rangle + \dot{a}_q \dot{a}^p \\ &= -\overline{a^p a_q} + \delta_q^p. \end{aligned} \quad (3.146)$$

To simplify the notation, the expectation value regarding  $|\Psi\rangle$  of an operator  $X$  will be denoted as

$$\langle X \rangle := \langle \Psi | X | \Psi \rangle. \quad (3.147)$$

In order to derive a formula for the 4-tuple contraction, one takes the expectation value regarding  $|\Psi\rangle$  of a product of four operators  $A_1, A_2, A_3$  and  $A_4$ . According to (3.125), the expectation value regarding  $|\Psi\rangle$  can be expressed as

$$\langle A_1 A_2 A_3 A_4 \rangle = \sum_{\pi \in \Pi} \text{sgn}(\pi) \overline{A_{\pi(1)} A_{\pi(2)}} \overline{A_{\pi(3)} A_{\pi(4)}} + \overline{A_1 A_2 A_3 A_4}, \quad (3.148)$$

where  $\text{sgn}(\pi)$  is the sign of the permutation  $\pi$  from the permutation set

$$\Pi := \left\{ \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 2 & 4 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 2 & 3 \end{pmatrix} \right\}. \quad (3.149)$$

By solving (3.148) for the 4-tuple contraction, one would obtain a formula for the 4-tuple contraction while the form is not convenient to prove the antisymmetry of the 4-tuple contraction. Thus, one is forced to insert the general relationship between the 2-tuple contraction with respect to  $|\Psi\rangle$  and  $|0\rangle$  (3.145) into (3.148), leading to

$$\begin{aligned} \langle A_1 A_2 A_3 A_4 \rangle &= \sum_{\pi \in \Pi} \text{sgn}(\pi) \langle N\{A_{\pi(1)} A_{\pi(2)}\} \rangle \langle N\{A_{\pi(3)} A_{\pi(4)}\} \rangle \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \langle N\{A_{\pi(1)} A_{\pi(2)}\} \rangle \dot{A}_{\pi(3)} \dot{A}_{\pi(4)} \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \dot{A}_{\pi(1)} \dot{A}_{\pi(2)} \langle N\{A_{\pi(3)} A_{\pi(4)}\} \rangle \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \dot{A}_{\pi(1)} \dot{A}_{\pi(2)} \ddot{A}_{\pi(3)} \ddot{A}_{\pi(4)} \\ &+ \overline{A_1 A_2 A_3 A_4}. \end{aligned} \quad (3.150)$$

Applying V-WT on the product of these four operators and taking the expectation value regarding  $|\Psi\rangle$  of it, one obtains

$$\begin{aligned} \langle A_1 A_2 A_3 A_4 \rangle &= \langle N\{A_1 A_2 A_3 A_4\} \rangle \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \langle N\{A_{\pi(1)} A_{\pi(2)}\} \rangle \dot{A}_{\pi(3)} \dot{A}_{\pi(4)} \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \dot{A}_{\pi(1)} \dot{A}_{\pi(2)} \langle N\{A_{\pi(3)} A_{\pi(4)}\} \rangle \\ &+ \sum_{\pi \in \Pi} \text{sgn}(\pi) \dot{A}_{\pi(1)} \dot{A}_{\pi(2)} \ddot{A}_{\pi(3)} \ddot{A}_{\pi(4)}, \end{aligned} \quad (3.151)$$

which is equivalent to (3.150). Comparing (3.150) with (3.151), all terms containing at least one contraction with respect to the vacuum cancel out. Hence, one immediately obtains a

formula for the 4-tuple contraction

$$\begin{aligned}
 \overline{A_1 A_2 A_3 A_4} &= \langle N\{A_1 A_2 A_3 A_4\} \rangle - \sum_{\pi \in \Pi} \text{sgn}(\pi) \langle N\{A_{\pi(1)} A_{\pi(2)}\} \rangle \langle N\{A_{\pi(3)} A_{\pi(4)}\} \rangle \\
 &= \langle N\{A_1 A_2 A_3 A_4\} \rangle - \langle N\{A_1 A_2\} \rangle \langle N\{A_3 A_4\} \rangle \\
 &\quad + \langle N\{A_1 A_3\} \rangle \langle N\{A_2 A_4\} \rangle - \langle N\{A_1 A_4\} \rangle \langle N\{A_2 A_3\} \rangle
 \end{aligned} \tag{3.152}$$

in a suitable form to proof the antisymmetry of the 4-tuple contraction.

**Corollary 3.1.** *The 4-tuple contraction is antisymmetric under permutation of two arbitrarily chosen operators  $A_i$  and  $A_j$  for all  $i, j \in \{1, 2, 3, 4\}$  with  $i \neq j$ , i.e.*

$$\overline{A_1 A_i A_j A_4} = -\overline{A_1 A_j A_i A_4}. \tag{3.153}$$

*Proof.* The first term in (3.152) is always antisymmetric because of the normal-ordering operator  $N$ . Furthermore, taking a closer look on it, one observes that one of the remaining three terms is antisymmetric depending on the choice of  $i$  and  $j$ , and the remaining two are antisymmetric to one another. Alternatively, the proof can be carried out going through all possibilities for  $i$  and  $j$ . As an example the operator  $A_1$  and  $A_4$  will be transposed. According to (3.152), it follows

$$\begin{aligned}
 \overline{A_4 A_2 A_3 A_1} &= \langle N\{A_4 A_2 A_3 A_1\} \rangle - \langle N\{A_4 A_2\} \rangle \langle N\{A_3 A_1\} \rangle \\
 &\quad + \langle N\{A_4 A_3\} \rangle \langle N\{A_2 A_1\} \rangle - \langle N\{A_4 A_1\} \rangle \langle N\{A_2 A_3\} \rangle
 \end{aligned} \tag{3.154}$$

Making use of the antisymmetry of the normal-ordering operator  $N$  and reordering the factors, one obtains

$$\begin{aligned}
 \overline{A_4 A_2 A_3 A_1} &= -\langle N\{A_1 A_2 A_3 A_4\} \rangle - (-)^2 \langle N\{A_2 A_4\} \rangle \langle N\{A_1 A_3\} \rangle \\
 &\quad + (-)^2 \langle N\{A_3 A_4\} \rangle \langle N\{A_1 A_2\} \rangle - (-) \langle N\{A_1 A_4\} \rangle \langle N\{A_2 A_3\} \rangle \\
 &= -\left( \langle N\{A_1 A_2 A_3 A_4\} \rangle + \langle N\{A_1 A_3\} \rangle \langle N\{A_2 A_4\} \rangle \right. \\
 &\quad \left. - \langle N\{A_1 A_2\} \rangle \langle N\{A_3 A_4\} \rangle - \langle N\{A_1 A_4\} \rangle \langle N\{A_2 A_3\} \rangle \right) \\
 &= -\overline{A_1 A_2 A_3 A_4}
 \end{aligned} \tag{3.155}$$

All other cases can be proven in a similar way.  $\square$

Corollary 3.1 implies the property

$$\overline{A_1 A_2 A_3 A_4} = \text{sgn}(\pi) \overline{N\{A_1 A_2 A_3 A_4\}}, \tag{3.156}$$

where  $N$  is the normal-ordering operator with respect to the vacuum and  $\text{sgn}(\pi)$  is sign of the permutation  $\pi$  which brings the product  $A_1 A_2 A_3 A_4$  in normal-order with respect to the vacuum. Hence, one only needs to consider the special case  $A_1 = a^p$ ,  $A_2 = a^r$ ,  $A_3 = a_s$  and

$A_4 = a_q$ . Inserting those operators in (3.152), it follows for the particle-number conserving 4-tuple contraction

$$\begin{aligned}
 \overline{a^p a^r a_s a_q} &= \langle N\{a_{qs}^{pr}\} \rangle - \langle N\{a^p a^r\} \rangle \langle N\{a_s a_q\} \rangle + \langle N\{a_s^p\} \rangle \langle N\{a_q^r\} \rangle - \langle N\{a_q^p\} \rangle \langle N\{a_s^r\} \rangle \\
 &= \langle a_{qs}^{pr} \rangle - \underbrace{\langle a^p a^r \rangle \langle a_s a_q \rangle}_{=0} + \langle a_s^p \rangle \langle a_q^r \rangle - \langle a_q^p \rangle \langle a_s^r \rangle \\
 &= \gamma_{qs}^{pr} - \left( \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r \right) =: \lambda_{qs}^{pr},
 \end{aligned} \tag{3.157}$$

which is equivalent to the two-body residual density matrix element  $\lambda_{qs}^{pr}$ , also called irreducible 2-particle density matrix element. The two-body residual density matrix element  $\lambda_{qs}^{pr}$  describes two-particle correlations. Note that

$$\gamma_{qs}^{pr} := \langle \Psi | a_{qs}^{pr} | \Psi \rangle \tag{3.158}$$

is the two-particle density matrix element with respect to  $|\Psi\rangle$ .

In a similar manner, a formula for the particle-number conserving 6-tuple contraction can be derived [Muk97]

$$\overline{a^p a^r a^t a_u a_s a_q} = \gamma_{qsu}^{prt} - \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) - \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) =: \lambda_{qsu}^{prt}, \tag{3.159}$$

which is equivalent to the residual three-particle density matrix element  $\lambda_{qsu}^{prt}$ , also called irreducible 3-particle density matrix element. Furthermore, the three-particle density matrix element with respect to  $|\Psi\rangle$  is denoted as

$$\gamma_{qsu}^{prt} := \langle \Psi | a_{qsu}^{prt} | \Psi \rangle, \tag{3.160}$$

and  $\mathbb{A}$  is the index antisymmetrizer collecting similar terms

$$\begin{aligned}
 \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) &= + \gamma_q^p \lambda_{su}^{rt} - \gamma_s^p \lambda_{qu}^{rt} - \gamma_u^p \lambda_{sq}^{rt} \\
 &\quad - \gamma_q^r \lambda_{su}^{pt} + \gamma_s^r \lambda_{qu}^{pt} - \gamma_u^r \lambda_{qs}^{pt} \\
 &\quad - \gamma_q^t \lambda_{us}^{pr} - \gamma_s^t \lambda_{qu}^{pr} + \gamma_u^t \lambda_{qs}^{pr},
 \end{aligned} \tag{3.161}$$

$$\begin{aligned}
 \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) &= + \gamma_q^p \gamma_s^r \gamma_u^t + \gamma_u^p \gamma_q^r \gamma_s^t + \gamma_s^p \gamma_u^r \gamma_q^t \\
 &\quad - \gamma_u^p \gamma_s^r \gamma_q^t - \gamma_s^p \gamma_q^r \gamma_u^t - \gamma_q^p \gamma_u^r \gamma_s^t.
 \end{aligned} \tag{3.162}$$

Summarizing all important results of this subsection, one obtains for the particle-number conserving 2-, 4- and 6-tuple contractions:

$$\overline{a^p a_q} = \gamma_q^p, \tag{3.163}$$

$$\overline{a^p a^r a_s a_q} = \gamma_{qs}^{pr} - \left( \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r \right) = \lambda_{qs}^{pr}, \tag{3.164}$$

$$\overline{a^p a^r a^t a_u a_s a_q} = \gamma_{qsu}^{prt} - \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) - \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) = \lambda_{qsu}^{prt}. \tag{3.165}$$

As expected the 4-tuple and 6-tuple contraction vanish for the special case of  $|\Psi\rangle$  consisting of a single Slater determinant

$$\overline{a^p a^r a_s a_q} = \gamma_{qs}^{pr} - (\gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r) \quad (3.166)$$

$$= \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r - (\gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r) = 0, \quad (3.167)$$

$$\overline{a^p a^r a^t a_u a_s a_q} = \gamma_{qsu}^{prt} - \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) - \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) \quad (3.168)$$

$$= \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) - 0 - \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) = 0, \quad (3.169)$$

using  $\gamma_{qsu}^{prt} = \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t)$  which is true for only a single-reference state.

### 3.5.6. Results for the One-, Two- and Three-Body Operators

The aim of this subsection is to express the one-, two- and three-body operators  $(a_q^p, a_{qs}^{pr}, a_{qsu}^{prt})$ , which are per definition in normal-order with respect to the vacuum, as sums of the one-, two- and three-body operator in MR-NO  $(\tilde{a}_q^p, \tilde{a}_{qs}^{pr}, \tilde{a}_{qsu}^{prt})$  which are defined in (3.116)–(3.118). Therefore, the MR-WT and the formulas derived for the 2-, 4- and 6-tuple contractions will be used.

For the one-body operator, one immediately obtains

$$a_q^p = \mathcal{N}\{a_q^p\} + \overline{a^p a_q} = \tilde{a}_q^p + \gamma_q^p. \quad (3.170)$$

Furthermore, for the two-body operator, one finds

$$\begin{aligned} a_{qs}^{pr} &= a^p a^r a_s a_q \\ &= \mathcal{N}\{a_{qs}^{pr}\} + \gamma_q^p \mathcal{N}\{a_s^r\} + \gamma_s^r \mathcal{N}\{a_q^p\} - \gamma_s^p \mathcal{N}\{a_q^r\} - \gamma_q^r \mathcal{N}\{a_s^p\} + \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r + \lambda_{qs}^{pr}. \end{aligned} \quad (3.171)$$

After applying the formula for the 4-tuple contraction and simplifying by means of the index antisymmetrizer, one obtains

$$\begin{aligned} a_{qs}^{pr} &= \tilde{a}_{qs}^{pr} + \gamma_q^p \tilde{a}_s^r + \gamma_s^r \tilde{a}_q^p - \gamma_s^p \tilde{a}_q^r - \gamma_q^r \tilde{a}_s^p + \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r + \gamma_{qs}^{pr} - (\gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r) \\ &= \tilde{a}_{qs}^{pr} + \mathbb{A}(\gamma_q^p \tilde{a}_s^r) + \gamma_{qs}^{pr}. \end{aligned} \quad (3.172)$$

For the three-body operator, it is advisable to clarify which possible combinations of particle-number conserving  $l$ -tuple contractions are relevant. These are single, double and triple 2-tuple contractions, single 4-tuple contractions, single 2-tuple combined with single

4-tuple contractions, and, of course, a single 6-tuple contraction, i.e.

$$\begin{aligned}
 a_{qsu}^{prt} &= \mathcal{N}\{a_{qsu}^{prt}\} + \gamma_q^p \mathcal{N}\{a_{su}^{rt}\} + \dots \\
 &\quad + \gamma_q^p \gamma_s^r \mathcal{N}\{a_u^t\} + \dots \\
 &\quad + \gamma_q^p \gamma_s^r \gamma_u^t + \dots \\
 &\quad + \lambda_{qs}^{pr} \mathcal{N}\{a_u^t\} + \dots \\
 &\quad + \gamma_q^p \lambda_{su}^{rt} + \dots \\
 &\quad + \lambda_{qsu}^{prt}.
 \end{aligned} \tag{3.173}$$

The first term is per definition  $\tilde{a}_{qsu}^{prt}$ . All terms including a single 2-tuple contractions can be expressed compactly using the index antisymmetrizer

$$\begin{aligned}
 \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) &= + \gamma_q^p \tilde{a}_{su}^{rt} - \gamma_s^p \tilde{a}_{qu}^{rt} - \gamma_u^p \tilde{a}_{sq}^{rt} \\
 &\quad - \gamma_q^r \tilde{a}_{su}^{pt} + \gamma_s^r \tilde{a}_{qu}^{pt} - \gamma_u^r \tilde{a}_{qs}^{pt} \\
 &\quad - \gamma_q^t \tilde{a}_{us}^{pr} - \gamma_s^t \tilde{a}_{qu}^{pr} + \gamma_u^t \tilde{a}_{qs}^{pr}.
 \end{aligned} \tag{3.174}$$

Furthermore, all terms including double 2-tuple contractions are given by

$$\begin{aligned}
 \mathbb{A}\left(\mathbb{A}(\gamma_q^p \gamma_s^r) \tilde{a}_u^t\right) &= + \mathbb{A}(\gamma_q^p \gamma_s^r) \tilde{a}_u^t - \mathbb{A}(\gamma_q^p \gamma_u^r) \tilde{a}_s^t - \mathbb{A}(\gamma_u^p \gamma_s^r) \tilde{a}_q^t \\
 &\quad - \mathbb{A}(\gamma_q^p \gamma_s^t) \tilde{a}_u^r + \mathbb{A}(\gamma_q^p \gamma_u^t) \tilde{a}_s^r - \mathbb{A}(\gamma_s^p \gamma_u^t) \tilde{a}_q^r \\
 &\quad - \mathbb{A}(\gamma_s^r \gamma_q^t) \tilde{a}_u^p - \mathbb{A}(\gamma_q^r \gamma_u^t) \tilde{a}_s^p + \mathbb{A}(\gamma_s^r \gamma_u^t) \tilde{a}_q^p \\
 &= - (\gamma_q^p \gamma_s^t - \gamma_s^p \gamma_q^t) \tilde{a}_u^r + (\gamma_q^p \gamma_u^t - \gamma_u^p \gamma_q^t) \tilde{a}_s^r - (\gamma_s^p \gamma_u^t - \gamma_u^p \gamma_s^t) \tilde{a}_q^r \\
 &\quad - (\gamma_s^r \gamma_q^t - \gamma_q^r \gamma_s^t) \tilde{a}_u^p - (\gamma_q^r \gamma_u^t - \gamma_u^r \gamma_q^t) \tilde{a}_s^p + (\gamma_s^r \gamma_u^t - \gamma_u^r \gamma_s^t) \tilde{a}_q^p,
 \end{aligned} \tag{3.175}$$

and all terms including single 4-tuple contractions

$$\begin{aligned}
 \mathbb{A}(\lambda_{qs}^{pr} \tilde{a}_u^t) &= + \lambda_{qs}^{pr} \tilde{a}_u^t - \lambda_{qu}^{pr} \tilde{a}_s^t - \lambda_{us}^{pr} \tilde{a}_q^t \\
 &\quad - \lambda_{qs}^{pt} \tilde{a}_u^r + \lambda_{qu}^{pt} \tilde{a}_s^r - \lambda_{su}^{pt} \tilde{a}_q^r \\
 &\quad - \lambda_{sq}^{rt} \tilde{a}_u^p - \lambda_{qu}^{rt} \tilde{a}_s^p + \lambda_{su}^{rt} \tilde{a}_q^p.
 \end{aligned} \tag{3.176}$$

The sum of (3.175) and (3.176) can be simplified using (3.164) and the linearity of the index antisymmetrizer to

$$\mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) = \mathbb{A}\left(\left(\mathbb{A}(\gamma_q^p \gamma_s^r) + \lambda_{qs}^{pr}\right) \tilde{a}_u^t\right) = \mathbb{A}\left(\mathbb{A}(\gamma_q^p \gamma_s^r) \tilde{a}_u^t\right) + \mathbb{A}(\lambda_{qs}^{pr} \tilde{a}_u^t).$$

All triple 2-tuple contractions results in

$$\begin{aligned}
 \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) &= + \gamma_q^p \gamma_s^r \gamma_u^t + \gamma_u^p \gamma_q^r \gamma_s^t + \gamma_s^p \gamma_u^r \gamma_q^t \\
 &\quad - \gamma_u^p \gamma_s^r \gamma_q^t - \gamma_s^p \gamma_q^r \gamma_u^t - \gamma_q^p \gamma_u^r \gamma_s^t.
 \end{aligned} \tag{3.177}$$

Terms including single 2- and 4-tuple contractions can be written as

$$\begin{aligned}
 \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) = & + \gamma_q^p \lambda_{su}^{rt} - \gamma_s^p \lambda_{qu}^{rt} - \gamma_u^p \lambda_{sq}^{rt} \\
 & - \gamma_q^r \lambda_{su}^{pt} + \gamma_s^r \lambda_{qu}^{pt} - \gamma_u^r \lambda_{qs}^{pt} \\
 & - \gamma_q^t \lambda_{us}^{pr} - \gamma_s^t \lambda_{qu}^{pr} + \gamma_u^t \lambda_{qs}^{pr}.
 \end{aligned} \tag{3.178}$$

The intermediate result states the following

$$a_{qsu}^{prt} = \tilde{a}_{qsu}^{prt} + \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) + \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) + \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) + \lambda_{qsu}^{prt}. \tag{3.179}$$

