Spectroscopic amplitudes and microscopic substructure effects in nucleon capture reactions

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Spectroscopic amplitudes play an important role in nuclear capture reactions. These amplitudes are shown to include both single-particle and polarization effects: the former through their spatial dependence and the latter through their normalization (the spectroscopic factors). Coupled-channels equations are developed for the spectroscopic amplitudes. These equations serve as a convenient starting point for the derivation of several approximations: Hartree, Hartree-Fock, and two different single-particle models. The single-particle models include antisymmetry in different ways, but both miss many-body effects. Therefore, cross sections calculated with either of these models need to be multiplied by the spectroscopic factor.

I. INTRODUCTION

Nucleon capture reactions at low energies, such as $^7\text{Be}(p,\gamma)^8\text{B}$, $^{16}\text{O}(p,\gamma)^{17}\text{F}^*$, or $^7\text{Li}(n,\gamma)^8\text{Li}$, play an important role in our understanding of astrophysical phenomena. For example, in the hydrogen-burning process in stars such as our sun, low-energy proton capture on beryllium takes place in the proton-proton chain, and the $^{16}\text{O}(p,\gamma)^{17}\text{F}^*$ reaction occurs in the carbon-nitrogen-oxygen cycle [1–3]. Exact knowledge of the reaction rates is necessary for modeling the energy generation and evolution of hydrogen-burning stars. In addition, the $^7\text{Be}(p,\gamma)^8\text{B}$ reaction at solar energies ($E_{\text{c.m.}} \lesssim 20$ keV) plays a key role in the "solar neutrino puzzle" since the neutrino event rate in the existing chlorine and water Cerenkov detectors is dominated by the high-energy neutrinos produced in the subsequent β decay of ^8B [1,2,4]. The $^7\text{Li}(n,\gamma)^8\text{Li}$ reaction is a key element of primordial nucleosynthesis in inhomogeneous big bang scenarios [1,5]. It initiates a sequence of reactions which bridge the mass gap at $A=8$ and thus its rate is crucial for determining the amounts of heavier elements produced in these models.

Direct measurements of capture reactions at energies corresponding to astrophysically relevant temperatures, however, are often very difficult, since the cross sections diminish exponentially at low energies. Thus, theoretical studies of these processes become very valuable. In addition to microscopic theories, such as the nuclear shell model or cluster models, one-body potential models provide a popular framework for such investigations. For example, the potential model was used in Ref. [6] to discuss the energy dependence of the reaction rates. In the one-body potential model, a single-particle wave function is used to calculate various observables; microscopic substructure effects are partially accounted for through the use of spectroscopic factors. This strategy, however, has recently been the subject of vivid discussions [7,8]. At issue is the proper normalization of the cross section. Csótó [7], for instance, maintains that spectroscopic factors should not be included in potential-model calculations of the $^7\text{Be}(p,\gamma)^8\text{B}$ cross section at low energies, since the reaction depends only on the asymptotic normalization coefficient of the ^8B bound-state wave function [9], whereas the spectroscopic factor arises from the short-range properties of the wave function. Mukhamedzhanov *et al.* [8,9] argue in favor of using a different approach, based on asymptotic normalization coefficients instead of spectroscopic factors, for determining the relevant cross sections. However, the asymptotic normalization coefficient contains short-range effects. It can actually be given in terms of an integral over the interior of the nucleus [10] and its interdependence with the spectroscopic factor has been noted in the earlier work of Locher and Mizutani [11] and of Lovas *et al.* [12].

These recent discussions have motivated us to revisit the question of the proper treatment of microscopic nuclear structure effects in one-body models. In the present work we focus on the role of spectroscopic amplitudes and factors. The use of spectroscopic factors in nuclear reaction calculations dates back to the early days of nucleon transfer reactions [13] and continues to be central in the interpretation of such processes [14]. With the renewed interest in nucleon capture reactions in the context of astrophysical scenarios, and the emerging need for very accurate reaction rates, it becomes necessary to review and clarify the assumptions associated with one of the most basic models of nuclear physics, the one-body potential model.

Before proceeding with the formalism, it is necessary to clarify the meaning of the terms spectroscopic amplitude, spectroscopic factor, and one-body model. For example, it is important to realize that there are many spectroscopic amplitudes and spectroscopic factors associated with an A-body

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system, namely, one corresponding to each excited state of the $(A-1)$-body system. The different amplitudes are not independent since they are related by a model-independent sum rule [15]. In addition, the spectroscopic amplitudes are related by a set of coupled-channels equations.

The question of what is meant by a one-body model is more complicated since different notions are associated with the term. The coupled-channels formalism presented here is used to derive two different one-body models and to study the connections between them. One approach, which uses either the Hartree or the Hartree-Fock approximation in an intermediate step, leads to A noninteracting nucleons in a one-body potential. This, strictly speaking, is not a one-body model since there are still A particles. However, the orbitals corresponding to the different particles decouple and the problem reduces to solving A one-body equations. The fact that we still have A nucleons explicitly present has the advantage that antisymmetry can be built in *ab initio* using a Slater determinant for the A-body wave function. Another method for generating a one-body model is based on integrating out the coordinates of $(A-1)$ nucleons, effectively projecting onto a low-dimensional space. In this approach antisymmetry is enforced separately for each channel in the coupled-channels equations. Truncating to a single channel results in the approximation advocated by Varga and Lovas *et al.* [16], who study the cluster substructure of ^{6}Li in this framework. Their work is based on the generator-coordinate method. The derivation presented here serves to clarify the relation between their model and other approximations.

In Sec. II, we define the terms spectroscopic amplitude and spectroscopic factor, derive coupled-channels equations for the amplitudes, and discuss several approximation schemes, including the first one-body model described above. An alternative approach to the spectroscopic amplitudes is considered in Sec. III, which includes details on the second one-body model mentioned above. In Sec. IV, we explore the physical aspects associated with the spatial dependence of the spectroscopic amplitude and its norm, the spectroscopic factor. We give an expression for the reaction matrix elements in terms of the spectroscopic amplitudes. For both single-particle models considered here the reactions rates need to be multiplied by a spectroscopic factor. Our conclusions are summed up in Sec. V, and various technical aspects of our work are included in the Appendixes.

