Computation of spectroscopic factors with the coupled-cluster method

O. Jensen,¹ G. Hagen,² T. Papenbrock,³,² D.J. Dean,² and J.S. Vaagen¹

¹Department of Physics and Technology, University of Bergen, N-5007 Bergen, Norway
²Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
³Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA

We present a calculation of spectroscopic factors within coupled-cluster theory. Our derivation of algebraic equations for the one-body overlap functions are based on coupled-cluster equation-of-motion solutions for the ground and excited states of the doubly magic nucleus with mass number \( A \) and the odd-mass neighbor with mass \( A - 1 \). As a proof-of-principle calculation, we consider \( ^{16}\text{O} \) and the odd neighbors \( ^{15}\text{O} \) and \( ^{15}\text{N} \), and compute the spectroscopic factor for nucleon removal from \( ^{16}\text{O} \). We employ a renormalized low-momentum interaction of the \( V_{\text{low-k}} \) type derived from a chiral interaction at next-to-next-to-next-to-leading order. We study the sensitivity of our results by variation of the momentum cutoff, and then discuss the treatment of the center of mass.

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I. INTRODUCTION

In the past two decades, \textit{ab initio} nuclear structure calculations have led to the development and test of high-precision models with predictive power \cite{1,2,3}. Recently, the application of effective field theory (EFT) \cite{4,5,6,7} and renormalization group techniques \cite{8,9,10,11} resulted in a model-independent approach to the nuclear interaction. These approaches have significantly deepened our understanding of nuclear forces and have also provided us with new technical means to simplify the solution of the nuclear many-body problem. The interactions from chiral EFT have been probed in light nuclei \cite{10,11,12,13} and selected medium-mass nuclei with different techniques \cite{14,15}. The focus of \textit{ab initio} calculations is not only on observables such as binding energies, radii, and low-lying excitation spectra, but also on transition rates and more detailed spectroscopic information. Very recently, \textit{ab initio} theory began to bridge the gap from nuclear structure to reactions \cite{17,18,19}. The inclusion of continuum effects, for instance, is necessary for the description of weakly bound and unbound nuclei. Direct reactions such as stripping and pickup of a single nucleon are rather well understood within phenomenological approaches (see, e.g. Ref. \cite{20}), but constitute a current frontier for \textit{ab initio} theory.

The interpretation of direct reactions within a given model or Hamiltonian is based on spectroscopic factors \cite{21,22}. The spectroscopic factor depends on wave function overlaps (see Eq. (16) below for a definition) and provides useful information that relates nuclear structure within a given model (i.e. within a given Hamiltonian) to stripping and transfer reactions \cite{21}. The spectroscopic factor is not an observable as it depends on the employed Hamiltonian or model. In nuclear physics, the high-momentum parts of the interaction are unconstrained and modeled in different ways. Thus, the short-ranged part of the wave function is model-dependent, and so is an overlap between wave functions. Therefore, the spectroscopic factor is merely a theoretical quantity and cannot be measured \cite{23,24}. However, the spectroscopic factor “provides a useful basis for the comparison of experiment and current nuclear models” \cite{21}. Its purpose thus lies in understanding a direct reaction within a certain model or Hamiltonian, and this interpretation might be useful and interesting \cite{25}.

In this paper, we develop the technical tools to compute spectroscopic factors within the coupled-cluster method \cite{26,27,28,29,30} (see Ref. \cite{31} for a recent review of this method), and perform a proof-of-principle calculation for \( ^{16}\text{O} \). The computation of the spectroscopic factor within coupled-cluster theory is not trivial (i) since the method does not readily yield a many-body wave function, and (ii) due to details related to the translation invariance of the coupled-cluster wave function. This paper is structured as follows. Section II is dedicated to a summary of the employed coupled-cluster method. The theoretical computation of spectroscopic factors within coupled-cluster theory is presented in Section III. We present our results and a discussion of the center-of-mass treatment in Section IV. Section V contains our conclusions and an outlook.