Inserting the formula for the 6-tuple contraction, it follows

$$\begin{aligned}
 a_{qsu}^{prt} = & \tilde{a}_{qsu}^{prt} + \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) + \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t) + \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) \\
 & + \gamma_{qsu}^{prt} - \mathbb{A}(\gamma_q^p \lambda_{su}^{rt}) - \mathbb{A}(\gamma_q^p \gamma_s^r \gamma_u^t).
 \end{aligned} \tag{3.180}$$

Finally, one obtains the 3-body operator as a sum of the zero-, one-, two- and three-body operators in MR-NO

$$a_{qsu}^{prt} = \tilde{a}_{qsu}^{prt} + \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) + \gamma_{qsu}^{prt}. \tag{3.181}$$

Summarizing the results, one obtains the one-, two- and three-body operators as sums of the zero<sup>-1</sup>, one-, two- and three-body operators in MR-NO:

$$a_q^p = \tilde{a}_q^p + \gamma_q^p, \tag{3.182}$$

$$a_{qs}^{pr} = \tilde{a}_{qs}^{pr} + \mathbb{A}(\gamma_q^p \tilde{a}_s^r) + \gamma_{qs}^{pr}, \tag{3.183}$$

$$a_{qsu}^{prt} = \tilde{a}_{qsu}^{prt} + \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) + \gamma_{qsu}^{prt}. \tag{3.184}$$

In the end, the requirements for the generalization (see [section 3.5.1](#)) will be verified. Therefore, (3.182)–(3.184) will be activated towards  $\tilde{a}_q^p$ ,  $\tilde{a}_{qs}^{pr}$  and  $\tilde{a}_{qsu}^{prt}$ , such a recursive formula is obtained for those operators, i.e.

$$\tilde{a}_q^p = a_q^p - \gamma_q^p, \tag{3.185}$$

$$\tilde{a}_{qs}^{pr} = a_{qs}^{pr} - \mathbb{A}(\gamma_q^p \tilde{a}_s^r) - \gamma_{qs}^{pr}, \tag{3.186}$$

$$\tilde{a}_{qsu}^{prt} = a_{qsu}^{prt} - \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) - \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) - \gamma_{qsu}^{prt}. \tag{3.187}$$

The second requirement can be easily verified by replacing the normal-ordering operator  $\mathcal{N}$  with  $\mathcal{N}_{\text{SR}}$ , and comparing the resulting equations with (3.103)–(3.105). In order to prove the first requirement, one should take the expectation value regarding  $|\Psi\rangle$  of those equations. It

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<sup>1</sup>A zero-body operator is always an operator in MR-NO due to requirement  $\mathcal{N}\{\lambda\} = \lambda$ .

is necessary for all  $p$  and  $q$

$$\begin{aligned}\langle \tilde{a}_q^p \rangle &= \langle a_q^p \rangle - \gamma_q^p \\ &= \gamma_q^p - \gamma_q^p = 0.\end{aligned}\tag{3.188}$$

Analogously, it is obtained for the other operators

$$\langle \tilde{a}_{qs}^{pr} \rangle = \langle a_{qs}^{pr} \rangle - \mathbb{A}(\gamma_q^p \langle \tilde{a}_s^r \rangle) - \gamma_{qs}^{pr} = \gamma_{qs}^{pr} - \gamma_{qs}^{pr} = 0,\tag{3.189}$$

$$\begin{aligned}\langle \tilde{a}_{qsu}^{prt} \rangle &= \langle a_{qsu}^{prt} \rangle - \mathbb{A}(\gamma_q^p \langle \tilde{a}_{su}^{rt} \rangle) - \mathbb{A}(\gamma_{qs}^{pr} \langle \tilde{a}_u^t \rangle) - \gamma_{qsu}^{prt} \\ &= \gamma_{qsu}^{prt} - \gamma_{qsu}^{prt} = 0\end{aligned}\tag{3.190}$$

for all  $p, r, t, q, s$  and  $u$ . Hence, the operators  $\tilde{a}_q^p$ ,  $\tilde{a}_{qs}^{pr}$  and  $\tilde{a}_{qsu}^{prt}$  are indeed in normal order with respect to  $|\Psi\rangle$ , as defined.



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## Chapter 4

# Multi-Reference Normal-Ordered $n$ -Body Approximation

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In this chapter, results obtained in the previous chapter will be used in order to derive normal-ordering approximations of any three-nucleon (3N) interaction.

By means of second quantization, any 3N interaction  $V_{3N}$  can be written as

$$V_{3N} = \frac{1}{36} \sum_{\substack{prt \\ qsu}} \langle prt | V_{3N} | qsu \rangle a_p^\dagger a_r^\dagger a_t^\dagger a_u a_s a_q, \quad (4.1)$$

where  $\langle prt | V_{3N} | qsu \rangle$  is the antisymmetrized three-body matrix element. Using the notation  $a_{qsu}^{prt}$  for the three-body operator  $a_p^\dagger a_r^\dagger a_t^\dagger a_u a_s a_q$  and the definition

$$v_{qsu}^{prt} := \langle prt | V_{3N} | qsu \rangle, \quad (4.2)$$

it can be rewritten in the compact form

$$V_{3N} = \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} a_{qsu}^{prt}. \quad (4.3)$$

Inserting (3.184) in (4.3), one obtains

$$\begin{aligned} V_{3N} &= \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} a_{qsu}^{prt} \\ &= \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \left( \tilde{a}_{qsu}^{prt} + \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) + \gamma_{qsu}^{prt} \right). \end{aligned} \quad (4.4)$$

It is convenient to define the following operators

$$\tilde{V}_3 := \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \tilde{a}_{qsu}^{prt}, \quad (4.5)$$

$$\tilde{V}_2 := \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}), \quad (4.6)$$

$$\tilde{V}_1 := \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t), \quad (4.7)$$

$$\tilde{V}_0 := \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qsu}^{prt}, \quad (4.8)$$

where  $\tilde{V}_i$  is called the  $i$ -body contribution in MR-NO of the given 3N interaction. Since  $v_{qsu}^{prt}$  and the terms including the index antisymmetrizer  $\mathbb{A}$  are antisymmetric, the product is symmetric. Consequently, by renaming the indices of the sum, the two- and one-body contribution in MR-NO can be simplified to

$$\tilde{V}_2 = \frac{9}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \tilde{a}_{su}^{rt} = \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \tilde{a}_{su}^{rt}, \quad (4.9)$$

$$\tilde{V}_1 = \frac{9}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} \tilde{a}_u^t = \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} \tilde{a}_u^t. \quad (4.10)$$

Hence, any 3N interaction can be written as a sum of the zero-, one-, two- and three-body contributions in MR-NO

$$\begin{aligned} V_{3N} &= \tilde{V}_0 + \tilde{V}_1 + \tilde{V}_2 + \tilde{V}_3 \\ &= \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qsu}^{prt} + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} \tilde{a}_u^t + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \tilde{a}_{su}^{rt} + \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \tilde{a}_{qsu}^{prt}, \end{aligned} \quad (4.11)$$

where this form is called the reference-state representation of the 3N interaction. For a general discussion of the  $m$ -nucleon interaction in reference-state representation see [appendix A](#).

Based on (4.11), an approximate lower-particle-rank form of the 3N interaction can be systematically defined by neglecting all many-body contributions beyond a given rank  $n$ . These approximations will be referred to as multi-reference normal-ordered  $n$ -body (MR-NO $n$ B) approximation. There are three possible MR-NO $n$ B approximations for any 3N interaction [[Rot+12](#)]

$$V_{3N}^{\text{MR-NO0B}} := \tilde{V}_0, \quad (4.12)$$

$$V_{3N}^{\text{MR-NO1B}} := \tilde{V}_0 + \tilde{V}_1, \quad (4.13)$$

$$V_{3N}^{\text{MR-NO2B}} := \tilde{V}_0 + \tilde{V}_1 + \tilde{V}_2, \quad (4.14)$$

where  $V_{3N}^{\text{MR-NO}n\text{B}}$  is the 3N interaction in MR-NO $n$ B approximation (here in reference-state representation).

Since the operators  $\tilde{a}_q^p$ ,  $\tilde{a}_{qs}^{pr}$  and  $\tilde{a}_{qsu}^{prt}$  are abstract objects, one has to transform the one- and two-body operator in MRNO into vacuum representation<sup>1</sup>. For that purpose, one needs to express  $\tilde{a}_q^p$  and  $\tilde{a}_{qs}^{pr}$  as sums of the one- and two-body operators in V-NO. According to (3.182) and (3.183), it follows for the one-body operator in MR-NO

$$\tilde{a}_q^p = a_q^p - \gamma_q^p, \quad (4.15)$$

and for the two-body operator in MR-NO

$$\begin{aligned} \tilde{a}_{qs}^{pr} &= a_{qs}^{pr} - \mathbb{A}(\gamma_q^p \tilde{a}_s^r) - \gamma_{qs}^{pr} \\ &= a_{qs}^{pr} - \mathbb{A}(\gamma_q^p (a_s^r - \gamma_s^r)) - \gamma_{qs}^{pr} \\ &= a_{qs}^{pr} - \mathbb{A}(\gamma_q^p a_s^r) + \mathbb{A}(\gamma_q^p \gamma_s^r) - \gamma_{qs}^{pr}. \end{aligned} \quad (4.16)$$

Using these results, the one-body and two interaction in MRNO can be transformed in vacuum representation. For the one-body contribution in MRNO in vacuum representation, one obtains

$$\begin{aligned} \tilde{V}_1 &= \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} \tilde{a}_u^t \\ &= \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} (a_u^t - \gamma_u^t) \\ &= -\frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} \gamma_u^t + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} a_u^t. \end{aligned} \quad (4.17)$$

Moreover, making use of the antisymmetry of the three-body matrix element, and by renaming the indices, the two-body contribution in MRNO in vacuum representation can be simplified to

$$\begin{aligned} \tilde{V}_2 &= \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \tilde{a}_{su}^{rt} \\ &= \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \left( a_{su}^{rt} - \mathbb{A}(\gamma_s^r a_u^t) + \mathbb{A}(\gamma_s^r \gamma_u^t) - \gamma_{su}^{rt} \right) \\ &= \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \left( a_{su}^{rt} - 4\gamma_s^r a_u^t + 4\gamma_s^r \gamma_u^t - \gamma_{su}^{rt} \right) \\ &= \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} (4\gamma_q^p \gamma_s^r \gamma_u^t - \gamma_q^p \gamma_{su}^{rt}) - \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \gamma_s^r a_u^t + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p a_{su}^{rt}. \end{aligned} \quad (4.18)$$

<sup>1</sup>The zero-body contribution in MRNO is per definition in reference-state as well as in vacuum representation. Since the three-body contribution in MRNO is neglected in MR-NO $n$ B approximation, it is not transformed here.

In the final step the terms have been sorted and summarized according to their particle-rank. Note that the one- and two-body contribution in MRNO contribute to lower-particle-rank interactions while transforming the 3N interaction in MR-NO $n$ B approximation into the vacuum representation.

Finally, inserting the one- and two-body contribution in MRNO denoted in vacuum representation (4.17) and (4.18) into (4.13) and (4.14), the 3N interaction in MR-NO $n$ B approximation denoted in vacuum representation for different maximum particle rank  $n$  reads

$$V_{3N}^{\text{MR-NO0B}} = \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qsu}^{prt} = \langle \Psi | V_{3N} | \Psi \rangle, \quad (4.19)$$

$$V_{3N}^{\text{MR-NO1B}} = \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} (\gamma_{qsu}^{prt} - 9\gamma_{qs}^{pr} \gamma_u^t) + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_{qs}^{pr} a_u^t, \quad (4.20)$$

$$\begin{aligned} V_{3N}^{\text{MR-NO2B}} &= \frac{1}{36} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} (\gamma_{qsu}^{prt} - 18\gamma_q^p \gamma_{su}^{rt} + 36\gamma_q^p \gamma_s^r \gamma_u^t) \\ &\quad + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} (\gamma_{qs}^{pr} - 4\gamma_q^p \gamma_s^r) a_u^t \\ &\quad + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p a_{su}^{rt}, \end{aligned} \quad (4.21)$$

where the terms have been sorted and summarized according to their particle rank.

As a cross-check, the special case of  $|\Psi\rangle$  consisting of a single Slater determinant will be considered. Especially, the three- and two-particle density matrix elements with respect to a single Slater determinant can be expressed as a function of the one-particle density matrix element, namely

$$\gamma_{qsu}^{prt} = \gamma_q^p \gamma_s^r \gamma_u^t + \gamma_u^p \gamma_q^r \gamma_s^t + \gamma_s^p \gamma_u^r \gamma_q^t - \gamma_q^p \gamma_u^r \gamma_s^t - \gamma_s^p \gamma_q^r \gamma_u^t - \gamma_u^p \gamma_s^r \gamma_q^t, \quad (4.22)$$

$$\gamma_{qs}^{pr} = \gamma_q^p \gamma_s^r - \gamma_s^p \gamma_q^r. \quad (4.23)$$

Hence, (4.19)–(4.21) can be simplified by renaming the indices and using the antisymmetry of the three-body matrix element  $v_{qsu}^{prt}$  to

$$V_{3N}^{\text{SR-NO0B}} := \frac{1}{6} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \gamma_s^r \gamma_u^t = \langle \phi | V_{3N} | \phi \rangle, \quad (4.24)$$

$$V_{3N}^{\text{SR-NO1B}} := -\frac{1}{3} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \gamma_s^r \gamma_u^t + \frac{1}{2} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \gamma_s^r a_u^t, \quad (4.25)$$

$$V_{3N}^{\text{SR-NO2B}} := \frac{1}{6} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \gamma_s^r \gamma_u^t - \frac{1}{2} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p \gamma_s^r a_u^t + \frac{1}{4} \sum_{\substack{prt \\ qsu}} v_{qsu}^{prt} \gamma_q^p a_{su}^{rt}. \quad (4.26)$$

These formulas are in general true for any single-reference state. For a proper choice of the basis, the one-particle density matrix element with respect to a single Slater determinant can be written as

$$\gamma_q^p = n_q \delta_q^p, \quad (4.27)$$

where  $n_q$  denotes the occupation number—being one if  $q$  labels an occupied state, otherwise zero. Assuming that  $i, j$  and  $k$  are hole indices, i.e. they label occupied states, and using the definition

$$w := \frac{1}{6} \sum_{ijk} v_{ijk}^{ijk}, \quad (4.28)$$

$$w_u^t := \frac{1}{2} \sum_{ij} v_{iju}^{ijt}, \quad (4.29)$$

$$w_{su}^{rt} := \sum_i v_{isu}^{irt}, \quad (4.30)$$

one obtains for the 3N interaction in SR-NO $n$ B approximation denoted in vacuum representation by a proper choice of the basis

$$V_{3N}^{\text{SR-NO0B}} = w, \quad (4.31)$$

$$V_{3N}^{\text{SR-NO1B}} = -2w + \sum_{tu} w_u^t a_u^t, \quad (4.32)$$

$$V_{3N}^{\text{SR-NO2B}} = w - \sum_{tu} w_u^t a_u^t + \frac{1}{4} \sum_{rtsu} w_{su}^{rt} a_{su}^{rt}. \quad (4.33)$$

Equation (4.33) is consistent with the results in [Rot<sup>+</sup>12].



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# Chapter 5

## Results

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This chapter starts with an overview of the calculations performed in this work. The starting point is a Hamiltonian  $H$  containing either the NN or NN+3N interaction from chiral effective field theory, where the NN interaction at N<sup>3</sup>LO are taken from Entem and Machleidt [EM03] and the three-nucleon interaction at N<sup>3</sup>LO in local form from Navrátil [Nav07]. The low-energy constants have been fitted to the ground-state energy and  $\beta$ -decay half-life of three-nucleon systems [GQN09]. Both Hamiltonians will be transformed using the similarity renormalization group (SRG), in order to enhance convergence behaviour regarding the model-space size  $N_{\max}$  [Rot+11]. The SRG transformation is performed in the 3B space.

Hence, the inputs for the many-body calculations in this work are the SRG-evolved chiral NN+3N-induced (2.13) and the NN+3N-full Hamiltonians (2.14). The 3N-interaction terms in both Hamiltonians have quite different characteristics, which makes them useful for benchmarking the MR-NO2B approximation. The matrix elements of the SRG-evolved 3N interaction are computed and stored in a  $JT$ -coupled scheme as described in [Ber+08]. In order to increase the number of test cases, each of these two Hamiltonians will be considered with two different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  and  $0.08 \text{ fm}^4$ . These two types of Hamiltonians with  $\alpha = 0.04 \text{ fm}^4$  and  $0.08 \text{ fm}^4$  are in the following referred as the hard and soft Hamiltonian, respectively.

For each of these four Hamiltonians, the MR-NO2B approximation with respect to a nucleus-specific reference state will be constructed. The choice of the reference state  $|\Psi_{\text{gs}}^{\text{ref}}\rangle$  is a priori not fixed, but it will be chosen as the ground state of the nucleus under consideration to obtain a first approximation of the considered system. In order to analyze the dependence on the reference state, several reference states  $|\Psi_{\text{gs}}^{\text{ref}}\rangle$  will be calculated for the ground state of the considered nucleus with the given Hamiltonian using the NCSM for small model spaces. The model-space size, in which the reference state has been calculated, will be denoted as  $N_{\max}^{\text{ref}}$ .

Consequently, several different approximations for each of these four Hamiltonians in MR-NO2B approximation with respect to  $|\Psi_{\text{gs}}^{\text{ref}}\rangle$  are obtained. For brevity, the following notations will be used: MR-NO2B approximation with respect to a reference state  $|\Psi_{\text{gs}}^{\text{ref}}\rangle$  calculated in a

model-space size  $N_{\max}^{\text{ref}}$  will be written as MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ). Note that for closed-shell nuclei the MR-NO2B( $0\hbar\Omega$ ) approximation is equivalent to the SR-NO2B approximation. This does not hold for open-shell nuclei.

Finally, importance-truncated NCSM (IT-NCSM) calculations for the Hamiltonian containing the explicit 3N interaction, and the corresponding MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximations are performed and energies of a few low-lying states depending on the model-space size  $N_{\max}$  are compared. For the closed-shell nuclei, only the ground-state energies will be of interest. The results and calculations performed with the Hamiltonian containing the explicit 3N interaction are in the following referred to exact results and exact calculations, respectively. Comparison to experiment is not carried out here to avoid confusion. The predictive power of chiral Hamiltonians have been shown before, e.g. in [Rot<sup>+</sup>11; Rot<sup>+</sup>12; Her<sup>+</sup>13].

## 5.1. Ground-State Energies

One starts with a direct comparison of IT-NCSM calculations for the ground-state energies. Firstly, results obtained for the closed-shell nuclei  $^4\text{He}$  and  $^{16}\text{O}$  which have been already investigated in the framework of the SR-NO2B approximation will be presented [Rot<sup>+</sup>12]. As mentioned before, this case is equivalent to MR-NO2B( $0\hbar\Omega$ ) for closed-shell nuclei. Furthermore, these results will be compared to results obtained with the MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximations for a range of  $N_{\max}^{\text{ref}}$  parameters with  $N_{\max}^{\text{ref}} > 0$  that correspond to non-trivial multi-reference states. The reference state contains information about the specific many-body system under consideration. The larger the parameter  $N_{\max}^{\text{ref}}$ , the more information the reference state contains. Hence, one expects that the quality of the MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximations should improve with increasing  $N_{\max}^{\text{ref}}$ .

Secondly, for the first time the open-shell nuclei  $^6\text{Li}$ ,  $^{10}\text{B}$  and  $^{12}\text{C}$  will be investigated in the framework of the MR-NO2B approximation. Especially  $^{10}\text{B}$  will be a very interesting test case for the MR-NO2B approximation, because the total angular momentum of the ground state is in agreement with experiment only if the NN+3N-full Hamiltonian is used [E C02]. The question is whether the NN+3N-full Hamiltonian in MR-NO2B approximation can capture this genuine 3N-interaction effect. Note that only MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximations with  $N_{\max}^{\text{ref}} > 0$  have been discussed, but in principle it is possible to calculate MR-NO2B( $0\hbar\Omega$ ) approximations, too.