II. SPECTROSCOPIC AMPLITUDES

In this section we expand an A-body wave function in terms of the ground and excited states of the $(A-1)$-body system and derive a set of coupled differential equations for the expansion coefficients, of which the spectroscopic amplitudes are a special case. The resulting equations of motion give insight into the long-range behavior of the A-body ground state wave function and lead to various approximation schemes. In particular, the Hartree and Hartree-Fock approximations and a one-body potential-model approach emerge naturally. For simplicity, spin and isospin degrees of freedom are suppressed and the Coulomb potential is neglected. Furthermore, we do not consider the center-of-mass

motion here; this subject is discussed in Appendix D.

Let $\Psi^n_{A-1}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{A-1})$ denote the nth (fully antisymmetric) eigenstate of the $(A-1)$-body Hamiltonian H_{A-1}. The collection of all Ψ^n_{A-1}, including both bound and continuum states, forms a complete set of states in the space of antisymmetric $(A-1)$-body wave functions. Using this set, $\{\Psi^n_{A-1}\}_{n=1,2,\ldots}$, one can construct a basis for the space of antisymmetric A-body wave functions by defining $_\mathcal{A}\Psi^{n,r}_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = \mathcal{A}\Psi^{n,r}_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$, where $\Psi^{n,r}_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) \equiv \Psi^n_{A-1}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{A-1})\delta(\boldsymbol{r}-\boldsymbol{r}_A)$ and $\mathcal{A}$ antisymmetrizes between the Ath coordinate, which occurs in the delta function, and the $(A-1)$ coordinates in Ψ^n_{A-1}. This ''intercluster'' antisymmetrization operator is normalized so as to satisfy $\mathcal{A}^2 = \sqrt{A}\,\mathcal{A}$.

The $\Psi^{n,r}_A$ span a space that includes both totally antisymmetric A-body states and mixed-symmetric states, which are antisymmetric in the first $A-1$ coordinates and symmetric under interchanges involving the Ath coordinate. The basis sets $\{\Psi^n_{A-1}\}$, $\{\Psi^{n,r}_A\}$, and $\{_\mathcal{A}\Psi^{n,r}_A\}$ are discussed in more detail in Appendix A.

An arbitrary antisymmetric A-body wave function ψ_A can then be expanded as

$$|\psi_A\rangle = \frac{1}{A}\sum_{n=1}^\infty \int d\boldsymbol{r}\,|_\mathcal{A}\Psi^{n,r}_A\rangle\phi_n(\boldsymbol{r})$$

$$= \frac{1}{\sqrt{A}}\sum_{n=1}^\infty \int d\boldsymbol{r}\,|\Psi^{n,r}_A\rangle\phi_n(\boldsymbol{r}) = \frac{1}{\sqrt{A}}\sum_{n=1}^\infty |\Psi^n_{A-1}\rangle|\phi_n\rangle$$

$$(2.1)$$

with expansion coefficients

$$\phi_n(r) = \langle _\mathcal{A}\Psi^{n,r}_A|\psi_A\rangle = \sqrt{A}\langle\Psi^{n,r}_A|\psi_A\rangle = \langle\Psi^n_{A-1}|a(\boldsymbol{r})|\psi_A\rangle.$$

$$(2.2)$$

Here $a(\boldsymbol{r})$ [$a^\dagger(\boldsymbol{r})$] is an annihilation [creation] operator which destroys [creates] a nucleon at position $\boldsymbol{r}$ and obeys the usual anticommutation relations. Note that only the first expansion in Eq. (2.1) is manifestly antisymmetric, while in the other two expressions the antisymmetry information is carried by the expansion coefficients. The coefficients are identical in all three expansions if and only if ψ_A is fully antisymmetric. In this case, the mixed-symmetry components of $\Psi^{n,r}_A$ do not contribute.

When ψ_A denotes a bound state, the $\phi_n(\boldsymbol{r})$ are called *spectroscopic amplitudes*, and the associated integrals

$$S_n = \int d\boldsymbol{r}\,|\phi_n(\boldsymbol{r})|^2 \qquad (2.3)$$

are the frequently used *spectroscopic factors* [17]. They obey the sum rule $\Sigma_{n=1}^\infty S_n = A$ [see Ref. [15] and also Eq. (A21)]. We observe that for a bound A-body state, there are many spectroscopic amplitudes (and thus many spectroscopic factors), namely, one for each excited state of the $(A-1)$-body nucleus. Given the structural information on the $(A-1)$-body system that enters the wave functions Ψ^n_{A-1}, the spectroscopic amplitudes completely determine the wave

function ψ_A. The spatial dependence of $\phi_n(r_A)$ is related to the properties of the single-particle orbital of the Ath nucleon in the larger system, and the norm of $\phi_n(r)$, the spectroscopic factor, provides a measure of the structural similarity of the nth excited $(A-1)$-body state and an $(A-1)$-body subcluster of the full A-nucleon system.

The interdependence of the spectroscopic amplitudes can be made explicit upon deriving a set of differential equations for the $\phi_n(r)$. For an A-body Hamiltonian H_A, which contains a kinetic energy term and a two-body potential, $H_A = -\Sigma_{i=1}^{A}(\nabla_{r_i}^2/2m_i) + \frac{1}{2}\Sigma_{i,j=1}^{A}V(|r_i-r_j|)$, we can write $H_A = H_{A-1} - (\nabla_{r_A}^2/2m_A) + \Sigma_{i=1}^{A-1}V(|r_i-r_A|)$, where H_{A-1} denotes the Hamiltonian of the $(A-1)$-body system and m_i is the mass of the ith nucleon (for simplicity we assume $m_i = m$ for $i = 1, \ldots, A$). Since $|\Psi_{A-1}^{n}\rangle$ and $|\psi_A\rangle$ are eigenstates of H_{A-1} and H_A, respectively, we have

$$\langle\Psi_{A-1}^{n}|H_A|\psi_A\rangle = E_A\langle\Psi_{A-1}^{n}|\psi_A\rangle = E_{A-1}^{n}\langle\Psi_{A-1}^{n}|\psi_A\rangle$$
$$+ \langle\Psi_{A-1}^{n}| -\frac{\nabla_{r_A}^2}{2m} + \sum_{i=1}^{A-1} V(|r_i-r_A|)|\psi_A\rangle.$$
(2.4)