II. EQUATION-OF-MOTION AND COUPLED-CLUSTER THEORY FOR NUCLEI

In this section we introduce the Hamiltonian and coupled-cluster theory \cite{26,27,28,29,30} for closed-shell and open-shell nuclei. Although our implementation of coupled-cluster theory has been presented elsewhere \cite{14,31,32}, we give a brief overview of the method since some details are needed for the calculation of spectroscopic factors.

We consider the intrinsic nuclear \( A \)-body Hamiltonian

\[
\hat{H} = \hat{T} - \hat{T}_{\text{cm}} + \hat{V}
\]

\[
= \sum_{1 \leq i < j \leq A} \left( \frac{(\hat{p}_i - \hat{p}_j)^2}{2mA} \right) + \hat{V}.
\]

Here \( T \) is the kinetic energy, \( T_{\text{cm}} \) is the kinetic energy of the center-of-mass coordinate, and \( V \) is the two-body
nucleon-nucleon interaction. In this paper we use low-momentum interactions $V_{\text{low-k}}$ with sharp cutoffs $\lambda = 1.6, 1.8, 2.0, 2.2$ fm$^{-1}$, respectively. For simplicity, we neglect any contributions of three-nucleon forces as we focus on a proof-of-principle calculation.

In coupled-cluster theory, one writes the ground-state many-body wave function as

$$\langle \psi_0 \rangle = e^T | \phi_0 \rangle .$$

(2)

Here, $| \phi_0 \rangle$ is a product state. The cluster operator $T$ introduces correlations as a linear combination of particle-hole excitations

$$T = T_1 + T_2 + \ldots + T_A .$$

(3)

Here, the $n$-particle-$n$-hole excitation operator is

$$T_n = \left( \frac{1}{n!} \right)^2 \sum_{\mu=1}^{n} t^{a_i \cdots a_i}_{a_i \cdots a_i} \cdots a_i \cdots a_i .$$

(4)

We employ the standard convention that indices $ijk \ldots$ refer to orbits below Fermi level (holes) and $abc \cdots$ above Fermi level (particles). Approximations in coupled-cluster theory are introduced by truncating the cluster operator $T$ at a certain particle-hole excitation level. In this work we truncate $T$ at the two-particle-two-hole excitation level, i.e. $T \approx T_1 + T_2$, which gives the coupled-cluster method with singles and doubles excitations (CCSD). This is the most commonly used approximation, as it provides a good compromise between computational cost on the one hand and accuracy on the other.

Within the CCSD approximation, the computational cost is given by $n_o^2 n_u^4$, where $n_o$ and $n_u$ denote the number of occupied and unoccupied orbitals, respectively. The correlated ground state solution is given by the amplitudes $t^{a}_{i}$ and $t^{ab}_{ij}$ that solve the nonlinear equations

$$\langle \phi_0^a | \overline{H} | \phi_0 \rangle = 0 ,$$

(5)

$$\langle \phi_0^{ab} | \overline{H} | \phi_0 \rangle = 0 .$$

(6)

Here, the bra states are particle-hole excitations of the reference Slater determinant, and $\overline{H}$ denotes the similarity-transformed Hamiltonian,

$$\overline{H} = e^{-T} H e^T = (He^T)_c .$$

(7)

The subscript $c$ indicates that only fully connected diagrams give non-zero contributions. Once $T$ is determined from the solution of the coupled-cluster equations [35], the correlated ground state (g.s.) energy is given by

$$E_0 = \langle \phi_0 | \overline{H} | \phi_0 \rangle .$$

(8)

The CCSD approach is known to work particularly well for the ground state of nuclei with closed (sub-) shells, as a Slater determinant provides a reasonable first approximation. In this work we use the Equation-of-Motion (EOM) [31, 36, 39] method to solve for the ground and excited states of the closed-shell nucleus $A$ and its odd neighbors with mass number $A - 1$.