For a quantitative analysis, it is convenient to define the absolute and relative deviation between the exact result and the corresponding MR-NO2B approximation

$$\Delta_{\text{abs}} := E_{\text{MR-NO2B}} - E_{\text{explicit-3N}}, \quad (5.1)$$

$$\Delta_{\text{rel}} := \frac{\Delta_{\text{abs}}}{E_{\text{explicit-3N}}} = \frac{E_{\text{MR-NO2B}}}{E_{\text{explicit-3N}}} - 1, \quad (5.2)$$

where  $E_{\text{explicit-3N}}$  and  $E_{\text{MR-NO2B}}$  denote the ground-state energy calculated with the explicit 3N interaction and the MR-NO2B approximation, respectively. Obviously, the absolute and relative deviations depend on the parameters  $N_{\max}^{\text{ref}}$  and  $N_{\max}$ . The MR-NO2B approximation

overbinds the exact ground-state energy if  $\Delta_{\text{rel}}$  is negative. In order to retain the overview of the following analysis, one refers to the relative deviation as the absolute value of it. The same holds for the absolute deviation. As aforementioned, the sign of  $\Delta_{\text{abs}}$  and  $\Delta_{\text{rel}}$  for a given  $N_{\text{max}}^{\text{ref}}$  and  $N_{\text{max}}$  only provides information whether over- or underbinding is present. Since  $E_{\text{explicit-3N}}$  and  $E_{\text{MR-NO2B}}$  contains error, error propagation needs to be considered:

$$\Delta(\Delta_{\text{abs}}) = \sqrt{(\Delta E_{\text{explicit-3N}})^2 - (\Delta E_{\text{MR-NO2B}})^2}, \quad (5.3)$$

$$\Delta(\Delta_{\text{rel}}) = \left| \frac{E_{\text{MR-NO2B}}}{E_{\text{explicit-3N}}} \right| \sqrt{\left( \frac{\Delta E_{\text{explicit-3N}}}{E_{\text{explicit-3N}}} \right)^2 + \left( \frac{\Delta E_{\text{MR-NO2B}}}{E_{\text{MR-NO2B}}} \right)^2}. \quad (5.4)$$

Absolute and relative deviations for all investigated nuclei are depicted in [appendix B.1](#) and [appendix B.2](#), relatively.

### 5.1.1. Closed-Shell Nuclei

In [figure 5.1](#) are presented the absolute ground-state energies of  ${}^4\text{He}$  as a function of the model-space size  $N_{\text{max}}$  calculated in the IT-NCSM for the NN+3N-induced and NN+3N-full Hamiltonian with different SRG flow parameter  $\alpha = 0.04 \text{ fm}^4$  and  $0.08 \text{ fm}^4$ . The same analysis is depicted for  ${}^{16}\text{O}$  in [figure 5.2](#). All calculations have been performed with the harmonic-oscillator frequency  $\hbar\Omega = 20 \text{ MeV}$ . The solid blue line corresponds to the Hamiltonian containing the explicit 3N interaction, dashed lines to the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}} \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters. Especially for  ${}^4\text{He}$ , MR-NO2B( $6\hbar\Omega$ ) approximations have been used, in order to analyze more precisely the dependence on the reference state. Error bars indicate the uncertainties of the threshold extrapolations of the IT-NCSM [[Rot09](#)].

#### Analysis for ${}^4\text{He}$ :

For the NN+3N-induced Hamiltonian, the larger the parameter  $N_{\text{max}}^{\text{ref}}$ , the better the agreement between the exact calculations and the MR-NO2B approximations for sufficiently large  $N_{\text{max}}$ . To quantify this observation, consider for the largest  $N_{\text{max}}$  the relative deviations between the exact and the approximations of the hard NN+3N-induced Hamiltonian which decreases monotonically with increasing  $N_{\text{max}}^{\text{ref}} = 0, 2, 4, 6$  from 2% to 1.7% to 1.2% and finally to 0.9%. Note that these are the absolute value of the relative deviations. The sign of these values is always negativ, meaning that the omitted 3B contribution is repulsiv. Similar patterns are observed for the soft NN+3N-induced Hamiltonian, where the relative deviations decrease from 1.4% to 1.0% to 0.5%, and then to 0.4%.

In contrast, the hard and soft NN+3N-full Hamiltonians do not show a clear pattern. Using the hard one for  $N_{\text{max}}^{\text{ref}} = 0$  and 6, the relative deviations is less than 0.1% for sufficiently large  $N_{\text{max}}$ . This value is significantly more accurate than the results for  $N_{\text{max}}^{\text{ref}} = 2$  and 4 both amounting to deviations of 0.4%. Using the soft NN+3N-full Hamiltonian, the MR-NO2B( $N_{\text{max}}^{\text{ref}} \hbar\Omega$ ) approximations with  $N_{\text{max}}^{\text{ref}} > 0$  are consistently more accurate than the MR-NO2B( $0\hbar\Omega$ ). The relative deviation at the level of 0.8% is reduced to 0.1% by going

from  $N_{\max}^{\text{ref}} = 0$  to  $N_{\max}^{\text{ref}} = 4$ . Furthermore, the relative deviation for  $N_{\max}^{\text{ref}} = 2$  and 6 results in 0.3% which is less than the relative deviation for  $N_{\max}^{\text{ref}} = 0$ , but larger than the one for  $N_{\max}^{\text{ref}} = 4$ . This observation implies that there is no universal pattern stating that the quality of the MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximation improves with increasing  $N_{\max}^{\text{ref}}$ . The largest relative deviation at the level of 2% is observed with the hard NN+3N-induced Hamiltonian.

### Analysis for $^{16}\text{O}$ :

For the NN+3N-induced Hamiltonian, there is a weak dependence on the parameter  $N_{\max}^{\text{ref}}$ , but the uncertainties of the threshold extrapolations makes a quantitative statement difficult. On the other hand, in the case of the soft NN+3N-full Hamiltonian, using  $N_{\max}^{\text{ref}} = 2$  produces a significant improvement of about 1.2 MeV compared to the  $N_{\max}^{\text{ref}} = 0$  for sufficiently large  $N_{\max}$ . Using  $N_{\max}^{\text{ref}} = 4$  leads to a negligible improvement. The largest relative deviation at the level of  $(2.0 \pm 0.7)\%$  is again observed with the hard NN+3N-induced Hamiltonian.

### Summary:

All MR-NO2B approximations are in a very good agreement with the exact calculations. The relative as well as the absolute deviations between the exact calculations and the MR-NO2B approximations vary in a very small range. The largest relative deviation at the level of  $(2.0 \pm 0.7)\%$  is observed with the hard NN+3N-induced Hamiltonian for  $^{16}\text{O}$ .

Using the NN+3N-induced Hamiltonian, the MR-NO2B approximations for all  $N_{\max}^{\text{ref}}$  always overbind the absolute ground-state energy of  $^4\text{He}$  and  $^{16}\text{O}$  for sufficiently large  $N_{\max}$ . This implies that the omitted normal-ordered 3-body contribution of the NN+3N-induced Hamiltonian is repulsive. This statement cannot be made for the NN+3N-full Hamiltonian, where one observes different characteristics of the omitted normal-ordered 3-body contribution depending on the parameters  $\alpha$  and  $N_{\max}^{\text{ref}}$ .

Contrary to expectations, there is no universal pattern relating the quality of the MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximation systematically with  $N_{\max}^{\text{ref}}$ . For instance, the MR-NO2B( $4\hbar\Omega$ ) approximation is consistently more accurate than the MR-NO2B( $6\hbar\Omega$ ) for  $^4\text{He}$  and  $N_{\max} \geq 4$  with the soft NN+3N-full Hamiltonian. But one can definitely say that the MR-NO2B approximation is robust with respect to variation of the reference state, controlled by the parameter  $N_{\max}^{\text{ref}}$ . Nonetheless, in the majority of cases, larger  $N_{\max}^{\text{ref}}$  indeed leads to better agreement towards the exact calculation for sufficiently large  $N_{\max}$ , e.g.  $^4\text{He}$  with the hard and soft NN+3N-induced Hamiltonian.

Finally, the angular momentum of the ground state in  $^4\text{He}$  and  $^{16}\text{O}$  calculated with the Hamiltonian in MR-NO2B approximation agrees with the exact calculations, which holds for all parameters  $N_{\max}^{\text{ref}}$  and  $N_{\max}$ . This is remarkable, because the translation invariance of the Hamiltonian in MR-NO2B has not been proven mathematically. The angular momenta calculated using the MR-NO2B approximations are not depicted in the figures.

In the next subsection, ground-state energies of open-shell nuclei will be analyzed.

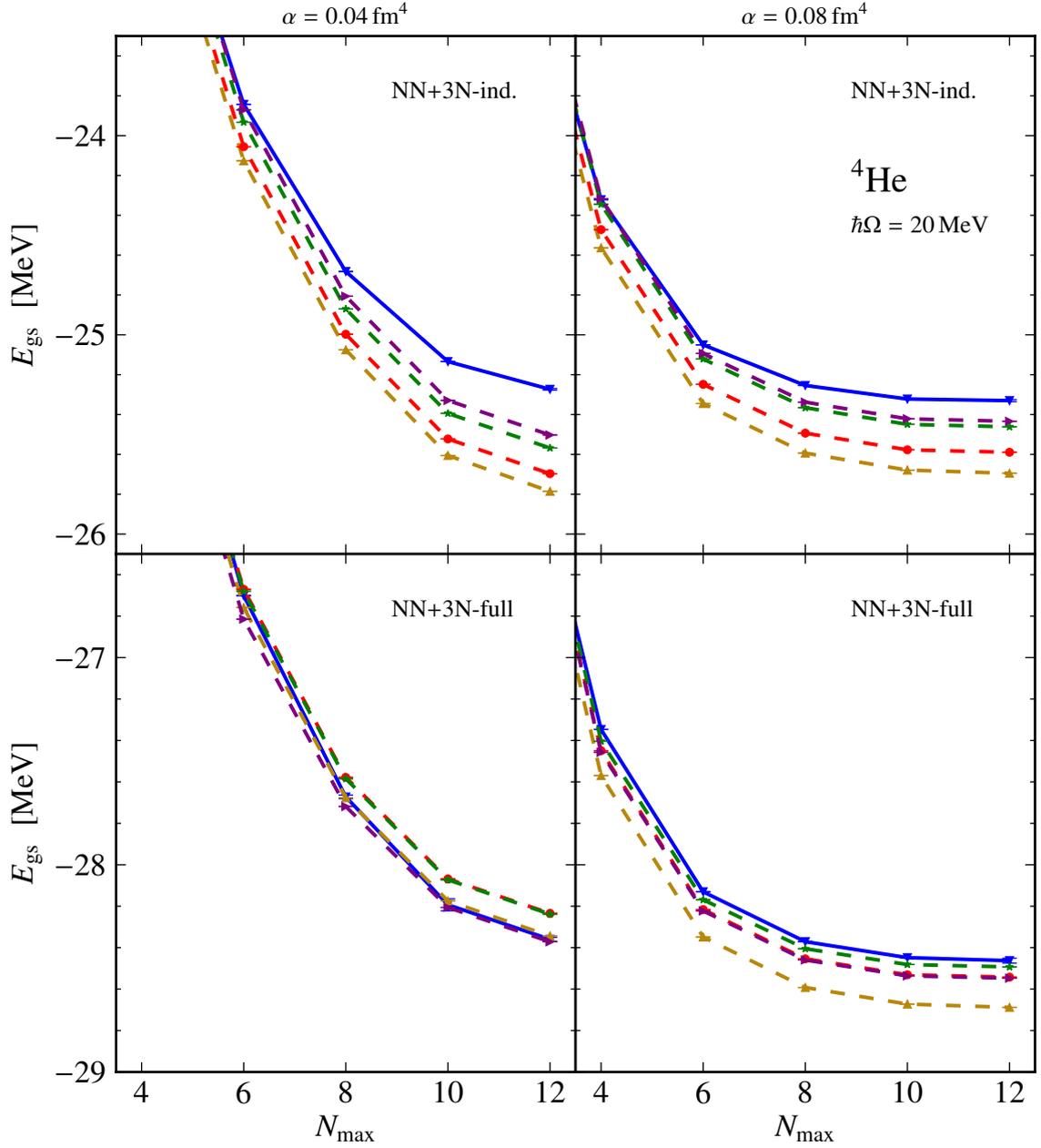


Figure 5.1.: (color online) IT-NCSM ground-state energies of  ${}^4\text{He}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right). The data points ( $\blacktriangledown$ ) connected by a solid blue line correspond to the explicit 3N interaction, dashed lines to MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 0$  ( $\blacktriangle$ ), 2 ( $\bullet$ ), 4 ( $\star$ ) and 6 ( $\blacktriangleright$ ).

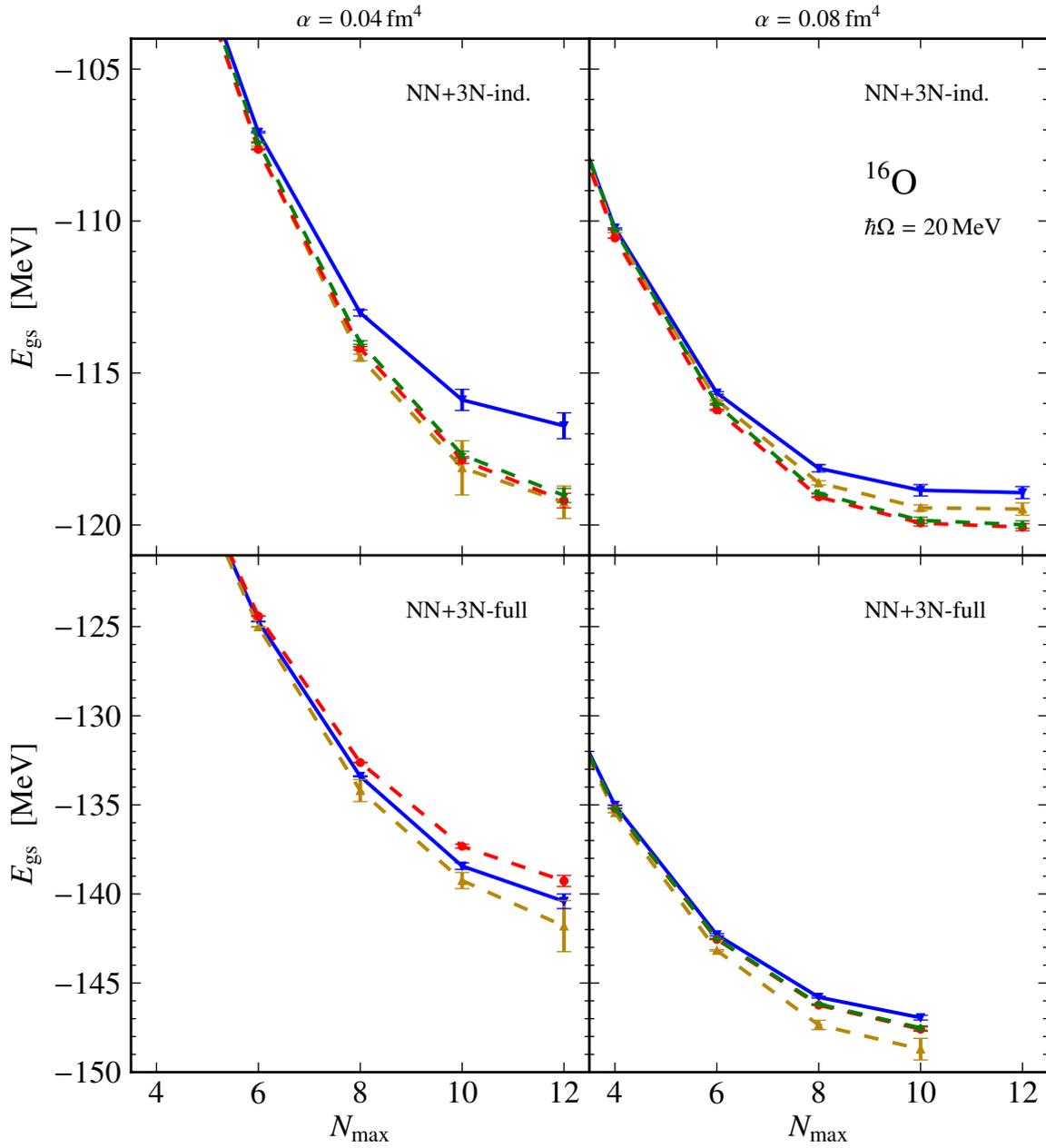


Figure 5.2.: (color online) IT-NCSM ground-state energies of  $^{16}\text{O}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right). The data points ( $\blacktriangledown$ ) connected by a solid blue line correspond to the explicit 3N interaction, dashed lines to MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 0$  ( $\blacktriangle$ ), 2 ( $\bullet$ ) and 4 ( $\blackstar$ ).

### 5.1.2. Open-Shell Nuclei

In [figure 5.3](#) are presented the absolute ground-state energies of  ${}^6\text{Li}$  as a function of the model-space size  $N_{\text{max}}$  calculated in the IT-NCSM for the NN+3N-induced Hamiltonian and NN+3N-full Hamiltonian with different SRG flow parameter  $\alpha = 0.04 \text{ fm}^4$  and  $0.08 \text{ fm}^4$ . The same analysis for  ${}^{10}\text{B}$  and  ${}^{12}\text{C}$  are shown in [figures 5.4](#) and [5.5](#), respectively. All calculations have been performed with the harmonic-oscillator frequency  $\hbar\Omega = 20 \text{ MeV}$ . The solid blue line corresponds to the Hamiltonian containing the explicit 3N interaction, dashed lines to the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}\hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters. Note that in principle MR-NO2B( $0\hbar\Omega$ ) approximations can be performed for open-shell nuclei, but they have not been considered here. Error bars indicate the uncertainties of the threshold extrapolations of the IT-NCSM.

#### Analysis for ${}^6\text{Li}$ :

For the NN+3N-induced Hamiltonian, larger  $N_{\text{max}}^{\text{ref}}$  lead to better agreement. The NN+3N-full Hamiltonian again shows a non-trivial dependence on  $N_{\text{max}}^{\text{ref}}$ . Furthermore, the MR-NO2B approximation behaves very robustly with respect to variation of the parameter  $N_{\text{max}}^{\text{ref}}$ . Finally, the largest relative deviation at the level of 1.9% is observed with the hard NN+3N-induced Hamiltonian. These observations are consistent with the investigated closed-shell nuclei.

#### Analysis for ${}^{10}\text{B}$ :

For the NN+3N-induced Hamiltonian in MR-NO2B approximations predicting a  $1^+$  for the ground state is in agreement with the angular momentum predicted by the NN+3N-induced Hamiltonian containing the explicit 3N interaction. The angular momentum of the ground state determined experimentally is a  $3^+$  which is correctly reproduced only by the NN+3N-full Hamiltonian. The corresponding MR-NO2B approximations reproduce this quantum number as well. This observation is an excellent confirmation for the quality and robustness of the MR-NO2B approximation, because the Hamiltonian in MR-NO2B approximation still contains adequate information to describe genuine 3N-interaction effects.

For a quantitative analysis, considering in the largest  $N_{\text{max}}$  the relative deviations for the hard NN+3N-induced Hamiltonian is at the order 3% for  $N_{\text{max}}^{\text{ref}} = 2$ . Using  $N_{\text{max}}^{\text{ref}} = 4$ , this deviation is halved. For the soft one, the relative deviations decrease from 3.8% to 3.1% with increasing  $N_{\text{max}}^{\text{ref}}$ . Note that for the hard and soft NN+3N-full only MR-NO2B( $2\hbar\Omega$ ) approximation has been performed. The maximum relative deviation for the NN+3N-full Hamiltonian amounts to 4% which is the largest observed relative deviation. So far, the hard NN+3N-induced Hamiltonian produced the largest relative deviations.

#### Analysis for ${}^{12}\text{C}$ :

For a quantitative analysis, considering in the largest  $N_{\text{max}}$  the relative deviations for the hard NN+3N-induced Hamiltonian that improves from 1.4% to 1.0% with increasing  $N_{\text{max}}^{\text{ref}}$ . Similar patterns are observed for the soft NN+3N-induced Hamiltonian where the relative

deviations decrease from 1.1% to 0.8%.