Inserting the expansion given in Eq. (2.1) for $|\psi_A\rangle$, we obtain a set of exact, Schrödinger-like coupled equations for the spectroscopic amplitudes:

$$(E_A - E_{A-1}^{n})\phi_n(r) = -\frac{\nabla_r^2}{2m}\phi_n(r)$$
$$+ \sum_{n'=1}^{\infty} \langle\Psi_{A-1}^{n}| \sum_{i=1}^{A-1} V(|r_i-r|)|\Psi_{A-1}^{n'}\rangle\phi_{n'}(r).$$
(2.5)

This set of equations, originally derived for stripping reactions (see, for example, Ref. [18]), is not sufficiently appreciated. In the form just given, these equations may be too complex for use directly in calculations, since the $V_{nn'}(r)$ $\equiv \langle\Psi_{A-1}^{n}|\Sigma_{i=1}^{A-1}V(|r_i-r|)|\Psi_{A-1}^{n'}\rangle$ couple an infinite set of coefficients. However, they allow us to discuss the long-range behavior of the A-body ground state wave function as well as derive commonly used approximations.

The solutions of Eq. (2.5) include not only the physically relevant completely antisymmetric states, but also the mixed-symmetric, i.e., unphysical, states. As long as the coupled equations are solved exactly this does not cause any problems since the two classes of states do not mix. However, when approximations are invoked one needs to ensure that the unphysical solutions are eliminated.

From Eq. (2.5) we can extract information on the long-range behavior of the A-body ground state wave function. The matrix element $V_{nn'}(r_A)$, for n or n' corresponding to an $(A-1)$-body bound state, has a range which is determined by the convolution of the (short-range) two-body potential with the bound-state wave function. Thus it falls off rapidly with increasing $r_A = |r_A|$. When both Ψ_{A-1}^{n} and

$\Psi_{A-1}^{n'}$ describe continuum states, the matrix element has a long-range, but infinitesimal, tail. Solving Eq. (2.5) outside the range of the potential, we find that the $\phi_n(r_A)$ decouple and fall off exponentially, $\phi_n(r_A) \propto \exp[-\sqrt{2m(E_{A-1}^{n}-E_A)}r_A]/r$. Since $(E_{A-1}^{n}-E_A)$ is smallest for $n=1$, the long-range behavior of the A-body wave function is dominated by $\phi_1(r_A)\Psi_{A-1}^{1}(r_1, \ldots, r_{A-1})$. Thus processes with reaction probabilities that are peaked in the asymptotic region depend only on the asymptotic normalization coefficient, $A_{nc} = \lim_{r\to\infty}\phi_1(r)r\exp[\sqrt{2m(E_A-E_{A-1}^{1})}r]$ (see also Refs. [8,9]). The asymptotic normalization coefficient is a property of the spectroscopic amplitude and hence implicitly includes the spectroscopic factor.

To obtain an explicit expression for the asymptotic normalization coefficient, we Fourier transform Eq. (2.5) [to include center-of-mass corrections, use Eq. (D11)]. This gives us

$$\tilde{\phi}_n(k) = \frac{1}{E_A - E_{A-1}^{n} - \frac{k^2}{2m}} \sum_{n'=1}^{\infty} \int dr e^{ikr}$$
$$\times \langle\Psi_{A-1}^{n}|\sum_{i=1}^{A-1} V(|r_i-r|)|\Psi_{A-1}^{n'}\rangle\phi_{n'}(r).$$
(2.6)

The pole in $\tilde{\phi}_n(k)$ is thus explicitly seen. It is this pole which is responsible for the upturn in the astrophysical S factor of the $^7\text{Be}(p,\gamma)^8\text{B}$ and $^{16}\text{O}(p,\gamma)^{17}\text{F*}$ reactions as the incident momentum goes to zero [6]. As shown in Ref. [10], the residue at this pole for $n=1$ is proportional to the asymptotic normalization coefficient. We have

$$A_{nc} = \lim_{k\to-i\kappa} 4m\pi^2 \sum_{n'=1}^{\infty} \int dr e^{ikr}$$
$$\times \langle\Psi_{A-1}^{1}|\sum_{i=1}^{A-1} V(|r_i-r|)|\Psi_{A-1}^{n'}\rangle\phi_{n'}(r),$$
(2.7)

where $\kappa = \sqrt{2m(E_A-E_{A-1}^{1})}$, i.e., the asymptotic normalization coefficient can be given as an integral over the interior of the nucleus [since Ψ_{A-1}^{1} has the spatial extent of the ground state of the $(A-1)$-body system]. The price paid is that there is a sum over all the spectroscopic amplitudes.

For arbitrary distances, we may consider approximating the Ψ_{A-1}^{n} in Eq. (2.5) by Slater determinants constructed from the spectroscopic amplitudes $\phi_i(r)$ with $i \in \{1, \ldots, A\}$. In this case, we obtain the Hartree-Fock equations in coordinate space. The A Hartree-Fock orbitals can thus be identified as approximations to the spectroscopic amplitudes and the Hartree-Fock single-particle energies approximate single-nucleon separation energies. The local (Hartree) term arises from the diagonal terms (V_{nn}) in Eq. (2.5), and the off-diagonal terms ($V_{nn'}$ with $n \neq n'$) give the nonlocal (exchange) potential, i.e., the Fock terms originate

from the channel coupling. If the off-diagonal elements ($V_{nn'}$, $n \neq n'$) are neglected we obtain the Hartree approximation.