In EOM, the ground and excited states of a nucleus with mass number $B$ are obtained by acting with an excitation operator $\Omega_\mu$ on the ground state wave function of a nucleus with mass number $A$, i.e. $\psi^B_\mu = \Omega_\mu \psi^A_0$. Here $\mu$ denotes quantum numbers such as spin, parity, and isospin projection. Within the EOM approach, the ground state wave function $\psi^A_0$ denotes the coupled-cluster wave function $e^T \phi_0$. In this work we choose either $B = A$, in which case we solve the excited states of closed-shell nucleus $A$, or $B = A - 1$, in which case we solve the ground and excited states of the $A - 1$ neighboring nucleus. To solve for the excited states of the closed-shell nucleus $A$, we define $\Omega_\mu$ by the excitation operators,

$$R^A = r_0 + \frac{1}{4} \sum_{ia} r_i^a a_i^\dagger a_i + \frac{1}{4} \sum_{ijab} r_{ijab}^a a_i^\dagger a_j^\dagger a_j a_i ,$$

(9)

$$L^A = 1 + \frac{1}{4} \sum_{ia} t_{i}^a a_i^\dagger a_i + \frac{1}{4} \sum_{ijab} t_{ijab}^a a_i^\dagger a_j^\dagger a_j a_i .$$

(10)

Here, we suppressed the index $\mu$, but it is understood that the operators $R^A$ and $L^A$ excite and de-excite states with quantum numbers $\mu$, respectively. For the ground and excited states of the nucleus with mass number $A - 1$, we define $\Omega_\mu$ by the particle removal operators

$$R^{A-1} = \sum_i r_i a_i + \frac{1}{2} \sum_{ija} r_{ija}^a a_i a_j a_i ,$$

(11)

$$L^{A-1} = \sum_i l_i^a a_i + \frac{1}{2} \sum_{ija} l_{ija}^a a_i a_j a_i .$$

(12)

Again, we suppressed the index $\mu$ labeling the quantum numbers. The operators $R_\mu = R^A (R_\mu = R^{A-1})$ commute with the cluster operator $T$, and the unknowns $r_i^a, r_{ijab}^a (r_i, r_{ijab}^a) \ldots$ solve the EOM equation

$$[\overline{H}, R_\mu] | \phi_0 \rangle = \omega_\mu R_\mu | \phi_0 \rangle ,$$

(13)

which defines an eigenvalue problem for the excitation operator $R_\mu$ with eigenvalue $\omega_\mu = E_\mu - E_0$. It is clear from the definitions [14] and [7] that $\overline{H}$ is non-Hermitian; dual space solutions need to be calculated explicitly. We obtain the de-excitation operators $L_\mu = L^A, L^{A-1}$ by solving the left eigenvalue problem

$$\langle \phi_0 | L_\mu \overline{H} = \langle \phi_0 | L_\mu \omega_\mu \cdots$$

(14)

The right and left eigenvectors form a bi-orthogonal set and are normalized in the following way

$$\langle \phi_0 | L_\mu R_{\mu'} | \phi_0 \rangle = \delta_{\mu \mu'} .$$

(15)

The EOM solution for the ground state of system $A$ is identical to the CC solution, so that $R^A_0 = r_0 = 1$. Ref [51] provides a detailed description of EOM.
III. OVERLAP FUNCTIONS AND SPECTROSCOPIC FACTORS FROM COUPLED-CLUSTER THEORY

The one-particle overlap function between two wave functions $\Psi_{A-1}$ and $\Psi_A$ of nuclei with mass number $A-1$ and $A$, respectively, is defined as [22]

$$O_{A-1}^{A}(\vec{x}) \equiv \sqrt{A} \int d^{3}(A-2)\xi\Psi_{A-1}(\vec{\xi})\Psi_{A}(\vec{x}, \vec{\xi}) .$$

(16)

Here $\xi$ represent the $3(A-2)$ translationally invariant position coordinates and the $A-1$ spin coordinates of $A-1$ particles present in both $\Psi_{A-1}$ and $\Psi_A$, while $\vec{x}$ labels the position and spin of the additional particle in the nucleus with mass number $A$ with respect to the center of mass of the nucleus with mass number $A-1$. The isospin coordinate has been suppressed.