For the soft NN+3N-full Hamiltonian, the largest relative deviation is at the level of 0.4%. The effect of increasing  $N_{\max}^{\text{ref}}$  cannot be quantified due to the relatively large error bars. Finally, the largest relative deviation at the level of 1.5% is observed with the hard NN+3N-induced Hamiltonian, consistent with the closed-shell case.

### Summary:

Similar to the closed-shell nuclei, all MR-NO2B approximations are in a very good agreement with the exact calculations. The relative as well as the absolute deviations between the exact calculations and the MR-NO2B approximations vary in a very small range, again. The largest relative deviation at the level of 4% is observed with the hard NN+3N-full Hamiltonian for  $^{10}\text{B}$ .

Consistent with the closed-shell nuclei, there is no universal pattern relating the quality of the MR-NO2B( $N_{\max}^{\text{ref}}\hbar\Omega$ ) approximation systematically with  $N_{\max}^{\text{ref}}$ . One observes a non-trivial dependence on the  $N_{\max}^{\text{ref}}$ .

The angular momentum of the ground states in all investigated open-shell nuclei calculated with the Hamiltonian in MR-NO2B approximation agrees with the exact calculations. This holds for all parameters  $N_{\max}^{\text{ref}}$  and  $N_{\max}$ . For instance, in  $^{10}\text{B}$  the hard as well as the soft NN+3N induced Hamiltonian in MR-NO2B( $2\hbar\Omega$ ) and MR-NO2B( $4\hbar\Omega$ ) approximation reproduce the angular momenta calculated with the initial NN+3N induced Hamiltonian within all model-space sizes  $N_{\max}$ . This is remarkable, since the  $2\hbar\Omega$  and  $4\hbar\Omega$  reference states used for the MR-NO2B approximations have different angular momenta. This observation again confirms the robustness of the MR-NO2B approximation with respect to variation of the reference state.

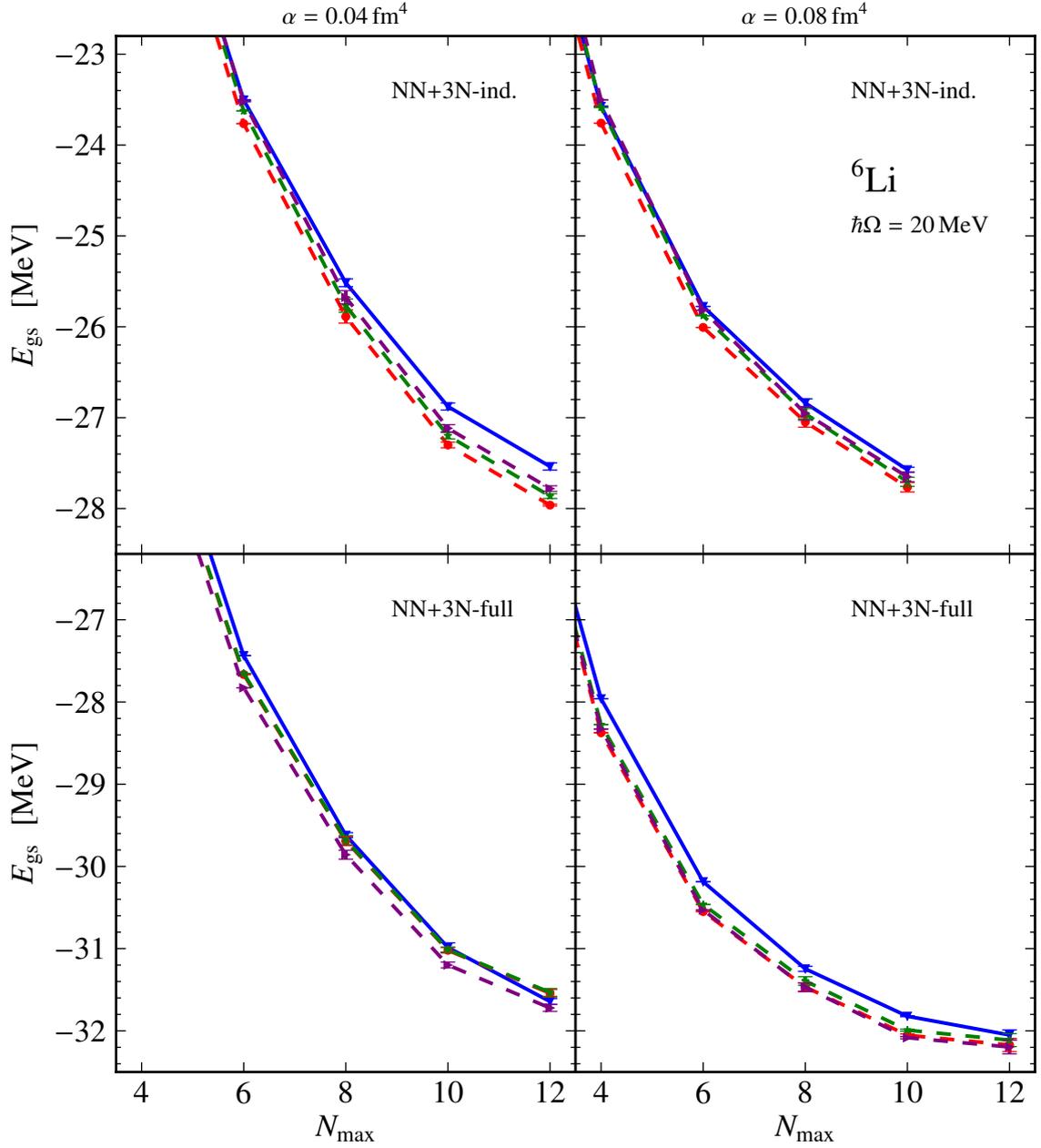


Figure 5.3.: (color online) IT-NCSM ground-state energies of  ${}^6\text{Li}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right). The data points ( $\blacktriangledown$ ) connected by a solid blue line correspond to the explicit 3N interaction, dashed lines to MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  ( $\bullet$ ), 4 ( $\star$ ) and 6 ( $\blacktriangleright$ ).

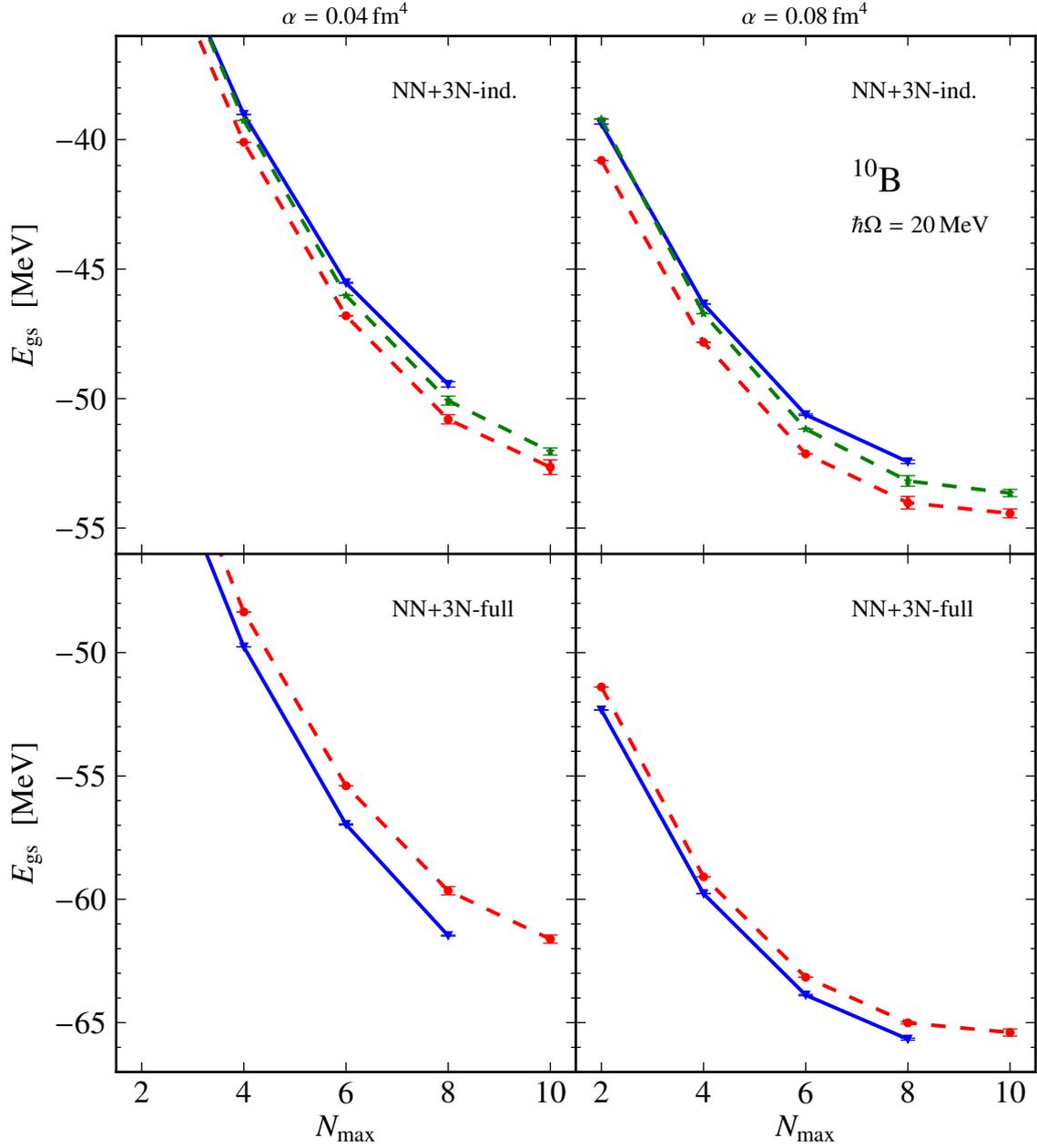


Figure 5.4.: (color online) IT-NCSM ground-state energies of  $^{10}\text{B}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right). The data points ( $\blacktriangledown$ ) connected by a solid blue line correspond to the explicit 3N interaction, dashed lines to MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  ( $\bullet$ ) and  $4$  ( $\star$ ).

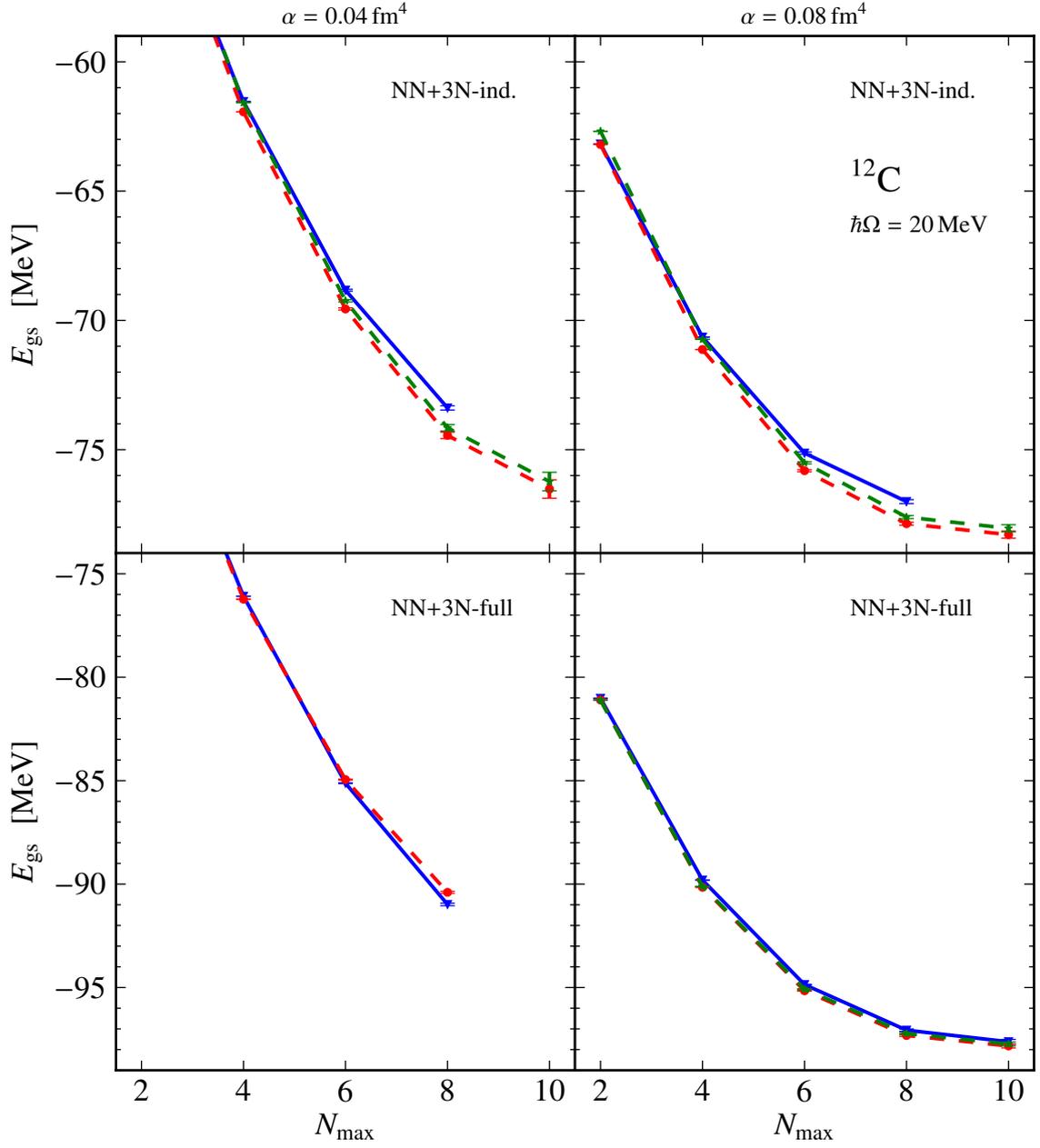


Figure 5.5.: (color online) IT-NCSM ground-state energies of  $^{12}\text{C}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right). The data points ( $\blacktriangledown$ ) connected by a solid blue line correspond to the explicit 3N interaction, dashed lines to MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  ( $\bullet$ ) and 4 ( $\star$ ).

## 5.2. Spectra

The spectra of  ${}^4\text{He}$  and  ${}^{16}\text{O}$  will not be considered. Here, only the open-shell nuclei  ${}^6\text{Li}$ ,  ${}^{10}\text{B}$  and  ${}^{12}\text{C}$  are of interest. It should be emphasized that in this section the same Hamiltonians used for the ground-state calculations are used. The reference states are still the ground states of the nucleus under consideration calculated with the considered Hamiltonian in different model-space sizes  $N_{\text{max}}^{\text{ref}}$ . Hence, no information about excited states enters the MR-NO2B approximation. Using these Hamiltonians, the three energetically low-lying excited states will be calculated and presented for each nucleus.

In figures 5.6–5.8 are presented the IT-NCSM excitation energies of  ${}^6\text{Li}$ ,  ${}^{10}\text{B}$  and  ${}^{12}\text{C}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced and NN+3N-full Hamiltonian with different SRG flow parameter  $\alpha = 0.04 \text{ fm}^4$  and  $0.08 \text{ fm}^4$ . All calculations for  ${}^6\text{Li}$  and  ${}^{12}\text{C}$  have been performed with the harmonic-oscillator frequency  $\hbar\Omega = 20 \text{ MeV}$ . For  ${}^{10}\text{B}$  additionally  $\hbar\Omega = 16 \text{ MeV}$  is considered. The blue lines correspond to the explicit 3N interaction, the other ones to MR-NO2B( $N_{\text{max}}^{\text{ref}}\hbar\Omega$ ) approximations with  $N_{\text{max}}^{\text{ref}} = 2$  and  $4$ . In order to analyze the dependence on the reference state, the MR-NO2B( $6\hbar\Omega$ ) approximation has been additionally performed for  ${}^6\text{Li}$ . Furthermore, the MR-NO2B( $4\hbar\Omega$ ) approximation has not been applied to the hard as well as to the soft NN+3N-full Hamiltonian for  ${}^{10}\text{B}$ , because the MR-NO2B approximation seems to be very robust with respect to variation of the parameter  $N_{\text{max}}^{\text{ref}}$  as seen in the previous section. Note that the excitation energies also contain errors which are not depicted in the spectra for simplicity. An error analysis reveals that the maximum error is at the level of  $0.07 \text{ MeV}$  which indeed can be neglected.

For a quantitative analysis—analogously the to ground-state analysis—absolute (relative) deviations between the exact and the MR-NO2B( $N_{\text{max}}^{\text{ref}}\hbar\Omega$ ) approximation will be analyzed in order to get a feeling how large the deviations are. As a reminder, the absolute deviation—now for a given excited state—is defined as the difference of the excitation energies between the exact calculation and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}\hbar\Omega$ ) approximation. Finally, the absolute deviation is divided by the exact excitation energy to calculate the relative deviation, denoted within the bracket. For this type of analysis no graphical illustration will be given.

### Analysis for ${}^6\text{Li}$ :

Similar patterns are observed for all Hamiltonians. Firstly, all excitation energies are described with a reasonable accuracy. Secondly, the order of all excited states is correctly reproduced. Thirdly, the MR-NO2B approximation shows a very robust behaviour with respect to variation of the parameter  $N_{\text{max}}^{\text{ref}}$  that is consistent to the ground-state analysis. Finally, all excitation energies are consistently overestimated by the MR-NO2B approximations.

Since there is nearly no dependence on the parameter  $N_{\text{max}}^{\text{ref}}$ , consider the absolute (relative) deviations for the MR-NO2B( $2\hbar\Omega$ ) approximation. For the largest  $N_{\text{max}}$ , the absolute (relative) deviations for the hard NN+3N-induced Hamiltonian and the corresponding MR-NO2B( $2\hbar\Omega$ ) approximation for the first, second and third excited states amount

to 0.12 MeV (3.9%), 0.10 MeV (2.5%) and 0.14 MeV (3.2%). For the soft one, one obtains 0.10 MeV (3.2%), 0.04 MeV (0.9%) and 0.08 MeV (1.8%).

The same analysis for the hard NN+3N-full Hamiltonian results in 0.25 MeV (9.9%), 0.24 MeV (6.0%) and 0.15 MeV (3.0%); and for the soft one 0.19 MeV (7.4%), 0.29 MeV (6.9%) and 0.10 MeV (1.9%). This analysis shows that the MR-NO2B approximation works more accurately for the NN+3N-induced than for the NN+3N-full Hamiltonian.

Finally, the maximum absolute deviation between the exact and the corresponding MR-NO2B approximation is at level of 0.1 MeV for the NN+3N-induced Hamiltonian, and 0.3 MeV for the NN+3N-full Hamiltonian. The maximum relative deviation is at level of 4% for the NN+3N-induced Hamiltonian, and 10% for the NN+3N-full Hamiltonian.

### Analysis for $^{10}\text{B}$ :

Using the hard NN+3N-induced Hamiltonian following observations are made: Firstly, all excitation energies are described with a reasonable accuracy. Secondly, the order of the first two excited states is correctly reproduced. This is remarkable because, as already mentioned, both reference states have a different structure, namely the angular momentum is  $3^+$  for  $N_{\text{max}}^{\text{ref}} = 2$ , and  $1^+$  for  $N_{\text{max}}^{\text{ref}} = 4$ . The angular momentum of the third state is not correctly described, but this could be related to the fact that the fourth excited state is energetically very close to the third one leading to level crossings. Thirdly, a weak dependence on the parameter  $N_{\text{max}}^{\text{ref}}$  is observed. Increasing  $N_{\text{max}}^{\text{ref}}$  does not necessarily lead to better agreement. For instance, the first and third excited states are better described by MR-NO2B( $2\hbar\Omega$ ) than MR-NO2B( $4\hbar\Omega$ ) approximation for  $N_{\text{max}} \geq 4$ . Finally, in contrast to  $^6\text{Li}$ , excitation energies are not consistently overestimated by the MR-NO2B approximations. Depending on  $N_{\text{max}}^{\text{ref}}$  and  $N_{\text{max}}$ , one obtains over- and underestimation for the same excited state. For instance, the excitation energy of the first excited state is underestimated by the MR-NO2B( $4\hbar\Omega$ ) approximation and overestimated by the MR-NO2B( $2\hbar\Omega$ ) approximation for  $N_{\text{max}} = 2$ . Going to larger  $N_{\text{max}}$ , the excitation energy of this state is underestimated by the MR-NO2B( $2\hbar\Omega$ ) approximation and overestimated by the MR-NO2B( $4\hbar\Omega$ ) approximation. The over- and underestimation is at the order of 0.2 MeV. The results for the soft NN+3N-induced Hamiltonian show a quite similar pattern as for the hard one.