A one-body potential model, which treats the nucleus as a system of A *noninteracting* nucleons, can be obtained from either the Hartree or the Hartree-Fock approximation. Starting from the Hartree equations, one can express the many-body wave functions Ψ^n_{A-1} as Slater determinants of the $\phi_i(\mathbf{r})$, $i \in \{1, \ldots, A\}$, and impose the condition that the one-body potential be the same for each single-particle orbital, $V_{nn}(\mathbf{r}) \Rightarrow V(\mathbf{r})$. Alternatively, beginning from the Hartree-Fock equations, one can dictate the replacement

$$V_{nn'}(\mathbf{r}) = \langle \Psi^n_{A-1} | \sum_{i=1}^{A-1} V(|\mathbf{r}_i - \mathbf{r}|) | \Psi^{n'}_{A-1} \rangle \Rightarrow V(\mathbf{r}) \delta_{nn'} . \tag{2.8}$$

In both cases, one obtains the following equation for the $\phi_n(\mathbf{r})$:

$$(E_A - E^n_{A-1}) \phi_n(\mathbf{r}) = -\frac{\nabla^2_r}{2m} \phi_n(\mathbf{r}) + V(\mathbf{r}) \phi_n(\mathbf{r}), \quad (2.9)$$

which defines a one-body potential model with A noninteracting nucleons in a common potential. Thus, the one-body potential model may be regarded as an approximation to either the Hartree or the Hartree-Fock approach. In this model, antisymmetry can be ensured in a straightforward manner: many-body wave functions, such as Ψ^n_{A-1} or ψ_A, are—like in the Hartree-Fock picture—Slater determinants constructed from A given single-particle wave functions.

The Slater determinants, in one-body potential models, usually play only a formal role and disappear from sight in actual calculations, to the extent that their existence is often forgotten causing conceptual confusion. For the matrix elements of a one-body operator, $\mathcal{O}(\mathbf{r})$, between states that differ only in one orbital, the remaining $(A-1)$-body orbitals integrate out leaving just the active orbitals. Thus we have a matrix element like $\int d\mathbf{r} \phi_m(\mathbf{r}) \mathcal{O}(\mathbf{r}) \phi_{m'}(\mathbf{r})$ where m and m' denote the active orbitals. At first sight this expression is a pure one-body expression that seems to have no antisymmetry present and indeed at the computational level this is true. In calculating the matrix elements of one-body operators there is no need to explicitly consider the Slater determinants. However, the Slater determinants did their job of ensuring antisymmetry before they were integrated out.

Since the single-particle Schrödinger equation, Eq. (2.9), originates from the coupled-channels equations for the expansion coefficients, Eq. (2.5), the bound-state single-particle wave functions of the potential-model discussed here approximate the spectroscopic amplitudes. Therefore, the potential-model approximation gives A nonzero spectroscopic amplitudes, all of which are normalized to one. Consequently, the associated spectroscopic factors are 1 and carry no information on the many-body correlations of the nuclei involved.

One can, however, move beyond the simple picture of A noninteracting particles in a common potential and include some many-nucleon correlations in a schematic manner. As a

first correction, one usually allows for single-particle orbitals which are different for the $(A-1)$-body and A-body systems. As a result, the expansion of ψ_A, Eq. (2.1), will have contributions from more than A terms. Consequently, the spectroscopic factors will be, on average, less than 1, and most individual factors will be smaller than 1.

Another important correction to be taken into account involves the treatment of the center-of-mass motion and leads to the introduction of an intrinsic spectroscopic amplitude (see Appendix D). In both the Hartree-Fock and the one-body potential-model approaches, the center of mass is erroneously confined in a potential. In potential models which are based on a harmonic oscillator potential the center-of-mass corrections can be taken into account exactly. In this case, the spectroscopic amplitudes corresponding to valence shell orbitals increase by a factor $[A/(A-1)]^{m/2}$, where m denotes the major oscillator shell under consideration, while the amplitudes associated with lower shells decrease accordingly [15]. The sum rule for the spectroscopic factors remains unaffected. The center-of-mass correction causes some of the spectroscopic factors to be greater than unity.

The above considerations illustrate that information on the structure of the A-body wave function of a nuclear system, which is lost in a simple one-body potential-model approach, can be in part recovered through the appropriate correction to the single-particle wave functions, that is, by multiplying by the spectroscopic factors. In Sec. IV we will discuss how the resulting deviations of the spectroscopic factors from 1 (or zero) affect physical observables such as the cross sections for external capture reactions.

III. AN ALTERNATIVE PERSPECTIVE

In this section we approach the spectroscopic amplitudes from a different perspective. Motivated by cluster-model results, we derive a set of coupled integral equations. While general cluster-model calculations involve two or more clusters of arbitrary size, we restrict ourselves to describing an A-body nucleus as an $(A-1)$-body cluster plus a single nucleon. The approach pursued in this section has the advantage that explicit channel coupling is no longer required to ensure antisymmetry. Again, various approximation schemes can be used to simplify the coupled equations. In particular, in one of these schemes the Hartree-Fock equations can be recovered; in another a one-body model emerges, which was previously discussed by various authors [16,19] and which differs from the model presented in the last section.

Starting with the Schrödinger equation for an A-body system, $H_A \psi_A = E_A \psi_A$, and expanding ψ_A in terms of the antisymmetric basis states $_\mathcal{A} \Psi^{n,r}_A$, we obtain

$$\sum_{n'=1}^{\infty} \int d\mathbf{r}' \langle _\mathcal{A} \Psi^{n,r}_A | H_A | _\mathcal{A} \Psi^{n',r'}_A \rangle \phi_{n'}(\mathbf{r}')$$

$$= E_A \sum_{n'=1}^{\infty} \int d\mathbf{r}' \langle _\mathcal{A} \Psi^{n,r}_A | _\mathcal{A} \Psi^{n',r'}_A \rangle \phi_{n'}(\mathbf{r}'), \quad (3.1)$$

or, equivalently

$$\sum_{n'=1}^{\infty} \int dr'_A \mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}') \phi_{n'}(\boldsymbol{r}')$$

$$= E_A \sum_{n'=1}^{\infty} \int dr' \mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}') \phi_{n'}(\boldsymbol{r}'), \qquad (3.2)$$