In our coupled-cluster approach, however, we do not employ coordinates with respect to the center of mass, as this would limit us to light systems [40]. Thus, the overlap can be associated with a specific nucleon represented by a second quantization operator,

$$O_{A-1}^{A}(\vec{x}) \equiv \langle A-1|a(\vec{x})|A \rangle .$$

(17)

Here, $|A\rangle$ and $|A-1\rangle$ denote eigenstates in the nucleus with mass $A$ and $A-1$, respectively. Typically, $|A\rangle$ is the ground state, and $|A-1\rangle$ is the ground state or an excited state. Our formalism will be kept general and is not limited to these cases. The radial overlap function $O_{A-1}^{A}(l; r)$ is derivied by expanding $\vec{x}$ in terms of partial waves,

$$a(\vec{x}) = (-)^{j-m}\sum_{ljm} a_{ljm}(r)Y_{ljm}(\hat{x}) .$$

(18)

Here, $Y_{ljm}(\hat{x})$ is the spin-orbital spherical harmonic

$$Y_{ljm}(\hat{x}) = [Y_{l}(\hat{r}) \otimes \chi_{1/2}(\sigma)]_{jm} ,$$

$Y_{l}(\hat{r})$ is the spherical harmonic of rank $l$ and $\chi_{1/2}(\sigma)$ is a fermionic spin function. The orbital angular momentum quantum number is denoted by $l$, while $j$ and $m$ denote the rank and projection, respectively, of $Y_{ljm}(\hat{x})$ as a spherical tensor. The hat denotes unit vectors, i.e., $\hat{x} \equiv \vec{x}/||\vec{x}||$. We have also introduced the spherical annihilation operator $\hat{a}_{ljm}(r) = (-)^{j+m}a_{ljm}(r)$. The radial overlap is now given by the reduced matrix element and the overlap becomes [43]

$$O_{A-1}^{A}(\vec{x}) = \sum_{j} (-)^{j-m} \langle J_{A}M_{Aj} - m | J_{A-1}M_{A-1} \rangle \times O_{A-1}^{A}(l; r)Y_{ljm}(\hat{x}) .$$

(19)

Here, $\langle \cdot | \cdot \rangle$ denotes a Clebsch-Gordan coefficient. The overlap is now expressed by a radial function associated with each tensorial component $Y_{ljm}(\hat{x})$

$$O_{A-1}^{A}(l; r) \equiv \langle A-1||\hat{a}_{ljm}(r)||A \rangle$$

(20)

$$= (-)^{j-m} \langle A-1|a_{ljm}(r)|AM_{A} \rangle \langle J_{A}M_{Aj} - m | J_{A-1}M_{A-1} \rangle .$$

This equation also defines the reduced matrix elements we employ.

The norm of the radial overlap function is the spectroscopic factor

$$S_{A-1}^{A}(lj) = \int dr^2 |O_{A-1}^{A}(l; r)|^2 .$$

(21)

The overlap functions can be expressed in an energy basis by inserting the expansions

$$a_{ljm}^{\dagger}(r) = \sum_{n} a_{nljm}^{\dagger}\phi_{nljm}(r) ,$$

$$a_{ljm}(r) = \sum_{n} a_{nljm}\phi_{nljm}^{*}(r) ,$$

(22)

(23)

where $n$ is the nodal quantum number and $\phi_{nljm}(r)$ is the radial single-particle wave function associated with the orbits $nljm$. While $a_{ljm}^{\dagger}(r)$ represents the creation of a particle at radial distance $r$, $a_{ljm}(r)$ represents the action of populating a single-particle orbit.