Considering the hard NN+3N-full Hamiltonian, all excitation energies are consistently underestimated maximally at the level of 0.8 MeV. Furthermore, level crossings depending on  $N_{\text{max}}$  are correctly described. For instance, the  $0^+$  state is the first excited state for  $N_{\text{max}} = 2$ . After some level crossings, it becomes the third excited state for  $N_{\text{max}} = 8$ . This behaviour is correctly described by the MR-NO2B approximation. For the largest calculated  $N_{\text{max}}$ , the absolute (relative) deviations of the first, second and third excited states amount to 0.40 MeV (26.2%), 0.80 MeV (38.4%) and 0.4 MeV (15.8%). Badly reproduced is the energy splitting between the first and second excited state that is at the order of 0.6 MeV in the largest  $N_{\text{max}}$  for the exact calculation, and 0.18 MeV for the MR-NO2B approximation. For the soft NN+3N-full Hamiltonian, a quite similar pattern as for the hard one is observed. The absolute (relative) deviation of the first excited state amounts to 0.25 MeV (15.9%), and

for the second excited state 0.50 MeV (27.2%) that is the maximum observed deviation. For the third, it is 0.20 MeV (8.9%). Badly reproduced again is the energy splitting between the first and second excited state that is at the order of 0.25 MeV in the largest  $N_{\max}$  for the exact calculation, and 0.03 MeV for the MR-NO2B approximation.

### Analysis for $^{12}\text{C}$ :

The hard and soft NN+3N-induced Hamiltonian show similar patterns: All excitation energies are described with a reasonable accuracy. The order of all excited states is correctly reproduced. Nearly no dependence on the parameter  $N_{\max}^{\text{ref}}$  is observed. All excitation energies are consistently overestimated by the MR-NO2B approximations. The maximum absolute deviation between the exact and the corresponding MR-NO2B approximation is at level of 0.4 MeV for the hard NN+3N-induced Hamiltonian, and 0.6 MeV for the soft one. The maximum relative deviation is at level of 3.8% for the hard NN+3N-induced Hamiltonian, and 5.5% for the soft one.

Using the soft NN+3N-full Hamiltonian, all excitation energies are described with a reasonable accuracy. Furthermore, the order of the first two excited states is correctly reproduced. The angular momentum of the third state is not correctly described. This could be related to the fact that the fourth excited state is energetically very close to third one. Again, nearly no dependence on the parameter  $N_{\max}^{\text{ref}}$  is observed. Excitation energies are consistently overestimated by the MR-NO2B approximations. Finally, the maximum absolute deviation between the exact and the corresponding MR-NO2B approximation is at level of 0.9 MeV for the soft NN+3N-induced Hamiltonian, and the maximum relative deviation is at level of 7.3%.

### Dependence on $\hbar\Omega$ :

In order to analyze the dependence on the harmonic-oscillator frequency  $\hbar\Omega$ , the same calculation is performed using the NN+3N-induced and NN+3N-full Hamiltonians both with  $\alpha = 0.08 \text{ fm}^4$  for  $^{10}\text{B}$  with  $\hbar\Omega = 16 \text{ MeV}$  which is actually the convenient choice for  $^{10}\text{B}$ . The results are compared to the previous results with  $\hbar\Omega = 20 \text{ MeV}$  in [figure 5.9](#). The upper and lower panels correspond to the soft NN+3N-induced and NN+3N-full Hamiltonian, respectively.

One starts with the soft NN+3N-induced Hamiltonian. Using the harmonic-oscillator frequency  $\hbar\Omega = 16 \text{ MeV}$ , the spectra are reproduced with a much higher accuracy. In this case, even the angular momentum of the third excited state is correctly described, which did not hold for  $\hbar\Omega = 20 \text{ MeV}$ . The clear dependence on the parameter  $N_{\max}^{\text{ref}}$  vanishes for  $\hbar\Omega = 16 \text{ MeV}$ . This is due to the fact the reference states used for the MR-NO2B approximation have quite similar structure, e.g. both have angular momentum  $1^+$ .

Considering the soft NN+3N-full Hamiltonian with  $\hbar\Omega = 16 \text{ MeV}$ , the second and third states are described with a reasonable accuracy. On the other hand, the deviation for the first excited state is only 0.4 MeV. Moreover, using the harmonic-oscillator frequency  $\hbar\Omega = 16 \text{ MeV}$ , the energy splitting between the first and second excited state is much better described as with  $\hbar\Omega = 20 \text{ MeV}$ .

Finally, for a precise investigation of the dependence of the MR-NO2B approximation on the harmonic-oscillator frequency  $\hbar\Omega$ , a systematic study is necessary by considering a large number of  $\hbar\Omega$  parameter.

**Summary:**

The Hamiltonians in MR-NO2B approximations reproduce the spectrum of the nucleus under consideration even though the reference state is just the ground state.

Consistent with the ground-state analysis, the MR-NO2B approximation shows a robust behaviour with respect to variation of the parameter  $N_{\max}^{\text{ref}}$ . Moreover, the hard and soft Hamiltonians show similar patterns. This observation implies that the MR-NO2B approximation is also robust with respect to variation of the SRG flow parameter.

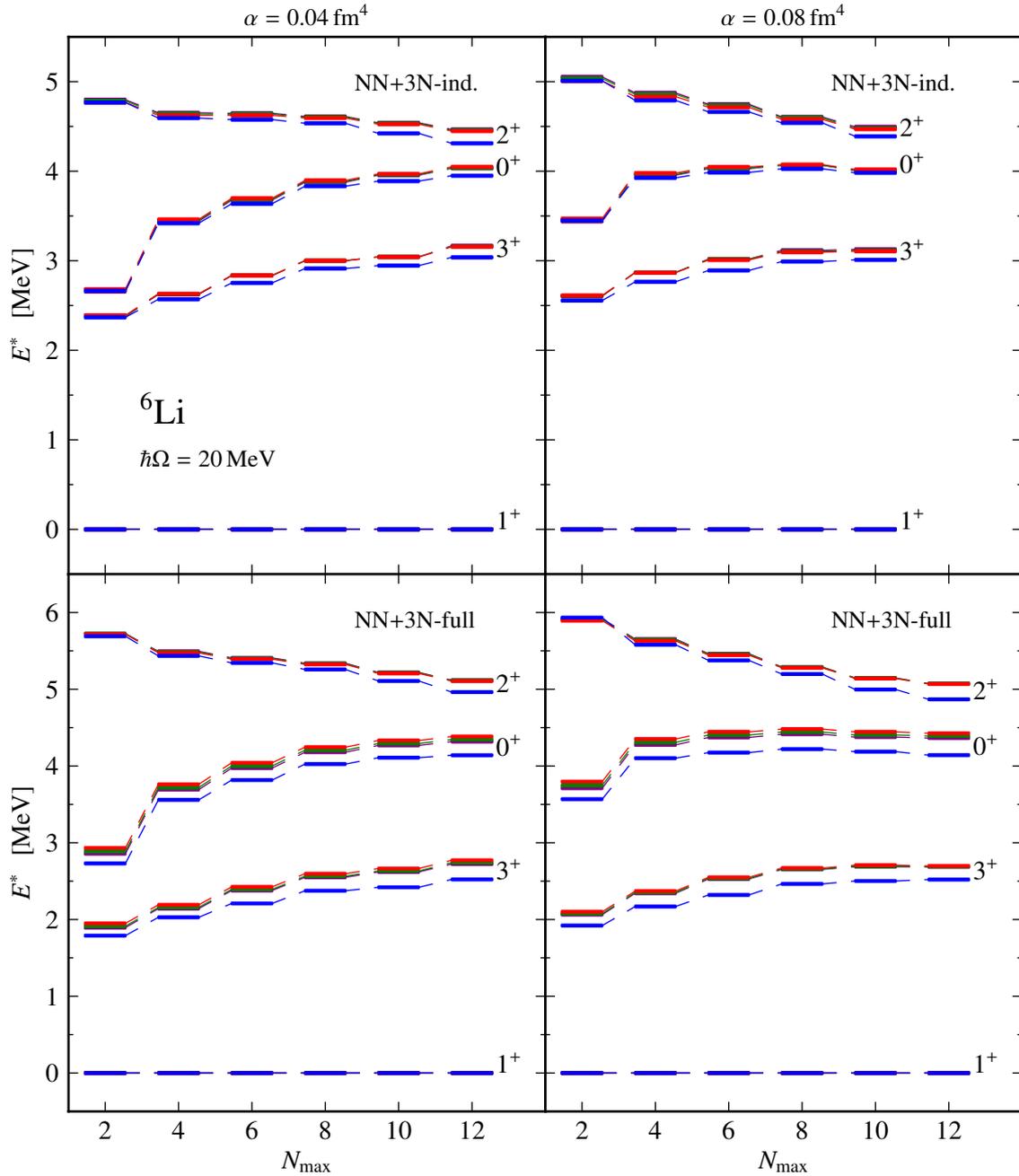


Figure 5.6.: (color online) IT-NCSM excitation energies of  ${}^6\text{Li}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $\alpha = 0.08 \text{ fm}^4$  (right). The blue lines correspond to the explicit 3N interaction, the other ones to MR-NO2B( $N_{\text{max}}^{\text{ref}} \hbar\Omega$ ) approximations with  $N_{\text{max}}^{\text{ref}} = 2, 4$  and  $6$ .

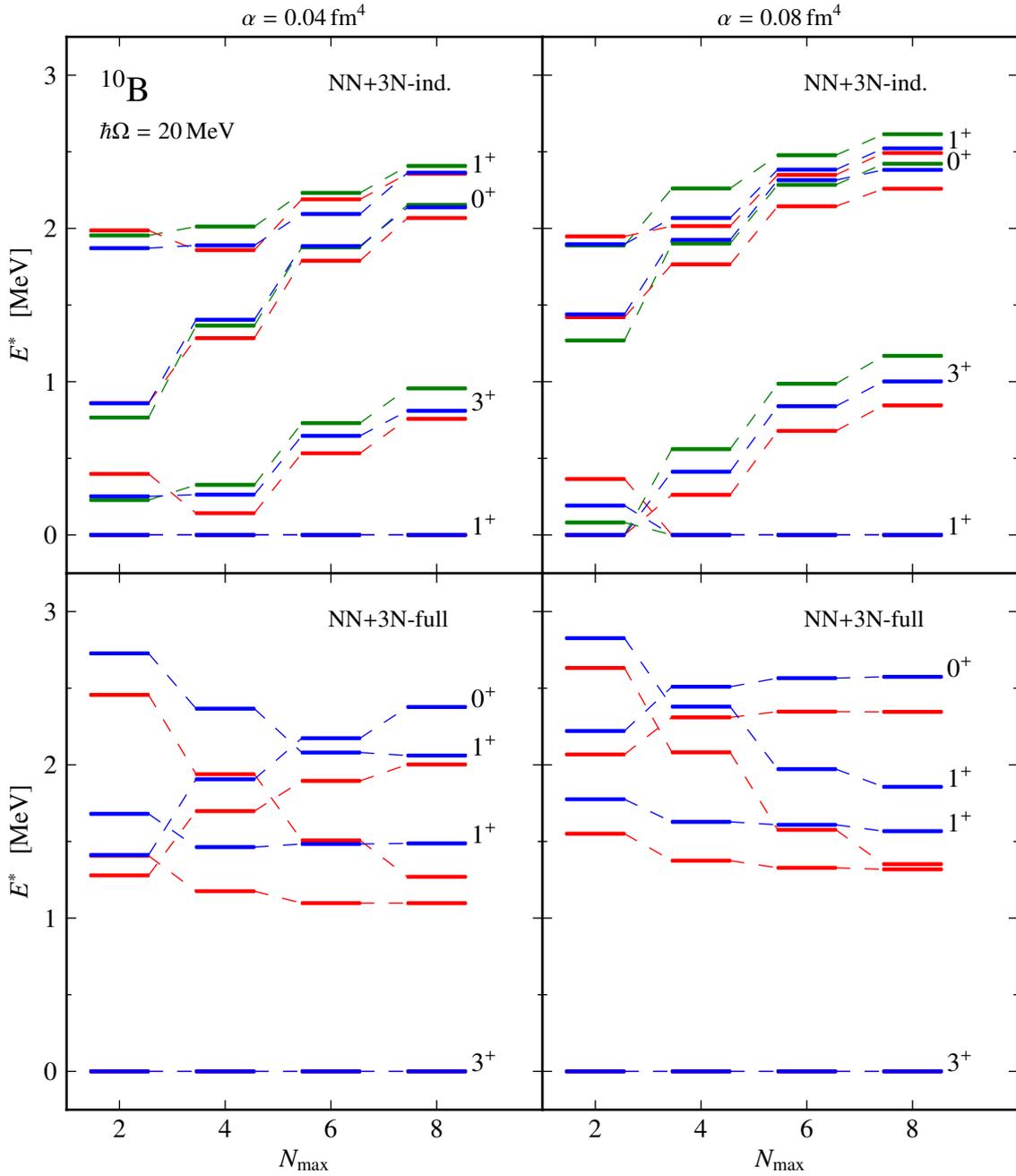


Figure 5.7.: (color online) IT-NCSM excitation energies of  $^{10}\text{B}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $\alpha = 0.08 \text{ fm}^4$  (right). The blue lines correspond to the explicit 3N interaction, the other ones to MR-NO2B( $N_{\text{max}}^{\text{ref}} \hbar\Omega$ ) approximations with  $N_{\text{max}}^{\text{ref}} = 2$  and  $4$ .

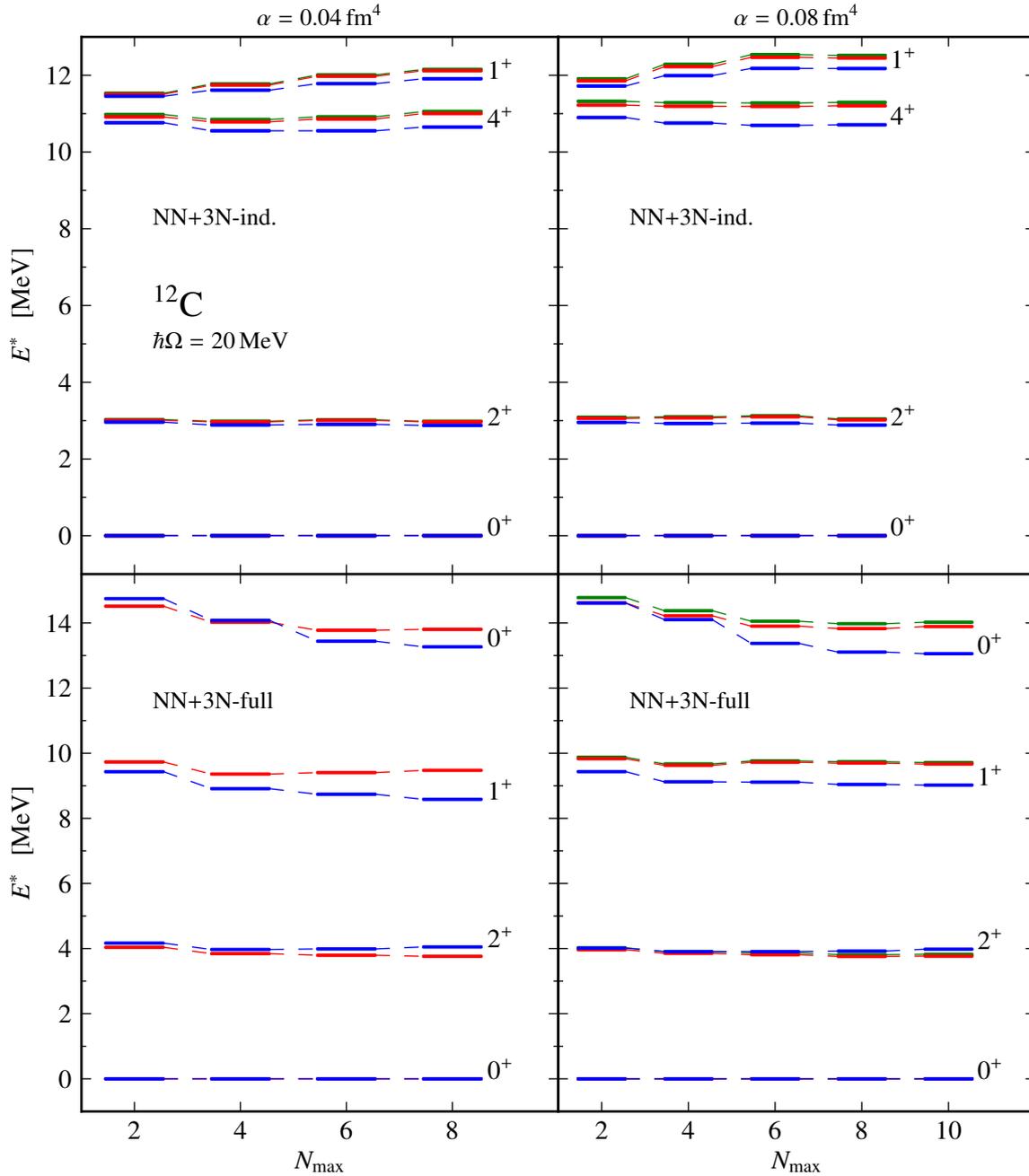


Figure 5.8.: (color online) IT-NCSM excitation energies of  $^{12}\text{C}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $\alpha = 0.08 \text{ fm}^4$  (right). The blue lines correspond to the explicit 3N interaction, the other ones to MR-NO2B( $N_{\text{max}}^{\text{ref}} \hbar\Omega$ ) approximations with  $N_{\text{max}}^{\text{ref}} = 2$  and  $4$ .