where $_A\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')=\langle _A\Psi_A^{n,r}|H_A|_A\Psi_A^{n',r'}\rangle$ and $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')=\langle _A\Psi_A^{n,r}|_A\Psi_A^{n',r'}\rangle$ denote the kernels of integral operators $_A\hat{\mathcal{H}}_{nn'}$ and $\hat{\mathcal{N}}_{nn'}$, respectively. The operator $\hat{\mathcal{I}}_{nn'}$ ($\hat{\mathcal{I}}_{nn'}=_A\hat{\mathcal{H}}_{nn'}$ or $\hat{\mathcal{N}}_{nn'}$), which is the (n,n') entry of an infinite-dimensional matrix $\hat{\mathcal{I}}$ ($\hat{\mathcal{I}}=_A\hat{\mathcal{H}}$ or $\hat{\mathcal{N}}$), acts as follows: $\hat{\mathcal{I}}_{nn'}f(\boldsymbol{r})\equiv\int d\boldsymbol{r}'\mathcal{I}(n,\boldsymbol{r},n',\boldsymbol{r}')f(\boldsymbol{r}')$. The matrix $\hat{\mathcal{N}}$ serves as the norm operator for the antisymmetrized basis $\{_A\Psi_A^{n,r}\}$ and has many interesting properties which are discussed in Appendix B. $\hat{\mathcal{N}}/A$ is a projection operator which projects an arbitrary many-body state into the set of completely antisymmetric wave functions. Thus, Eqs. (3.1) and (3.2) contain an explicit projection onto completely antisymmetric states, in contrast to the coupled differential equations discussed in the previous section, Eq. (2.5). This projection means that the solutions of Eq. (3.2), $\phi_n^{(sol)}(\boldsymbol{r})$, can contain arbitrary contributions from mixed-symmetric states while still satisfying the equations of motion. Thus the projected state, $\phi_n=(1/A)\sum_{n'=1}^{\infty}\int d\boldsymbol{r}'\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')\phi_{n'}^{(sol)}(\boldsymbol{r}')$, rather than $\phi_n^{(sol)}(\boldsymbol{r})$, corresponds to the physical state.

With Eq. (3.1) [or, equivalently, Eq. (3.2)], we have derived a set of coupled-channels (integral) equations, analogous to the system of coupled differential equations in the previous section, Eq. (2.5). In the present approach, however, antisymmetry is explicitly enforced, resulting in a set of equations which contain a projection operator and a complicated expression for the effective Hamiltonian. To illustrate this, we compare the Hamiltonian kernel in the nonantisymmetrized basis, $\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')$, with the corresponding expression in the antisymmetrized basis, $_A\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')$. The former is local, i.e., diagonal, in the spatial coordinate, although not in the discrete variable n,

$$\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')=\langle\Psi_A^{n,r}|H_A|\Psi_A^{n',r'}\rangle \qquad (3.3)$$

$$= \delta(\boldsymbol{r}-\boldsymbol{r}')\left[\delta_{nn'}\left(E_{A-1}^n-\frac{\nabla_{r'}^2}{2m}\right)\right.$$

$$\left.+\langle\Psi_{A-1}^n|\sum_{i=1}^{A-1}V(|\boldsymbol{r}_i-\boldsymbol{r}|)|\Psi_{A-1}^{n'}\rangle\right], \quad (3.4)$$

whereas the latter has off-diagonal contributions from both $\boldsymbol{r}$ and n:

$$_A\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')=\sum_{n''=1}^{\infty}\int d\boldsymbol{r}''\mathcal{H}(n,\boldsymbol{r},n'',\boldsymbol{r}'')\mathcal{N}(n'',\boldsymbol{r}'',n',\boldsymbol{r}')$$

$$(3.5)$$

$$=\left(E_{A-1}^n-\frac{\nabla_r^2}{2m}\right)\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$$

$$+\delta(\boldsymbol{r}-\boldsymbol{r}')\langle\Psi_{A-1}^n|\sum_{i=1}^{A-1}V(|\boldsymbol{r}_i-\boldsymbol{r}|)|\Psi_{A-1}^{n'}\rangle$$

$$-(A-1)\int\prod_{i=2}^{A-1}dr_i\Psi_{A-1}^{n*}(\boldsymbol{r}',\boldsymbol{r}_2,\ldots,\boldsymbol{r}_{A-1})$$

$$\times\left[V(|\boldsymbol{r}'-\boldsymbol{r}|)+\sum_{i=2}^{A-1}V(|\boldsymbol{r}_i-\boldsymbol{r}|)\right]\Psi_{A-1}^{n'}(\boldsymbol{r},\boldsymbol{r}_2,\ldots,\boldsymbol{r}_{A-1}).$$

$$(3.6)$$

Imposing antisymmetry via the projection operator associated with $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$ leads to exchange terms in the effective potential.

For the special case of a one-body Hamiltonian, $H=\Sigma_{i=1}^{A}H(\boldsymbol{r}_i)$, we obtain the Hamiltonian kernels $\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')=\delta_{nn'}\delta(\boldsymbol{r}-\boldsymbol{r}')(E_{A-1}^n+H(\boldsymbol{r}))$ and $_A\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')=\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')(E_{A-1}^n+H(\boldsymbol{r}))$, and Eq. (3.2) reduces to the single-particle Schrödinger equation. The kernel $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$ guarantees that only expansion coefficients originating from an antisymmetric A-body wave function are considered, i.e., $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$ ensures that the associated single-particle orbitals are not among the occupied states of the $(A-1)$-body system. This can be trivially taken into account in the calculations. Nevertheless, even in a case as simple as this one, $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$ is not diagonal in n,n'.