Assuming orthogonality of the single-particle wave functions, the spectroscopic factor is written as,

$$S_{A-1}^{A}(lj) = \sum_{n}|\langle A-1|a_{nljm}|A \rangle|^2$$

$$= \sum_{n}\frac{|\langle A-1|a_{nljm}|A \rangle|^2}{(J_{A}M_{Aj} - m | J_{A-1}M_{A-1})^2} .$$

(24)

Here we used the Wigner-Eckhart theorem for the reduced matrix elements. Eq. (21) is our starting point since we work in an uncoupled ($m$-scheme) basis. Using the EOM-CCSD solutions for the right and left eigenvalue problems for the $A$ and the $A-1$ systems, and employing the ground state solutions for system $A$, Eq. (21) takes the form,

$$S_{A-1}^{A}(lj) = \sum_{n} \frac{\langle \phi_{0}|L_{A}^{*\dagger}a_{nljm}^{\dagger}R_{A}^{A-1}|\phi_{0} \rangle \langle \phi_{0}|L_{A}^{*\dagger}\sigma_{nljm}R_{A}^{A-1}|\phi_{0} \rangle}{(J_{A}M_{Aj} - m | J_{A-1}M_{A-1})^2} .$$

(25)

This gives the equation for the spectroscopic factors as defined within coupled-cluster theory. We note that this equation is unambiguously and uniquely defined in terms of the left and right eigenstates of the nuclei with mass numbers $A$ and $A-1$. This is clear since the spectroscopic factor is given by the absolute value squared of the one-body overlap matrix element, so any ambiguity related to the normalization condition [15] is removed.

In Eq. (25) we have introduced the similarity-transformed creation and annihilation operators,

$$\overline{a}_{p}^{T} = e^{-T}a_{p}^{*}e^{T} ,$$

(26)

$$\overline{\sigma}_{p} = e^{-T}a_{p}e^{T} .$$

(27)

Using the Baker-Campbell-Hausdorff commutator expansion, we can derive algebraic expressions for $\overline{a}_{p}$ and $\overline{\sigma}_{p}$.
in terms of the “bare” creation and annihilation operators \( a_p \) and \( a_p \) and the particle-hole excitations amplitudes \( t_i^a \) and \( t_{ij}^{ab} \):

\[
\begin{align*}
\overline{a}_p^a &= a_p^a - \sum_b t_{ij}^{bc} a_b^c - \frac{1}{2} \sum_{jbc} t_{ij}^{bc} a_b^c a_j^a a_j^a, \\
\overline{a}_p &= a_p + \sum_i t_i^p a_i + \frac{1}{2} \sum_{ijc} t_{ij}^{pc} a_j^a a_i^a.
\end{align*}
\]

(28)

(29)

These equations can also be given in a diagrammatic form, which provides a convenient bookkeeping system for the available Wick contractions in the expressions.

The coupled-cluster diagrams are similar to Goldstone diagrams. An algebraic Wick contraction corresponds to the diagrammatic connection of two directed lines, but the interpretation rules are slightly different. We refer the reader to Refs. [31, 41] for a complete introduction to the diagrammatic approach. Here we will only present the few concepts necessary to introduce the novel extensions of the formalism used in the context of spectroscopic factors.

Diagrammatic representations of the excitation and particle-removal operators \( T, L_\mu, \) and \( R_\mu \) are displayed in Table I. Lines with arrows pointing up (down) represent particle (hole) orbits. These lines have implicit indices \( a, b, c, \ldots \) (\( i, j, k, \ldots \)).

TABLE I: The left panel lists algebraic symbols for the particle-hole excitation operators and particle removal operators. Corresponding diagrammatic representations are displayed on the right. Arrows pointing up (down) represent particle (hole) orbits with implicit summation indices \( a, b, c, \ldots \) (\( i, j, k, \ldots \)).