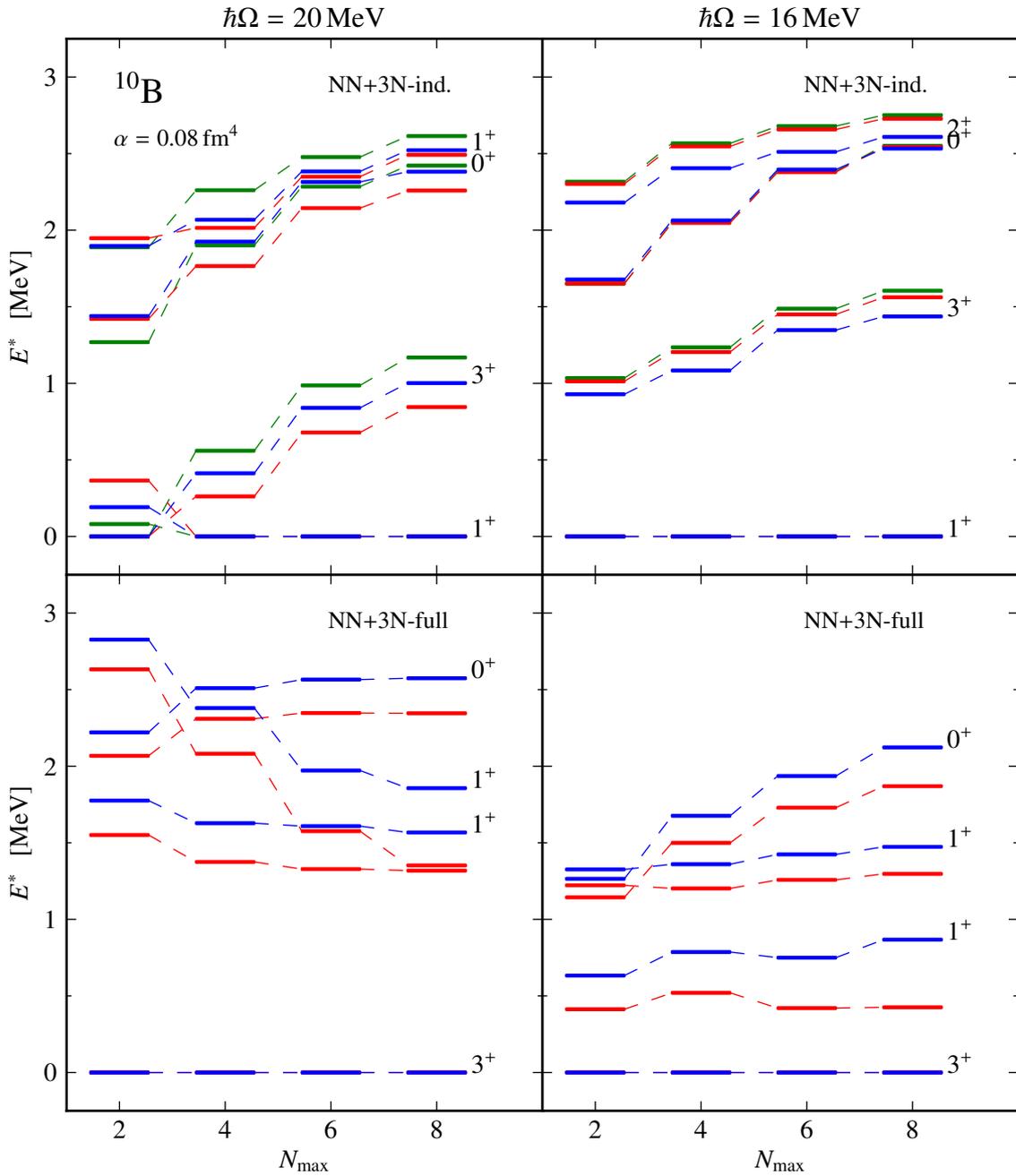


Figure 5.9.: (color online) IT-NCSM excitation energies of  $^{10}\text{B}$  as a function of  $N_{\max}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with  $\alpha = 0.08 \text{ fm}^4$  and different harmonic-oscillator frequencies  $\hbar\Omega = 20$  MeV (left) and  $\hbar\Omega = 16$  MeV (right). The blue lines correspond to the explicit 3N interaction, the other ones to MR-NO2B( $N_{\max}^{\text{ref}}, \hbar\Omega$ ) approximations with  $N_{\max}^{\text{ref}} = 2$  and  $4$ .



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# Chapter 6

## Summary and Outlook

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In this work, normal ordering and Wick's Theorem with respect to the vacuum, a single-reference and a multi-reference state have been introduced with specific attention to the mathematical formulation. Starting from the Wick's Theorem with respect to a multi-reference state taken from [Muk97], an explicit mathematical proof is given that particle-number non-conserving  $l$ -tuple contractions vanish, and that the 4-tuple contraction is antisymmetric under permutation of two arbitrarily chosen operators. Unfortunately, a general mathematical proof of the antisymmetry of the  $l$ -tuple contraction could not be worked out. Moreover, all necessary formulas for the normal-ordered  $n$ -body approximation used in this work have been derived, and their validity has been checked with [KM97].

Furthermore, the multi-reference normal-ordered  $n$ -body (MR-NO $n$ B) approximation has been derived. For the first time, it has been demonstrated that the MR-NO2B approximation allows for accurate nuclear-structure calculations using SRG-evolved chiral NN+3N Hamiltonians for open-shell nuclei—explicitly demonstrated for  ${}^6\text{Li}$ ,  ${}^{10}\text{B}$  and  ${}^{12}\text{C}$ . The obtained results show that the MR-NO2B approximation works very well for ground as well as excited states. Moreover, the MR-NO2B approximation is very robust with respect to variations of the reference state, controlled by the parameter  $N_{\text{max}}^{\text{ref}}$ . Contrary to expectations, there is no universal pattern relating the quality of the MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximation with  $N_{\text{max}}^{\text{ref}}$ .

For future investigations, there are some open tasks related to this work. The way the normal-ordering operator has been defined in this work, it is not an operator in the mathematical sense. Hence, a mathematical construction of the domain and codomain for the normal-ordering operator is necessarily needed to have a mathematical correct definition of the normal-ordering operator. Moreover, a general mathematical proof of the antisymmetry of the  $l$ -tuple contraction is left.

In this work, only nucleus-specific ground states have been used as reference states for the MR-NO2B approximation. In this manner, no explicit information about excited states enters the NO $n$ B approximation. Alternatively, one can construct reference states which contain information about excited states, e.g. a linear combination of a few low-lying excited states. In order to make use of all formulas derived in this work, one should normalize the constructed

reference state. A second way could be to perform MR-NO2B approximation with respect to the  $i$ -th excited state, in order to calculate the  $i$ -th excited state. This approach represents also a consistent possible way to choose the reference state.

In order to complete the picture of the dependence of the MR-NO2B approximation on the reference state, one should perform MR-NO2B( $0\hbar\Omega$ ) approximation for the open-shell nuclei, and for the closed-shell nuclei using the multi-reference code where the same—except numerical uncertainties—results are expected as with the single-reference code.

Using the MR-NO2B approximation, one can investigate medium-mass nuclei, where the inclusion of the complete 3N interaction is computationally too demanding. This has been done only in the case of closed-shell nuclei [Rot<sup>+</sup>12], but it remains for open-shell nuclei. Going one step farther, one can include 4N interactions by means of the MR-NO2B or MR-NO3B approximation for the 4N interaction. This is subject of present research, at least for closed-shell nuclei. By means of the NO $n$ B approximation, one avoids formal and computational challenges of including explicit 4N terms in many-body calculations. All necessary formulas to perform MR-NO2B or MR-NO3B approximation for 4N interactions with respect to a multi-reference state have been already derived in [appendix A](#). For the NO3B approximation of the 4N interaction, the three-particle density matrix elements will be needed explicitly which will increase the computational cost. One possible way to overcome this problem is calculate the three-particle density matrix elements on-the-fly while as much as possible is stored. Such an optimized method or function making use of all symmetries of the three-particle density matrix element is already implemented and is ready for use.

Finally, one should benchmark other observables, e.g. electromagnetic transition strengths that are more sensitive to the structure of the nucleus under consideration.

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# Appendix A

## $m$ -Nucleon Interaction in Reference-State Representation

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The aim of this chapter is to formulate the  $m$ -nucleon ( $mN$ ) interaction in reference-state representation, where the reference-state  $|\Psi\rangle$  is a multi-determinantal state, and to simplify it as far as possible. Furthermore, some special cases will be considered to confirm its validity.

The starting point for the derivation is the  $mN$  interaction in second quantization that reads

$$V_{mN} = \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} a_{q_1 \dots q_m}^{p_1 \dots p_m}, \quad (\text{A.1})$$

where  $v_{q_1 \dots q_m}^{p_1 \dots p_m} := \langle p_1 \dots p_m | V_{mN} | q_1 \dots q_m \rangle$  denotes the antisymmetrized  $m$ -body matrix element, and  $a_{q_1 \dots q_m}^{p_1 \dots p_m}$  the  $m$ -body operator in tensor notation. Note that the sum runs over all upper and lower indices, but this has been left out to retain overview.

As a reminder, the results obtained for the one-, two- and three-body operator expressed as a sum of the zero-, one-, two- and three-body operator in MR-NO from (3.182)–(3.184) are given by

$$a_q^p = \tilde{a}_q^p + \gamma_q^p, \quad (\text{A.2})$$

$$a_{qs}^{pr} = \tilde{a}_{qs}^{pr} + \mathbb{A}(\gamma_q^p \tilde{a}_s^r) + \gamma_{qs}^{pr}, \quad (\text{A.3})$$

$$a_{qsu}^{prt} = \tilde{a}_{qsu}^{prt} + \mathbb{A}(\gamma_q^p \tilde{a}_{su}^{rt}) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{a}_u^t) + \gamma_{qsu}^{prt}, \quad (\text{A.4})$$

where  $\mathbb{A}$  is the index antisymmetrizer defined in section 3.2. Taking a closer look, this result can be—without proof—generalized to an  $m$ -body operator as follows

$$a_{q_1 \dots q_m}^{p_1 \dots p_m} = \tilde{a}_{q_1 \dots q_m}^{p_1 \dots p_m} + \sum_{i=1}^{m-1} \mathbb{A} \left( \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \right) + \gamma_{q_1 \dots q_m}^{p_1 \dots p_m}. \quad (\text{A.5})$$

Before inserting this generalization into (A.1), it is convenient to introduce the  $i$ -body contribution in MR-NO  $\tilde{V}_i$  for a given  $m$ N interaction as follows

$$\tilde{V}_m := \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \tilde{a}_{q_1 \dots q_m}^{p_1 \dots p_m}, \quad (\text{A.6})$$

$$\tilde{V}_i := \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \mathbb{A} \left( \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \right), \quad i = 1, 2, \dots, m-1 \quad (\text{A.7})$$

$$\tilde{V}_0 := \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_m}^{p_1 \dots p_m}. \quad (\text{A.8})$$

Note that the 0-body contribution in MR-NO is equivalent to the expectation value of the  $m$ N interaction regarding  $|\Psi\rangle$ , i.e.

$$\tilde{V}_0 = \langle \Psi | V_{mN} | \Psi \rangle. \quad (\text{A.9})$$

This observation is helpful to simplify numerical calculations because the expectation value of the  $m$ N interaction with respect to  $|\Psi\rangle$  can be calculated using the Slater-Condon rules [Sla29; Con30] that is computationally less demanding than calculating the 0-body contribution using its definition. Hence, the  $m$ -particle density matrix element is not explicitly needed.

Since  $v_{q_1 \dots q_m}^{p_1 \dots p_m}$  and the index antisymmetrizer  $\mathbb{A}$  in (A.7) are antisymmetric, the product is symmetric. Consequently, by renaming the indices of the sum in (A.8), one obtains for the  $i$ -body contribution in MR-NO

$$\begin{aligned} \tilde{V}_i &= \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \mathbb{A} \left( \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \right) \\ &= \frac{1}{(m!)^2} \left( \frac{(m!)^2}{(i!)^2 ((m-i)!)^2} \right) \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \end{aligned} \quad (\text{A.10})$$

$$= \frac{1}{(i!)^2 ((m-i)!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m}. \quad (\text{A.11})$$

The factor in (A.10) follows directly from the definition of the index antisymmetrizer  $\mathbb{A}$ . First, all possible permutations of the  $m$  upper and  $m$  lower indices generates  $(m!)^2$  terms. If  $\mathbb{A}$  acts on a quantity, one needs to consider that every permuted term appears with coefficient unity. The  $i$ -particle density matrix element  $\gamma_{q_1 \dots q_i}^{p_1 \dots p_i}$  is per definition antisymmetric with respect to transpositions of the upper and lower indices, one obtains  $(i!)^2$  terms of the same form which can be simplified by renaming the indices. Analogously, acting with  $\mathbb{A}$  on the  $(m-i)$ -body operator  $\tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m}$  produces  $((m-i)!)^2$  terms. Due to combinatorial analysis, one needs to divide  $(m!)^2$  by the product of  $(i!)^2$  and  $((m-i)!)^2$ .

Hence, the  $mN$  interaction in reference-state representation reads

$$\begin{aligned}
V_{mN} &= \tilde{V}_m + \sum_{i=1}^{m-1} \tilde{V}_i + \tilde{V}_0 \\
&= \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \tilde{a}_{q_1 \dots q_m}^{p_1 \dots p_m} \\
&\quad + \sum_{i=1}^{m-1} \left( \frac{1}{(i!)^2 ((m-i)!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \right) \\
&\quad + \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_m}^{p_1 \dots p_m}.
\end{aligned} \tag{A.12}$$

Finally, two special cases will be considered:

As a cross-check, consider the case of  $m = 3$  that has been extensively discussed in [section 3.5.6](#). It follows immediately from (A.12)

$$\begin{aligned}
V_{3N} &= \frac{1}{36} \sum v_{q_1 q_2 q_3}^{p_1 p_2 p_3} \tilde{a}_{q_1 q_2 q_3}^{p_1 p_2 p_3} \\
&\quad + \frac{1}{4} \sum v_{q_1 q_2 q_3}^{p_1 p_2 p_3} \gamma_{q_1}^{p_1} \tilde{a}_{q_2 q_3}^{p_2 p_3} + \frac{1}{4} \sum v_{q_1 q_2 q_3}^{p_1 p_2 p_3} \gamma_{q_1 q_2}^{p_1 p_2} \tilde{a}_{q_3}^{p_3} \\
&\quad + \frac{1}{36} \sum v_{q_1 q_2 q_3}^{p_1 p_2 p_3} \gamma_{q_1 q_2 q_3}^{p_1 p_2 p_3},
\end{aligned} \tag{A.13}$$

which is consistent with the results obtained in (4.11).

Finally, the special case of  $|\Psi\rangle$  consisting of a single Slater determinant will be considered. For this case, the reference state does not contain any correlations, i.e. the  $i$ -particle density matrix element  $\gamma_{q_1 \dots q_i}^{p_1 \dots p_i}$  factorizes in a product of one-particle density matrix elements, each of them corresponding to a Kronecker's delta, i.e.

$$\begin{aligned}
\gamma_{q_1 \dots q_i}^{p_1 \dots p_i} &= \mathbb{A} \left( \gamma_{q_1}^{p_1} \dots \gamma_{q_i}^{p_i} \right) \\
&= \mathbb{A} \left( \delta_{q_1}^{p_1} \dots \delta_{q_i}^{p_i} \right) \\
&= \begin{cases} \mathbb{A} \left( \delta_{\beta_1}^{\alpha_1} \dots \delta_{\beta_i}^{\alpha_i} \right), & \text{if for all } p_j \in \{\alpha_1, \dots, \alpha_i\} \\ & \text{and } q_j \in \{\beta_1, \dots, \beta_i\} \\ 0, & \text{else.} \end{cases}
\end{aligned} \tag{A.14}$$

Here, the indices  $\alpha_1, \dots, \alpha_i$  and  $\beta_1, \dots, \beta_i$  are hole indices, i.e. they label states occupied in  $|\phi\rangle$ . Hence, the  $i$ -body operator in MR-NO can be simplified to

$$\begin{aligned}
\tilde{V}_i &= \frac{1}{(i!)^2 ((m-i)!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_i}^{p_1 \dots p_i} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \\
&= \frac{1}{(i!)^2 ((m-i)!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \mathbb{A} \left( \delta_{\beta_1}^{\alpha_1} \dots \delta_{\beta_i}^{\alpha_i} \right) \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \\
&= \frac{1}{(i!)^2 ((m-i)!)^2} i! \sum v_{\alpha_1 \dots \alpha_i q_{i+1} \dots q_m}^{\alpha_1 \dots \alpha_i p_{i+1} \dots p_m} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \\
&= \frac{1}{i! ((m-i)!)^2} \sum v_{\alpha_1 \dots \alpha_i q_{i+1} \dots q_m}^{\alpha_1 \dots \alpha_i p_{i+1} \dots p_m} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m}.
\end{aligned} \tag{A.15}$$

The factor  $\frac{(i!)^2}{i!} = i!$  can be derived with the same combinatorial analysis as explained above, but taking into account that all quantities within  $\mathbb{A}$  have the same label which produces the factor  $i!$  in the denominator. Note that the sum in (A.15) still runs over the indices  $\alpha_1, \dots, \alpha_i, p_{i+1}, \dots, p_m$  and  $q_{i+1}, \dots, q_m$ . Analogously, one obtains

$$\tilde{V}_0 = \frac{1}{(m!)^2} \sum v_{q_1 \dots q_m}^{p_1 \dots p_m} \gamma_{q_1 \dots q_m}^{p_1 \dots p_m} = \frac{1}{m!} \sum v_{\alpha_1 \dots \alpha_m}^{\alpha_1 \dots \alpha_m}. \quad (\text{A.16})$$

Introducing the notation

$$W_{q_1 \dots q_m}^{p_1 \dots p_m} := v_{q_1 \dots q_m}^{p_1 \dots p_m}, \quad (\text{A.17})$$

$$W_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} := \frac{1}{i!} \sum_{\alpha_1 \dots \alpha_i} v_{\alpha_1 \dots \alpha_i q_{i+1} \dots q_m}^{\alpha_1 \dots \alpha_i p_{i+1} \dots p_m}, \quad (\text{A.18})$$

$$W := \frac{1}{m!} \sum_{\alpha_1 \dots \alpha_m} v_{\alpha_1 \dots \alpha_m}^{\alpha_1 \dots \alpha_m}, \quad (\text{A.19})$$

it follows from (A.12) for the  $mN$  interaction in **single** reference-state representation

$$\begin{aligned} V_{mN} &= \frac{1}{(m!)^2} \sum W_{q_1 \dots q_m}^{p_1 \dots p_m} \tilde{a}_{q_1 \dots q_m}^{p_1 \dots p_m} \\ &+ \sum_{i=1}^{m-1} \left( \frac{1}{((m-i)!)^2} \sum_{\substack{p_{i+1} \dots p_m \\ q_{i+1} \dots q_m}} W_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \tilde{a}_{q_{i+1} \dots q_m}^{p_{i+1} \dots p_m} \right) \\ &+ W. \end{aligned} \quad (\text{A.20})$$

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# Appendix B

## Plots for Deviations of the Ground-State Energies

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### B.1. Absolute Deviations

As a reminder, the definition of the absolute deviation between the exact and the corresponding MR-NO2B approximation

$$\Delta_{\text{abs}} := E_{\text{MR-NO2B}} - E_{\text{explicit-3N}}, \quad (\text{B.1})$$

$$\Delta_{\text{rel}} := \frac{\Delta_{\text{abs}}}{E_{\text{explicit-3N}}} = \frac{E_{\text{MR-NO2B}}}{E_{\text{explicit-3N}}} - 1, \quad (\text{B.2})$$

where  $E_{\text{explicit-3N}}$  and  $E_{\text{MR-NO2B}}$  denote the ground-state energy calculated with the explicit 3N interaction and the MR-NO2B approximation, respectively. Obviously, the absolute deviations depend on the parameters  $N_{\text{max}}^{\text{ref}}$  and  $N_{\text{max}}$ . The MR-NO2B approximation overbinds the exact ground-state energy if  $\Delta_{\text{abs}}$  is negative. Since  $E_{\text{explicit-3N}}$  and  $E_{\text{MR-NO2B}}$  contains error, error propagation needs to be considered:

$$\Delta(\Delta_{\text{abs}}) = \sqrt{(\Delta E_{\text{explicit-3N}})^2 - (\Delta E_{\text{MR-NO2B}})^2}. \quad (\text{B.3})$$

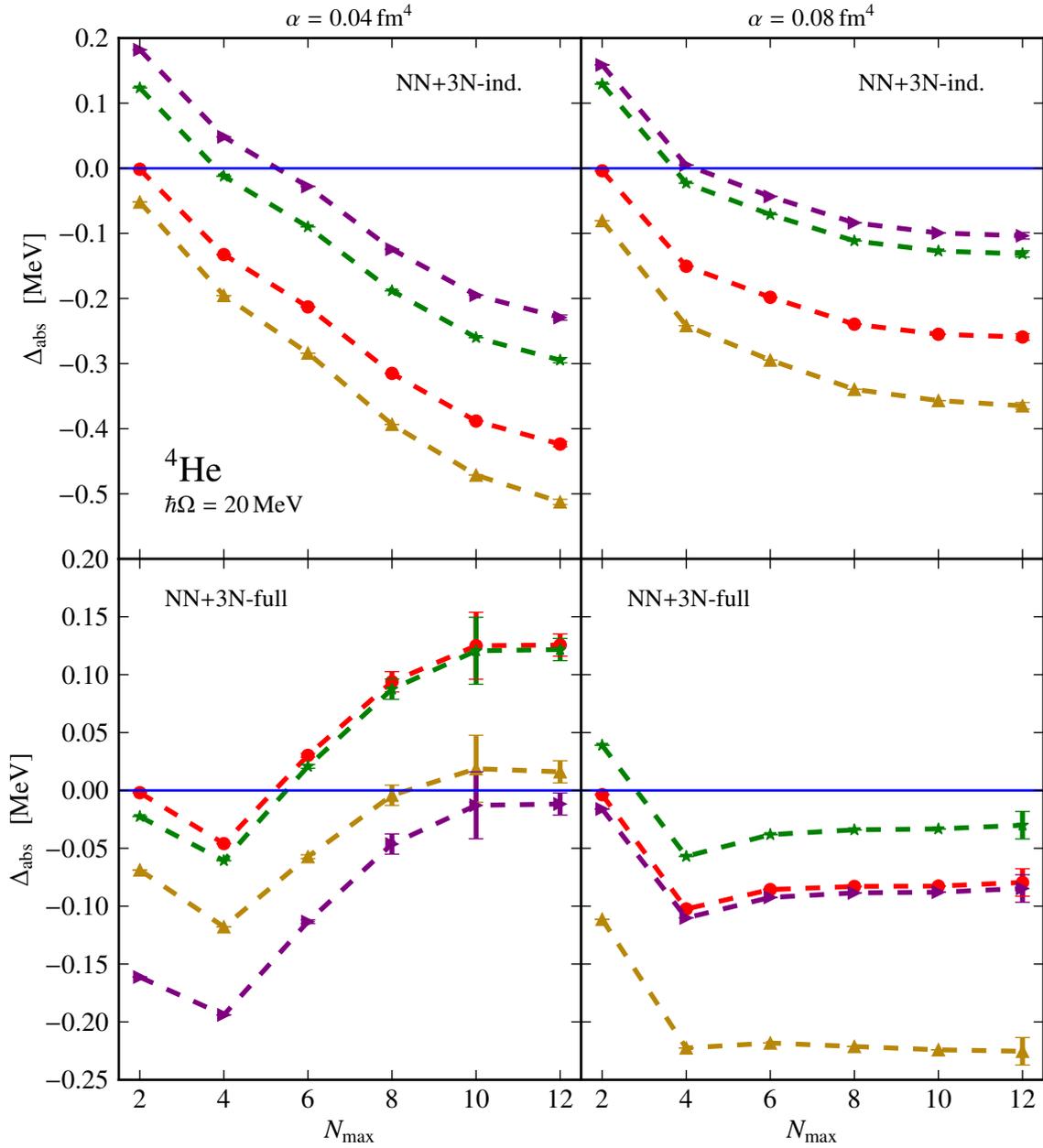


Figure B.1.: (color online) Absolute deviations for  ${}^4\text{He}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 0$  ( $\blacktriangle$ ), 2 ( $\bullet$ ), 4 ( $\star$ ) and 6 ( $\blacktriangleright$ ).