In order to facilitate working with the above (exact) set of coupled integral equations, Eq. (3.2), various approximations may be considered. For example, the Hartree-Fock equations are recovered by taking the $(A-1)$-body basis states, Ψ_{A-1}^n, to be Slater determinants constructed from the expansion coefficients $\phi_n(\boldsymbol{r})$. In contrast to the approach presented in the previous section, the current method does not require channel coupling to obtain the Fock terms. Instead, the nonlocal (exchange) terms are now explicitly present in the effective potential, as can be seen in the last line of Eq. (3.6). Thus, the advantage of using antisymmetric basis states — coupled channels are not needed to include the Fock term contributions — is offset by additional complications in the resulting equations of motion: the Hamiltonian kernel is no longer local and the antisymmetry operator appears explicitly in Eq. (3.2). Note also that in the Hartree-Fock approximation the channels are implicitly coupled through the use of expansion coefficients in the $(A-1)$-body Slater determinants.

Another approximation method leads to equations which were previously obtained by Varga and Lovas *et al.* [16] in the framework of the cluster model. In this approach, we ignore those terms in $_A\mathcal{H}(n,\boldsymbol{r},n',\boldsymbol{r}')$ and $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$ that couple different values of the discrete variable, i.e., contributions for which $n\neq n'$ holds. The equations of motion for the coefficients $\phi_n(\boldsymbol{r})$ then take the following form:

$$\int d\boldsymbol{r}'_A\mathcal{H}(n,\boldsymbol{r},n,\boldsymbol{r}')\phi_n(\boldsymbol{r}')=E\int d\boldsymbol{r}'\mathcal{N}(n,\boldsymbol{r},n,\boldsymbol{r}')\phi_n(\boldsymbol{r}'),$$

$$(3.7)$$

that is, we have effectively integrated out the coordinates of $(A-1)$ particles to obtain a set of one-body equations. This equation is more general than Hartree-Fock, but the Hartee-Fock approximation can be recovered by taking the $(A-1)$-body wave functions to be Slater determinants composed from the spectroscopic amplitudes. We can then derive the one-body potential model, Eq. (2.9), as in the previous section. In these cases antisymmetry can be exactly imposed through the use of Slater determinants and the explicit projection operator, $\hat{\mathcal{N}}$, is not needed.

A second one-body equation can be obtained by taking the $(A-1)$-body wave functions from an external source independent of the spectroscopic amplitudes. This can go beyond Slater determinants and Hartree-Fock since the $(A-1)$-body wave functions can include many-body correlations; in principle they can even be exact. The quality of this approximation will depend on how well the $(A-1)$-body wave functions are chosen. In this approach the orbitals can be considered one at a time. The price paid for this convenience is twofold. First, the expressions for the Hamiltonian become more complicated; compare Eqs. (3.4) and (3.6). Secondly, when we move beyond Slater determinants, $\hat{\mathcal{N}}$ is explicitly required and, moreover, its diagonal element, $\hat{\mathcal{N}}_{nn}$, is no longer a projection operator (see Appendix B), so antisymmetry is not explicit.

The one-body models associated with Eqs. (2.9) and (3.7) differ, but in most situations both lead to a decoupling of the expansion coefficients. The exceptions are the Hartree-Fock approximation and other self-consistent models in which the $(A-1)$-body wave functions are constructed from the expansion coefficients. While the decoupling is in many ways advantageous, it also implies that we have lost the information on the relative normalizations of the $\phi_n(r)$. If we assume that A of the coefficients are nonzero we may take them to be individually normalized to one. This is consistent with the overall normalization condition $A = \sum_{n'=1}^{\infty} \sum_{n=1}^{\infty} \int dr dr' \, \phi_n^*(r) \mathcal{N}(n,r,n',r') \phi_{n'}(r')$.

In the work of Lovas *et al.*, Eq. (3.7) was considered for the case $n = n' = 1$. The Hamiltonian operator $\hat{h} = (\hat{\mathcal{N}}_{11})_{\mathcal{A}}^{-1/2} \hat{\mathcal{H}}_{11} (\hat{\mathcal{N}}_{11})^{-1/2}$ and the wave function $\chi_l = (\hat{\mathcal{N}}_{11})^{1/2} \phi_1$ were defined. These redefinitions have the advantage of leading to an equation which takes the same form as the standard Schrödinger equation, $\hat{h}\chi_l = E\chi_l$. The χ_l provides a better approximation to the true spectroscopic amplitude than the model ϕ_1 [the solution of Eq. (3.7)] since it includes the effect of $(\hat{\mathcal{N}}_{11})^{1/2}$, an approximate projection operator onto antisymmetric states. As noted previously, a projection operator may be needed and this is amplified in the discussion of Ref. [7] in the next section. It is also χ_l (normalized to one) that in this approach should be identified with the single-particle wave function, both because of this better correspondence with the true spectroscopic amplitude and because of the form of the equation which it satisfies.

IV. SPECTROSCOPIC AMPLITUDES AND REACTION RATES

In this section we discuss how the spectroscopic amplitudes can be used to calculate reaction rates and elaborate on their physics content. We show that the spatial dependence of the spectroscopic amplitude and its norm, the spectroscopic factor, describe different physical aspects of the many-nucleon system, namely, single-particle properties of the Ath particle and distortions of the $(A-1)$-body system, respectively. We make the connection to the potential-model approach and find that both aspects are included, at least approximately, when spectroscopic factors are employed to scale the wave functions. Since our findings contradict the conclusions of Ref. [7], we explore the claims made in that paper.

To calculate the relevant reaction cross sections, we expand both the A-body bound state, $|\psi_A(r_1, \ldots, r_A)\rangle$, and the wave function in the incident channel, $|\psi_A^K(r_1, \ldots, r_A)\rangle$, as in Eq. (2.1). Here K specifies the asymptotic momentum of the incident particle relative to the $(A-1)$-body target nucleus. The corresponding expansion coefficients are given by $\phi_n(r) = \sqrt{A}\langle \Psi_A^{n,r}|\psi_A(r_1, \ldots, r_A)\rangle$ and $\phi_n^K(r) = \sqrt{A}\langle \Psi_A^{n,r}|\psi_A^K(r_1, \ldots, r_A)\rangle$, respectively. The expansion coefficient $\phi_1^K(r)$, associated with the continuum wave function, is the optical model wave function [20,21]. Thus the formalism based on expansion coefficients is sufficiently general to include both spectroscopic amplitudes and optical model wave functions. It will be useful whenever we are dealing with one-body operators. The matrix element for the one-body transition operator $\mathcal{O}(r)$ can then be written as

$$\mathcal{M} \equiv \langle \psi_A | \sum_{i=1}^{A} \mathcal{O}(r_i)|\psi_A^K\rangle = A\langle \psi_A|\mathcal{O}(r_A)|\psi_A^K\rangle \quad (4.1)$$

$$= \sum_{n=1}^{\infty} \int dr \, \phi_n^*(r)\mathcal{O}(r)\phi_n^K(r). \quad (4.2)$$