In this section we present our results for the calculation of the spectroscopic factor using \( ab \text{ initio} \) coupled-cluster theory. We study the spectroscopic factor of nucleon removal from \(^{16}\text{O}\) by calculating the one-body overlap functions of \(^{16}\text{O}\) with the odd mass neighbors \(^{15}\text{O}\) and \(^{15}\text{N}\) using the PR-EOM-CCSD approach to the ground and excited states of the \( A - 1 \) nuclei. The CCSD approximation is used to calculate the ground state of \(^{16}\text{O}\).

Our model space is spanned by oscillator states. We label the model space by the largest principal quantum number. The overall sign of a diagram is determined according to standard rules [11]. The negative sign of the second and third term in Eq. (28) is reflected in the \( a_i^T \) diagrams by the internal hole-lines that connect the small circle with the \( T \) operators. To determine the overall sign correctly for the spectroscopic factor diagrams, a sequence of directed lines ending or starting in a small circular vertex must be counted as a loop.

The diagrams shown in Tables II and III are the basic building blocks for the computation of the spectroscopic factor. We compute the matrix elements of the overlap function as products of the components \( R_\mu, L_\mu \) and either \( \overline{a}_p^a \) or \( \overline{a}_p^a \). The only non-vanishing contributions to the spectroscopic factor come from the diagrams in which all directed lines can be connected. These diagrams and the corresponding algebraic interpretation are shown in Table III. We assume an implicit summation over repeated indices.

The computational cost of the spectroscopic factor diagrams has the very gentle scaling, \( n_a^2 n_a^2 \), so the cost is completely dominated by the CC and EOM calculations. In the case that \( |A\rangle \) is the ground state of the closed-shell nucleus, we have \( r_i^a = 0 = r_{ij}^{ab} \) and several diagrams vanish.

IV. RESULTS

In this section we present our results for the calculation of the spectroscopic factor using \( ab \text{ initio} \) coupled-cluster theory. We study the spectroscopic factor of nucleon removal from \(^{16}\text{O}\) by calculating the one-body overlap functions of \(^{16}\text{O}\) with the odd mass neighbors \(^{15}\text{O}\) and \(^{15}\text{N}\) using the PR-EOM-CCSD approach to the ground and excited states of the \( A - 1 \) nuclei. The CCSD approximation is used to calculate the ground state of \(^{16}\text{O}\).

Our model space is spanned by oscillator states. We label the model space by the largest principal quantum number.
number $N$ that is included in the single-particle (s.p.) basis, so that the maximum s.p. energy is $E_N = (N + \frac{1}{2})\hbar\omega$, and the number of major oscillator shells is $N + 1$. In Fig. 1 we show the convergence of the ground-state of $^{16}\text{O}$ with increasing size of the model space for a wide range of oscillator frequencies $\hbar\omega$, using $V_{\text{low}}-k$ with momentum cutoff $\lambda = 2.0 \text{fm}^{-1}$. In Fig. 2 we show the convergence of the ground-state energies of $^{15}\text{O}$ and $^{15}\text{N}$ relative to the ground-state energy of $^{16}\text{O}$.

Our results shown in Figs. 1 and 2 show a weak dependence on $\hbar\omega$ in the largest model space. We estimate that our results for the ground state energies are converged within a few MeV in our largest model. We note that the CCSD ground-state for $^{16}\text{O}$ is overbound by $\sim 15 \text{MeV}$ as compared to experiment. However, the energy difference between the ground-states of $^{15}\text{O}$ and $^{15}\text{N}$ is about $\sim 4 \text{ MeV}$, which is very close to the experimental value of 3.5 MeV. It thus seems that energy differences are better reproduced than absolute energies.