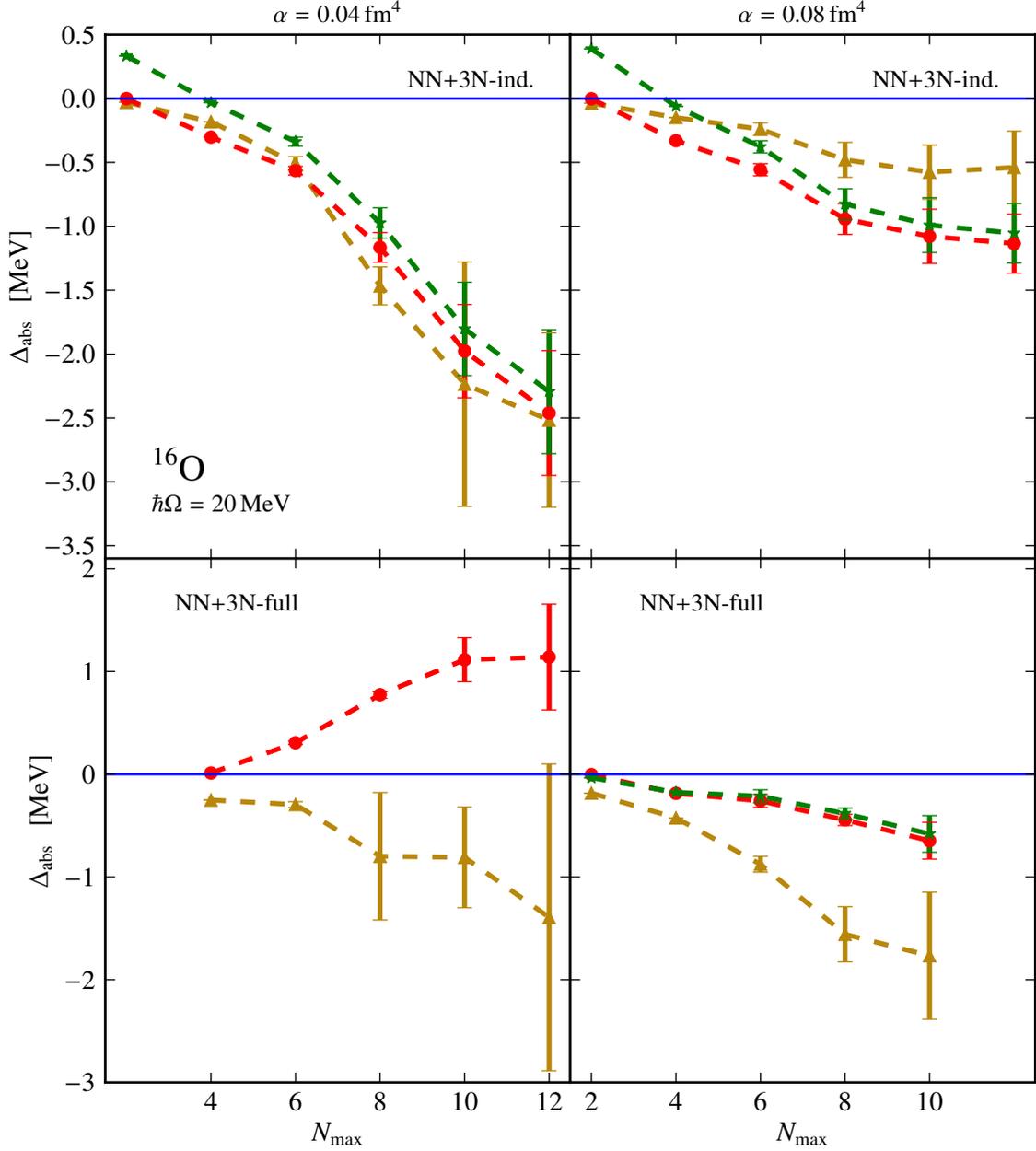


Figure B.2.: (color online) Absolute deviations for  $^{16}\text{O}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 0$  ( $\blacktriangle$ ), 2 ( $\bullet$ ) and 4 ( $\star$ ).

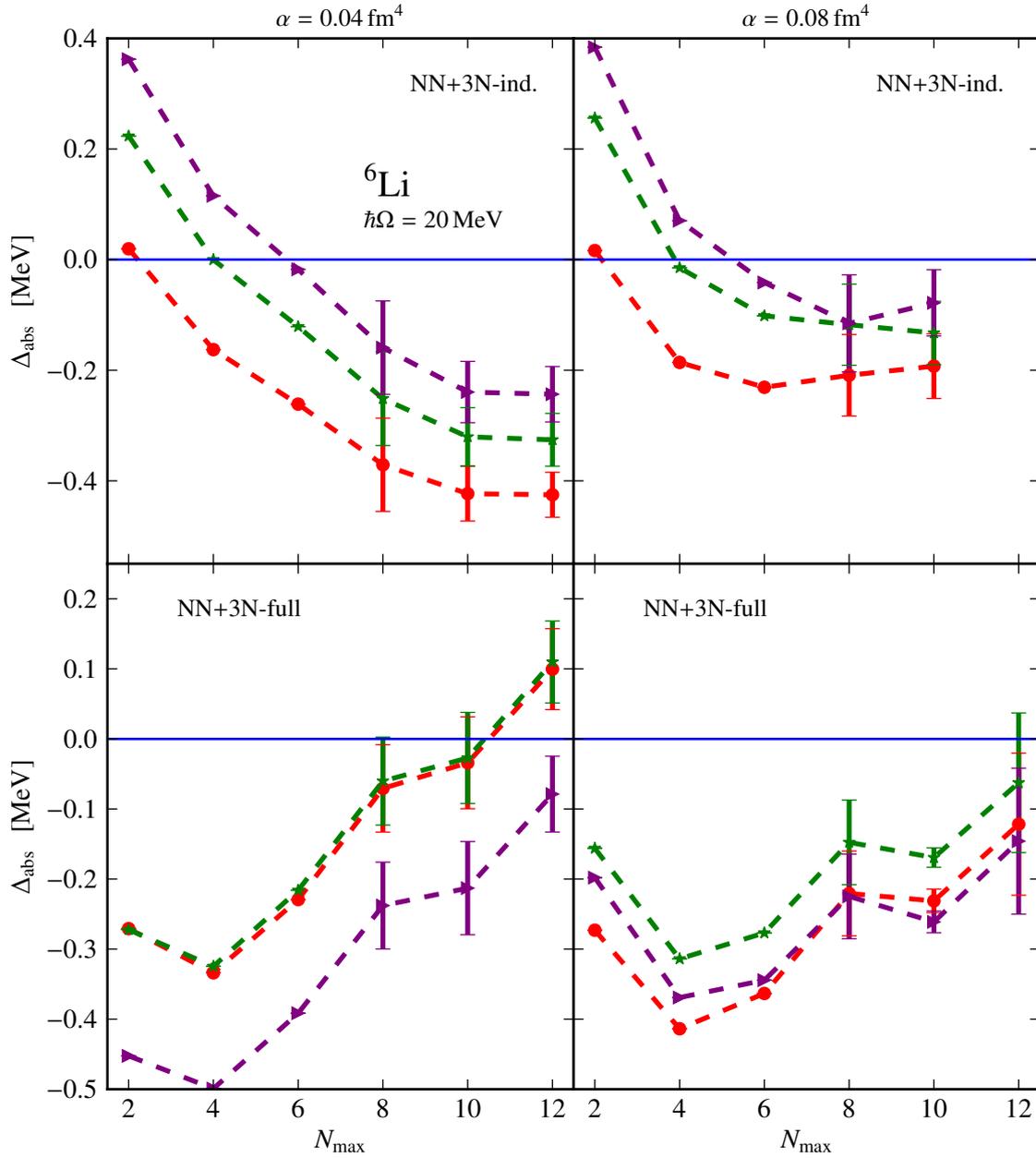


Figure B.3.: (color online) Absolute deviations for  ${}^6\text{Li}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  (●) and 4 (★) and 6 (▲).

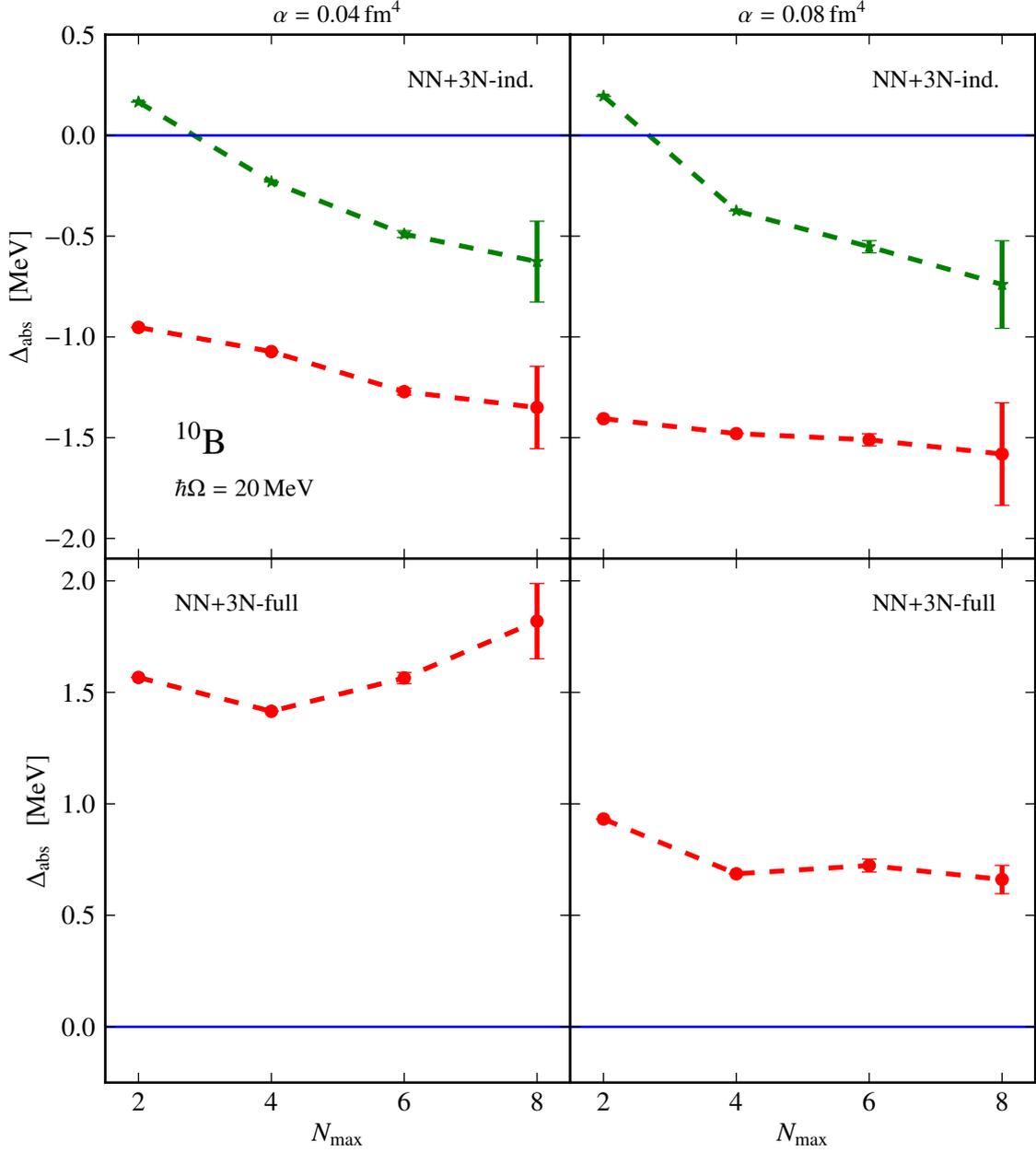


Figure B.4.: (color online) Absolute deviations for  $^{10}\text{B}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  (●) and 4 (★).

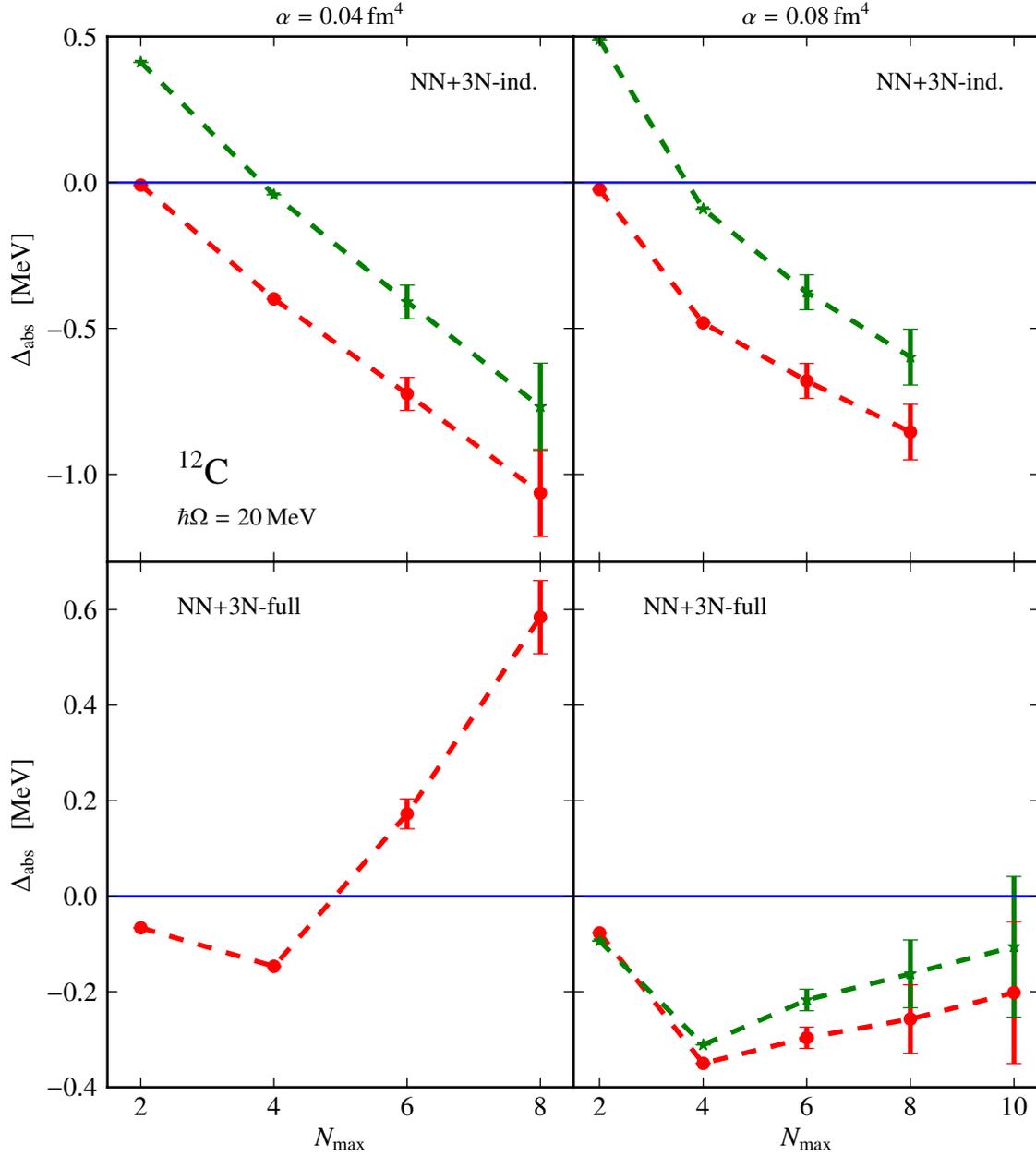


Figure B.5.: (color online) Absolute deviations for  $^{12}\text{C}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  (●) and 4 (★).