To make the connection with the potential model we separate the spatial dependence of the spectroscopic amplitude and its normalization, $\sqrt{S_n}$, as follows:

$$\phi_n(r) = \sqrt{S_n}\,\tilde{\phi}_n(r), \quad (4.3)$$

where $\int dr |\tilde{\phi}_n(r)|^2 = 1$. In Sec. II, we have shown that the potential-model wave functions approximate the spectroscopic amplitudes. Since the norm of $\tilde{\phi}_n(r)$ is one, whereas that of $\phi_n(r)$ is S_n, the $\tilde{\phi}_n(r)$, rather than the $\phi_n(r)$, should be identified with the potential-model wave functions. There is no equivalent normalization factor associated with the scattering state; ψ_A^K is normalized asymptotically.

The transition matrix element given in Eq. (4.2) can now be written as $\mathcal{M} = \sum_{n=1}^{\infty} \sqrt{S_n}\int dr \, \tilde{\phi}_n^*(r)\mathcal{O}(r)\phi_n^K(r)$. Both the $^7\text{Be}(p,\gamma)^8\text{B}$ and $^{16}\text{O}(p,\gamma)^{17}\text{F}^*$ reactions at threshold are peripheral, i.e., the capture processes take place at large distances from the center of the target nucleus, which is in its ground state. In such situations, as for all direct capture reactions, only the first expansion coefficient for ψ_A^K contributes and the matrix element reduces to $\mathcal{M} \rightarrow \sqrt{S_1}\int dr \, \tilde{\phi}_1^*(r)\mathcal{O}(r)\phi_1^K(r)$. Since the cross section is proportional to $|\mathcal{M}|^2$, the spectroscopic factor associated with the ground state of the $(A-1)$-body system, S_1, occurs lin-

early in the expression for the reaction rate. Thus we conclude that when a potential-model wave function (or any other function normalized to one) is used to calculate the transition matrix element $\mathcal{M}$, the resulting cross section needs to be multiplied by the associated spectroscopic factor in order to account for (some of) the many-body correlations in the nuclei involved. The implications of this for the asymptotic normalization are discussed at the end of this section.

The separation introduced in Eq. (4.3) is motivated by the realization that the spatial dependence of the spectroscopic amplitude $\phi_n(r_A)$, and its norm, the spectroscopic factor S_n, describe different physical properties of the nuclear many-body system. The former is related to the shape of the single-particle orbital of the Ath nucleon in the system, and can therefore be expressed through the normalized amplitude $\tilde{\phi}_n(r)$. The latter provides a measure of the structural similarity of the nth excited $(A-1)$-body state and an $(A-1)$-body subcluster of the larger system. Equivalently, the set of spectroscopic factors associated with the expansion of ψ_A, Eq. (2.1), can be viewed as describing the distortion of the $(A-1)$-body core due to the presence of an extra nucleon. This can be seen, for example, by casting S_n into the following form:

$$S_n = \int dr |\phi_n(r)|^2 \qquad (4.4)$$

$$= A \int \left(\prod_{i=1}^{A-1} dr_i \right) \int \left(\prod_{i=1}^{A-1} dr_i' \right)$$

$$\times \Psi_{A-1}^{n*}(r_1,\ldots,r_{A-1}) \Psi_{A-1}^{n}(r_1',\ldots,r_{A-1}')$$

$$\times \left[\int dr \psi_A^*(r_1,\ldots,r_{A-1},r) \psi_A(r_1',\ldots,r_{A-1}',r) \right]. \qquad (4.5)$$

In the last line (expression in square brackets) we have integrated out the dependence on the Ath particle. We are left with expressions involving wave functions of the $(A-1)$-body system. The extra particle's influence is still present in the modification it has induced in the $(A-1)$-body cluster. Upon decoupling the equations of motion for the expansion coefficients, as required in our derivation of the one-body models, this information on the last particle's influence is lost; the many-body correlations contained in the integrals S_n disappear and the spectroscopic factors become 1.

The spectroscopic factors carry information both on the dynamical distortions induced by the interaction between the $(A-1)$-body system and the extra particle and on antisymmetry effects. Specifically, as shown in Appendix C, the spectroscopic factor can be written as

$$S_n = N_n \langle \psi_A^{\|,n} | \psi_A^{\|,n} \rangle, \qquad (4.6)$$

where $\langle \psi_A^{\|,n} | \psi_A^{\|,n} \rangle$ reflects the influence of the distortions, and the normalization factor N_n contains antisymmetry effects. Specifically, N_n keeps track of the requirement that the

nucleon orbitals in the nth excited $(A-1)$-body state must be orthogonal to the orbital $\tilde{\phi}_n(r)$ of the Ath particle [for details see Eq. (C5)]. When center-of-mass corrections are taken into account, N_n may be greater than 1, otherwise it is less than or equal to 1. The matrix element $\langle \psi_A^{\|,n} | \psi_A^{\|,n} \rangle$ is always less than or equal to one. Consequently, when center-of-mass corrections are ignored, we have the restriction $S_n \leq 1$ for the spectroscopic factor. The influence of these corrections are discussed in detail in Appendix D.