The $\hbar\omega$ dependence provides some information about how the finite size of the model space affects the solutions. For high values of $\hbar\omega$, the model space includes high-momentum states beyond the momentum cutoff $\lambda$ of the interaction, but is not sufficiently extended in position space to accommodate a nucleus. For small values of $\hbar\omega$, the model space is sufficiently wide in position space for the extension of the nucleus but does not contain sufficient high-momentum modes to resolve the cutoff $\lambda$ of the interaction. Close to the minimum, in the largest model spaces considered, a good compromise is realized.

We also studied the energy levels using $V_{\text{low}}-k$ for various momentum cut-offs in the range $\lambda = 1.6-2.2 \text{ fm}^{-1}$. The calculated ground-state energies for $^{16}\text{O}$, $^{15}\text{O}$, and $^{15}\text{N}$ are sensitive to the cut-off, implying that induced three-body forces and short-ranged forces of higher rank would contribute significantly to the calculated energies.

Let us turn to the spectroscopic factor for nucleon removal from $^{16}\text{O}$. Figure 3 shows the spectroscopic factor

$$SF(1/2^-) \equiv S_{1/2}^{16}(l = 1, j = 1/2)$$

(30)

for the removal of a proton with quantum numbers $l = 1, j = 1/2$. The spectroscopic factor is given by

$$S_{1/2}^{16}(l = 1, j = 1/2)$$

The individual components of these diagrams are explained in Tables I and II.
$J^\pi = 1/2^-$ from $^{16}$O using a low-momentum interaction $V_{\text{low-k}}$ with a cut-off $\lambda = 2.0\,\text{fm}^{-1}$. Evidently, the spectroscopic factor is well converged and depends very weakly on the size of the model space and the oscillator frequency $\hbar \omega$. It varies less than 1% over a wide range of oscillator frequencies. The spectroscopic factor SF$(1/2^-)$ for neutron removal from $^{16}$O is almost identical to the SF$(1/2^-)$ for proton removal. Recall that isospin is approximately conserved in light nuclei.

The dependence on momentum cut-off $\lambda$ is displayed in Fig. 4. Note that the spectroscopic factor increases with decreasing cutoff. This is expected, since by lowering the cutoff the system becomes less correlated and the product state $|\phi_0\rangle$ becomes an increasingly good approximation, and the single-particle picture becomes more and more valid. Note also that isospin is approximately a good quantum number, as the spectroscopic factors for proton and neutron removal are almost identical.

Let us also study the center-of-mass problem. The intrinsic Hamiltonian (1) depends on the mass number $A$ of the nucleus, and the calculation of the spectroscopic factor requires us to employ identical Hamiltonians for the nuclei with mass numbers $A$ and $A - 1$. This constitutes dilemma, since no choice of actual value for the parameter $A$ can satisfy the parent and daughter nuclei simultaneously. It is thus necessary to investigate how strongly the spectroscopic factor depends on this value. Figure 5 shows the spectroscopic factor (in a model space $N = 4$ for a momentum cutoff $\lambda = 2.0\,\text{fm}^{-1}$) for different values of the mass number $A$ of the intrinsic Hamiltonian. The dependence on $A$ is very weak, and it is similar in size to the dependence on the parameters of the model space.

For an intrinsic Hamiltonian, the coupled-cluster wave function of a closed-shell nucleus factorizes into an intrinsic part and Gaussian for the center of mass of coordinate $\nu$. Following the procedure of Ref. 42, we confirmed that this factorization is present for the ground states of $^{15}$O and $^{15}$N in the largest model space we considered. We found that this factorization even takes place if the value $A = 16$ for the mass number is employed in the intrinsic Hamiltonian (1) for the computation of the nuclei $^{15}$O and $^{15}$N. These results suggest that our approach to calculate spectroscopic factors within the coupled-cluster method is practically free of any center-of-mass contamination.