## B.2. Relative Deviations

As a reminder, the definition of the relative deviation between the exact and the corresponding MR-NO2B approximation

$$\Delta_{\text{rel}} := \frac{\Delta_{\text{abs}}}{E_{\text{explicit-3N}}} = \frac{E_{\text{MR-NO2B}}}{E_{\text{explicit-3N}}} - 1, \quad (\text{B.4})$$

where  $E_{\text{explicit-3N}}$  and  $E_{\text{MR-NO2B}}$  denote the ground-state energy calculated with the explicit 3N interaction and the MR-NO2B approximation, respectively. Obviously, the relative deviations depend on the parameters  $N_{\text{max}}^{\text{ref}}$  and  $N_{\text{max}}$ . The MR-NO2B approximation overbinds the exact ground-state energy if  $\Delta_{\text{rel}}$  is negative. Since  $E_{\text{explicit-3N}}$  and  $E_{\text{MR-NO2B}}$  contains error, error propagation needs to be considered:

$$\Delta(\Delta_{\text{rel}}) = \left| \frac{E_{\text{MR-NO2B}}}{E_{\text{explicit-3N}}} \right| \sqrt{\left( \frac{\Delta E_{\text{explicit-3N}}}{E_{\text{explicit-3N}}} \right)^2 + \left( \frac{\Delta E_{\text{MR-NO2B}}}{E_{\text{MR-NO2B}}} \right)^2}. \quad (\text{B.5})$$

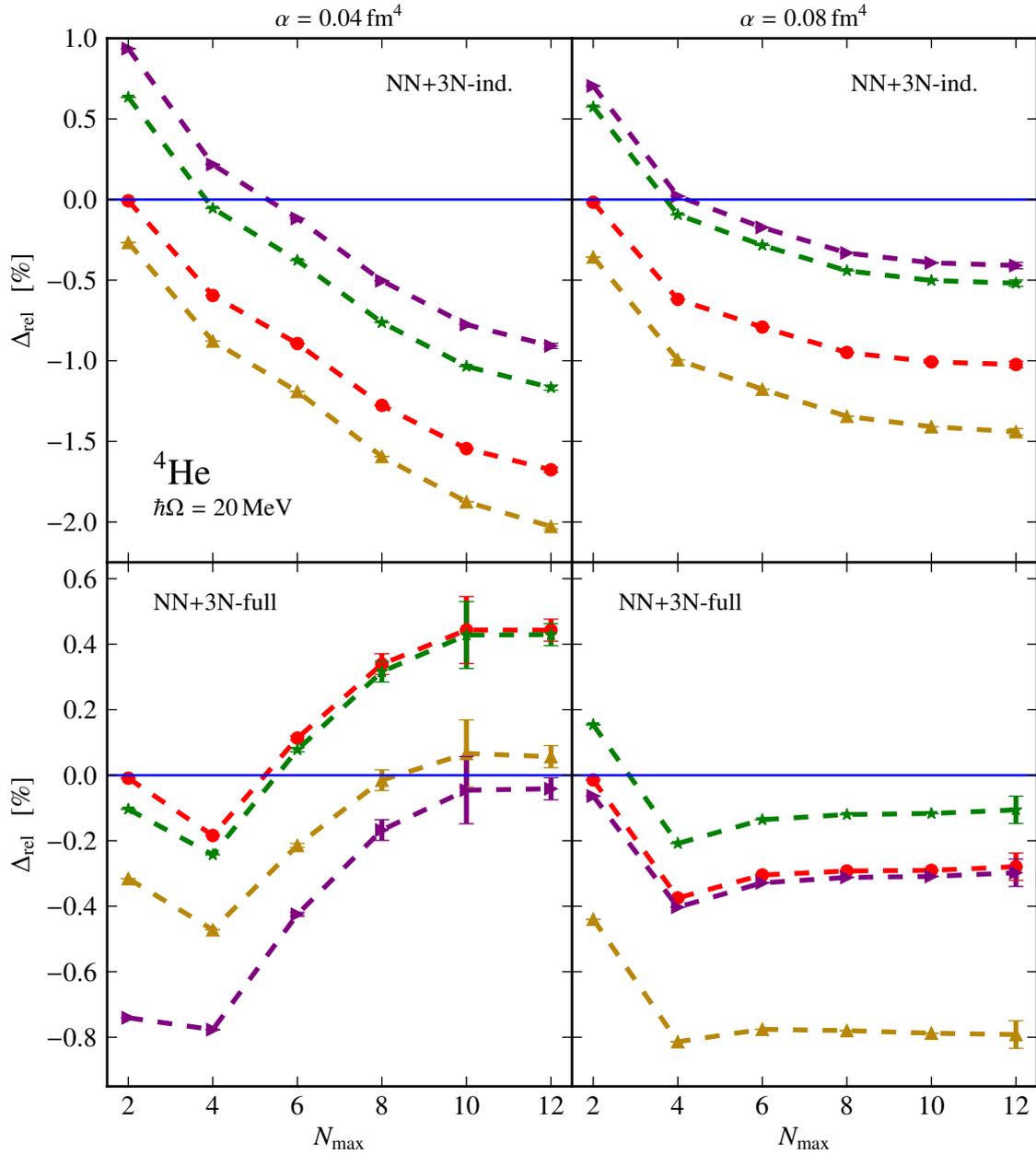


Figure B.6.: (color online) Relative deviations for  ${}^4\text{He}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 0$  ( $\blacktriangle$ ), 2 ( $\bullet$ ), 4 ( $\star$ ) and 6 ( $\blacktriangleright$ ).

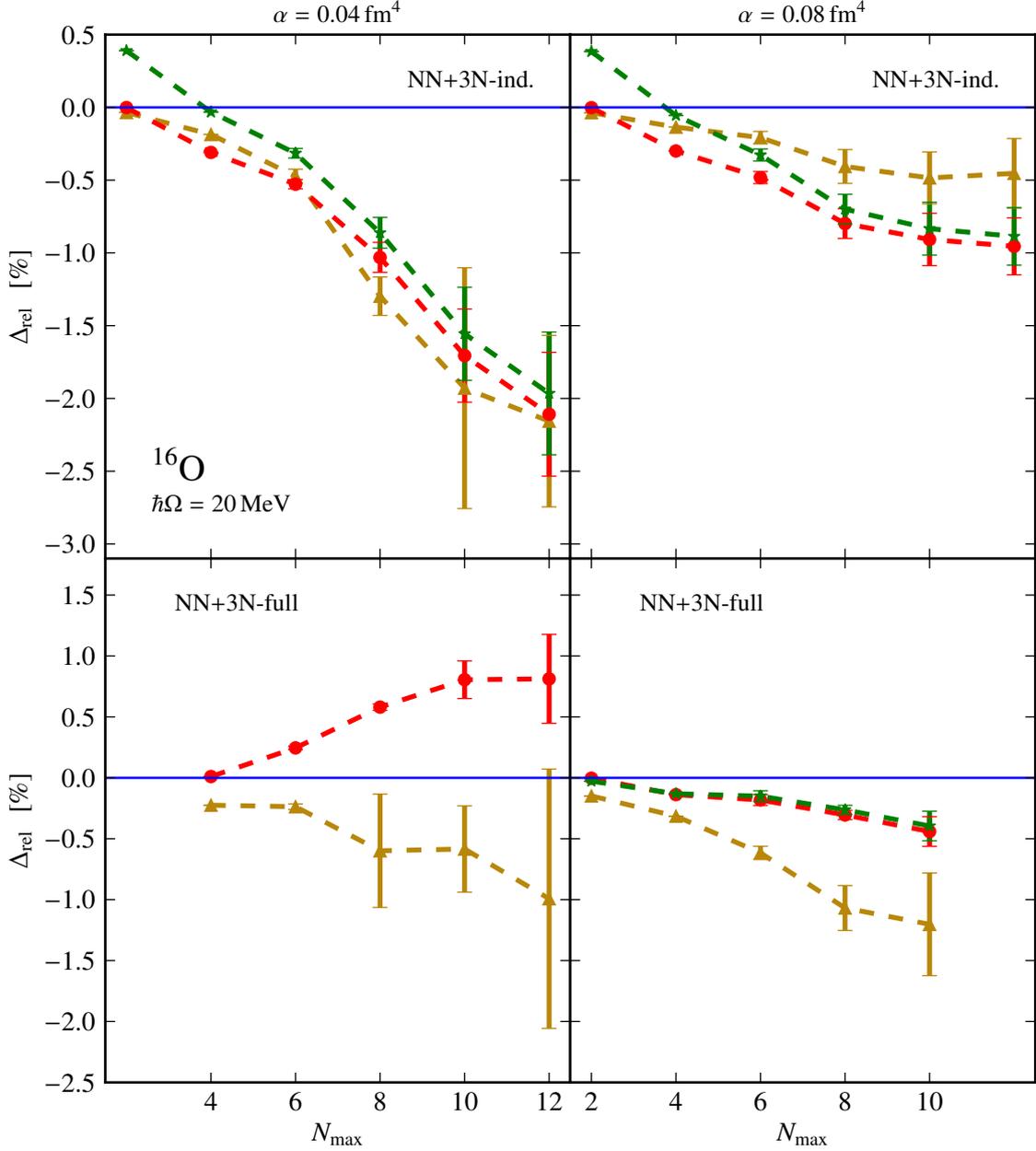


Figure B.7.: (color online) Relative deviations for  $^{16}\text{O}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 0$  ( $\blacktriangle$ ), 2 ( $\bullet$ ) and 4 ( $\blackstar$ ).

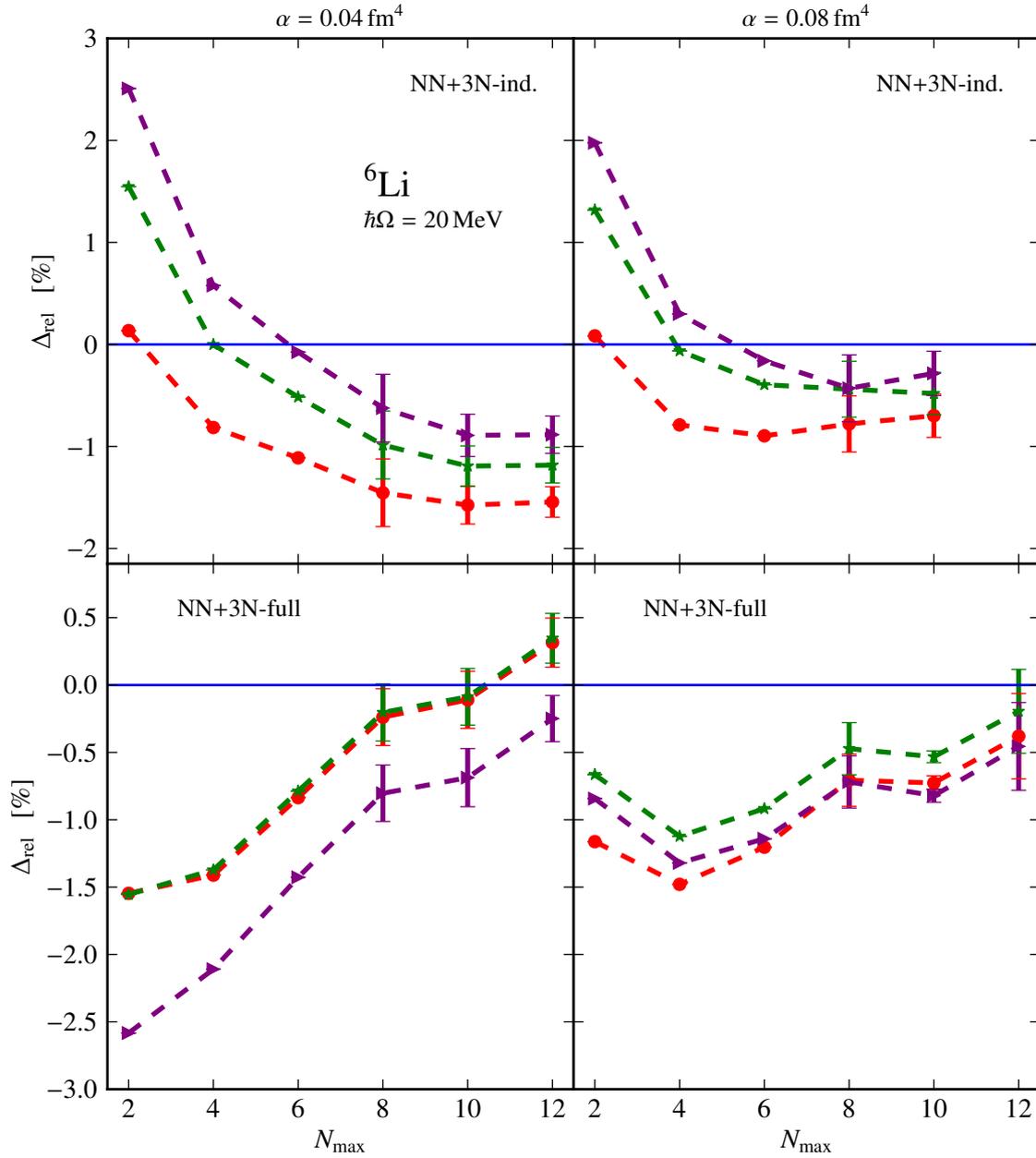


Figure B.8.: (color online) Relative deviations for  ${}^6\text{Li}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  ( $\bullet$ ) and 4 ( $\star$ ) and 6 ( $\blacktriangleright$ ).

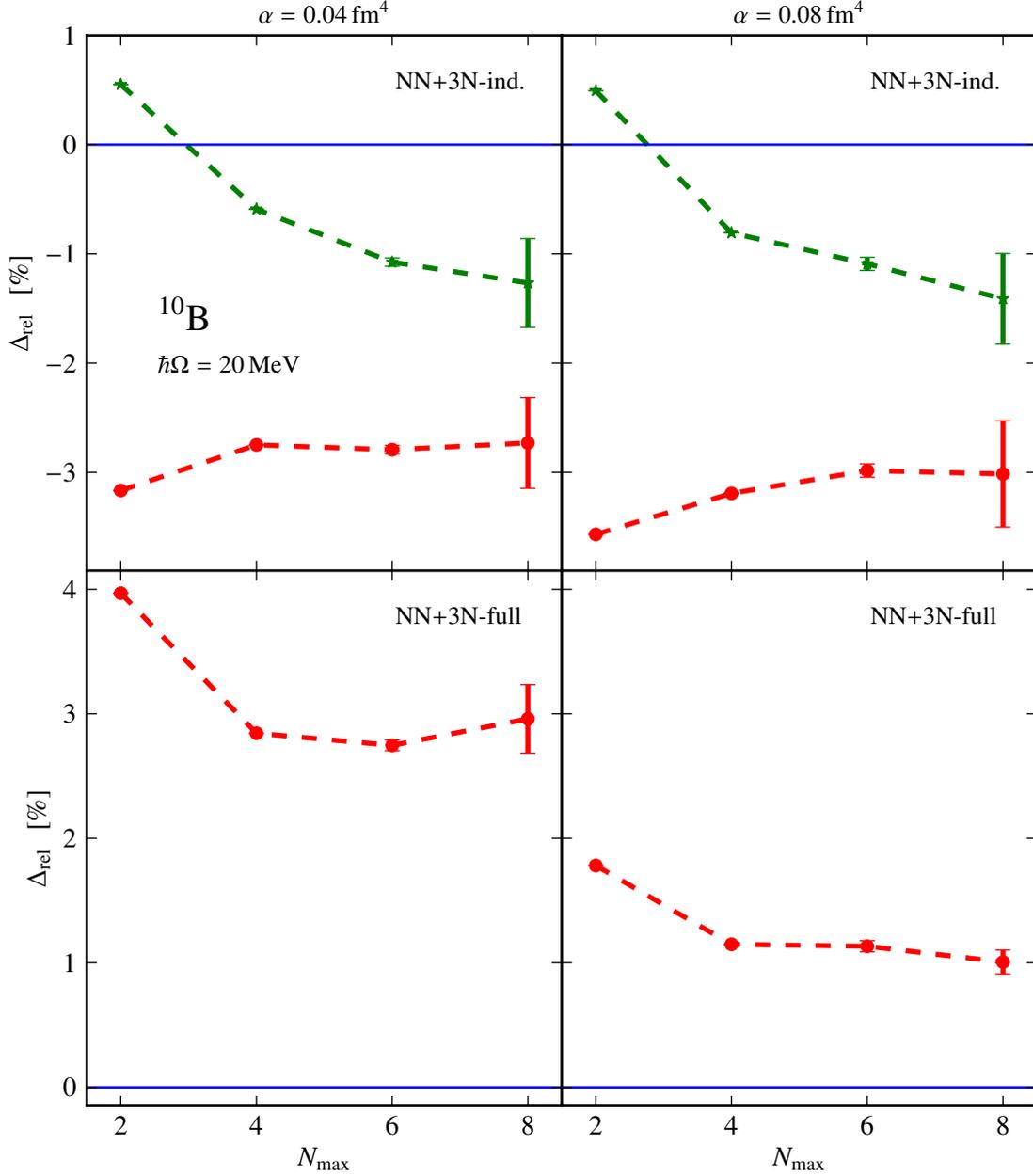


Figure B.9.: (color online) Relative deviations for  $^{10}\text{B}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}}, \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  (●) and 4 (★).

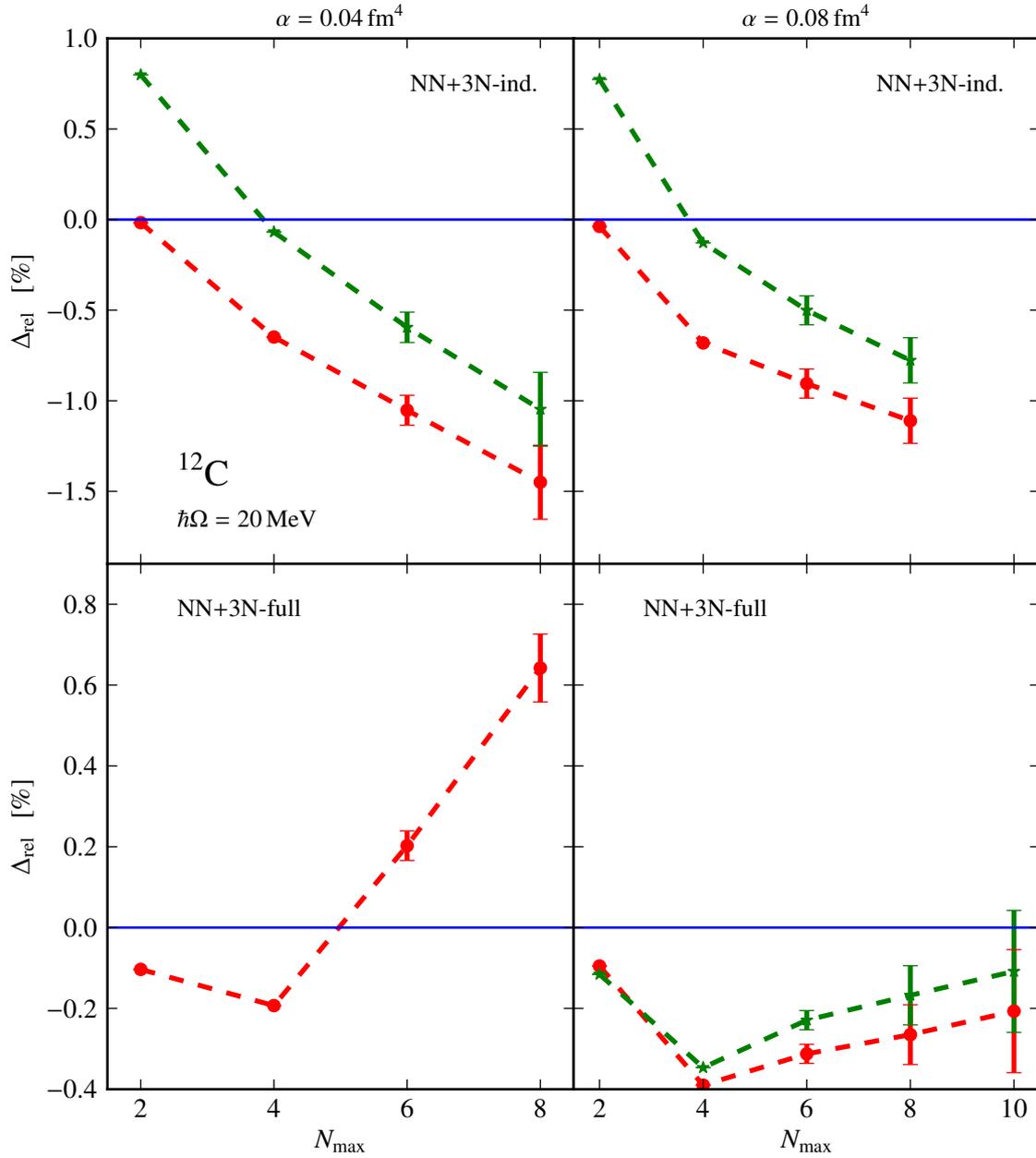


Figure B.10.: (color online) Relative deviations for  $^{12}\text{C}$  as a function of  $N_{\text{max}}$  for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with different SRG flow parameters  $\alpha = 0.04 \text{ fm}^4$  (left) and  $0.08 \text{ fm}^4$  (right) between the results obtained with the explicit 3N interaction and the corresponding MR-NO2B( $N_{\text{max}}^{\text{ref}} \hbar\Omega$ ) approximations for a range of  $N_{\text{max}}^{\text{ref}}$  parameters:  $N_{\text{max}}^{\text{ref}} = 2$  (●) and 4 (★).

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# Erklärung zur Eigenständigkeit

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Hiermit versichere ich, die vorliegende Arbeit ohne Hilfe Dritter nur mit den angegebenen Quellen und Hilfsmitteln angefertigt zu haben. Alle Stellen, die aus diesen Quellen entnommen wurden, sind als solche kenntlich gemacht worden. Diese Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen.

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Ort und Datum

Eskendr Gebrerufael



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