So far, we focused on the spectroscopic factors for removal of a $J^\pi = 1/2^-$ proton and neutron from $^{16}$O. We finally also compute the spectroscopic factor for removal of a neutron and proton from $^{16}$O as a function of the oscillator spacing $\hbar \omega$ for nucleon-nucleon interactions with different cutoffs in a model space with $N = 6$.

![Figure 3](image3.png)

FIG. 3: (Color online) Spectroscopic factor SF$(1/2^-)$ for proton removal from $^{16}$O as a function of the oscillator spacing $\hbar \omega$ for different model spaces consisting of $(N + 1)$ oscillator shells and a low-momentum interaction with cutoff $\lambda = 2.0\,\text{fm}^{-1}$.

![Figure 4](image4.png)

FIG. 4: (Color online) Spectroscopic factor SF$(1/2^-)$ for neutron and proton removal as a function of the oscillator spacing $\hbar \omega$ for nucleon-nucleon interactions with different cutoffs in a model space with $N = 6$.

![Figure 5](image5.png)

FIG. 5: (Color online) Spectroscopic factor SF$(1/2^-)$ for proton removal from $^{16}$O as a function of the oscillator spacing $\hbar \omega$ computed for different values of the mass number $A$ employed in the intrinsic Hamiltonian (1). The model space consists of $N + 1 = 5$ oscillator shells, and the momentum cutoff of the nucleon-nucleon interaction is $\lambda = 2.0\,\text{fm}^{-1}$.
moval of a $J^\pi = 3/2^-$ proton and a (deeply bound) $J^\pi = 1/2^+$ proton from $^{16}$O. The result is shown in Fig. 6 for different model spaces. As before, the results are well converged with respect to the size of the model space, and display only a mild dependence on the oscillator frequency. We find that the spectroscopic factor SF(3/2−) is similar in size to SF(1/2−). This is an interesting result. Barbieri and Dickhoff [25] also found in their computation of spectroscopic factors that SF(1/2−) ≈ SF(3/2−) for nucleon removal from $^{16}$O. As expected, the spectroscopic factor of the $J^\pi = 1/2^+$ state is very small. The removal of a deeply bound $J^\pi = 1/2^+$ proton from $^{16}$O yields a highly excited state of $^{15}$N that is a rather complex superposition of many $n$-particle–($n+1$)-hole states and thus has little overlap with a one-hole state.

\[ \text{FIG. 6: (Color online) Spectroscopic factors SF(3/2−) and SF(1/2+) for proton removal from } ^{16}\text{O as a function of the oscillator spacing } \hbar \omega. \text{ The employed model spaces have } N+1 \text{ oscillator shells, and the momentum cutoff of the nucleon-nucleon interaction is } \lambda = 2.0 \text{ fm}^{-1}. \]

V. CONCLUSION AND OUTLOOK

We have extended the coupled-cluster method for the computation of spectroscopic factors. To this purpose, we derived diagrammatic and algebraic expressions of the one-body overlap functions based on equation-of-motion methods for the ground and excited states of the closed-shell nucleus with mass number $A$ and the neighboring nuclei with mass number $A−1$. We implemented the equations in an uncoupled $m$-scheme, and presented proof-of-principle calculations of the spectroscopic factor for proton and neutron removal from $^{16}$O. The calculated spectroscopic factors are well converged in model spaces consisting of six oscillator shells for low-momentum nucleon-nucleon interactions. Within the coupled-cluster approach, the same intrinsic Hamiltonian has to be employed in the nuclei with mass numbers $A$ and $A−1$. We found that the spectroscopic factor is insensitive to the actual value of the mass number that is employed in the intrinsic Hamiltonian.

We plan to implement the computation of the spectroscopic factor also in a spherical formulation of nuclear coupled-cluster theory. This will allow us to employ much larger model spaces, and we plan to apply the techniques to physically interesting nuclei, such as $^{22,24}$O, $^{48,52}$Ca, and $^{56,78}$Ni.

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