At this point we would like to reassert that it is correct and necessary to include spectroscopic factors in potential-model cross sections of nuclear capture reactions. This procedure was questioned in Ref. [7]. The author of that paper argues that the short-range correlations contained in the spectroscopic factor should modify the bound-state wave function only in the nuclear interior and have no effect on the asymptotic behavior. Since multiplying the potential-model wave function by $\sqrt{S_n}$, however, affects its overall normalization, including in the tail region, the usual procedure of treating microscopic correlations in the potential model, viz. through spectroscopic factors, is pronounced to be incorrect. To illustrate his point, the author compares a wave function $\chi_c(r)$, which describes the relative motion of ^{7}Be and p in ^{8}B, to the spectroscopic amplitude function of the ^{7}Be$+p$ configuration in ^{8}B (Note that this χ_c is different from the wave function χ_l introduced by Lovas *et al.* [16] and discussed in the previous section). The wave functions χ_c considered individually do not contain Pauli effects but, when used in cluster-model calculations, appear behind an antisymmetrization operator. The spectroscopic amplitudes, on the other hand, are calculated from properly antisymmetrized wave functions. The two functions are shown to agree with each other and with the appropriately normalized Coulomb-Whittaker function in the asymptotic region, but they differ at small radii, as can be seen in Fig. 2 of Ref. [7]. Their difference is interpreted as a measure of the Pauli effects. Since multiplying $\chi_c(r)$ by a spectroscopic factor would affect both its short-range and asymptotic behaviors, the author concludes that this cannot be the proper procedure for incorporating microscopic substructure effects in potential-model calculations.

The argument presented in Ref. [7] is not correct. The function $\chi_c(r)$ does not, in general, correspond to a potential-model wave function. First, unlike the one-body wave functions we have considered, it already includes the spectroscopic factor through the normalization of the A-body wave function. Moreover, very little physics can be associated with χ_c outside the context of its usual use as a component in a properly antisymmetrized cluster-model wave function. To show this, we consider an arbitrary product state $\psi_A^P(r_1,\ldots,r_A) = \varphi(r_A) \psi_{A-1}^P(r_1,\ldots,r_{A-1})$. In the nonantisymmetrized basis, it has expansion coefficients

$$\phi_n^P(r) = \sqrt{A} \langle \Psi_A^{n,r} | \psi_A^P \rangle = \varphi(r) \sqrt{A} \langle \Psi_{A-1}^{n} | \psi_{A-1}^P \rangle, \quad (4.7)$$

and the associated antisymmetrized, i.e., physical

state, has expansion coefficients $\phi_n(\mathbf{r})$ $=(1/A)\sum_{n'=1}^{\infty}\int d\mathbf{r}\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')\phi_{n'}^P(\mathbf{r})$. In the product given above, $\varphi(\mathbf{r})$ can be taken to correspond to the relative-motion function $\chi_c(\mathbf{r})$ of Ref. [7]. As discussed in the previous section, $\mathcal{N}$ enforces antisymmetry by projecting onto a completely antisymmetric state. Thus, the choice of $\varphi(\mathbf{r})$ is somewhat arbitrary, since many functions lead to the same physical state. We may, for example, consider the case in which ψ_{A-1}^P and Ψ_{A-1}^n are Slater determinants and $\psi_{A-1}^P = \Psi_{A-1}^1$. If we then take $\varphi(\mathbf{r})$ to be orthogonal to the orbitals in ψ_{A-1}^P, the antisymmetry requirement will turn the product into a Slater determinant and we obtain $\phi_1(\mathbf{r}) = \phi_1^P(\mathbf{r})/\sqrt{A} = \varphi(\mathbf{r})$. On the other hand, if $\varphi(\mathbf{r})$ is not orthogonal to the occupied orbitals, the nonorthogonal components will be projected out as well. In the extreme case of $\varphi(\mathbf{r})$ being a linear combination of the occupied states, $\phi_1(\mathbf{r})$ is zero. From these considerations we conclude that the difference between $\varphi(\mathbf{r})$ and the associated physical state has no particular significance. The effect that antisymmetrization has on $\varphi(\mathbf{r})$ is not pertinent to the one-body models considered in this paper since both already include antisymmetry, at least approximately. [The effect of antisymmetry on the shape of the spectroscopic amplitudes is distinct from the effect of antisymmetry contained in the N_n of Eq. (4.6).] A more useful comparison would be between the spectroscopic amplitude and $(\hat{\mathcal{N}}_{11})^{1/2}\varphi(\mathbf{r}')$, since this would measure the influence of the off-diagonal matrix elements of $\hat{\mathcal{N}}$ and thus test the validity of the single-particle model based on Eq. (3.7). Neither comparison clarifies the role of the spectroscopic factors since, as previously noted, the spectroscopic factor is contained in both χ_c and the spectroscopic amplitudes.

At this point it is useful to return to the asymptotic normalization, A_{nc}, of the spectroscopic amplitude. For the low-energy $^7\text{Be}(p,\gamma)^8\text{B}$ and $^{16}\text{O}(p,\gamma)^{17}\text{F}^*$ reactions, for example, the capture occurs at large radii. Thus the asymptotic normalization of the spectroscopic amplitude is sufficient for describing the bound state in the physically relevant region. This is in line with the conclusions of Refs. [8,9]. As explained above, there are two different physical effects included in the spectroscopic amplitude and hence in its asymptotic normalization: one is related to the distortions of the $(A-1)$-body cluster due to the presence of an additional nucleon and is contained in the spectroscopic factor and the other is related to the single-particle properties of that extra particle and is described by the spatial dependence of the amplitude. Both are needed.

V. CONCLUSIONS

Spectroscopic amplitudes play a central role in the description of single-particle transfer reactions such as radiative nucleon capture. The amplitudes contain both single-particle and many-nucleon aspects of the nuclear many-body problem and can be, in principle, obtained from a fully microscopic model. We have presented two alternative approaches, each based on a set of coupled-channels equations, and have shown how one-body approximations can be de-

rived in a systematic manner. We obtained two different single-particle models. In both cases, the single-particle wave function was found to be an approximation to the spectroscopic amplitude but normalized to one rather than to the spectroscopic factor. The quality of the one-body approximation depends on how well it describes the spatial dependence of the spectroscopic amplitude. However, even the best single-particle wave function will miss the spectroscopic factor.

The first one-body approximation considered here results in A noninteracting particles in a single-particle potential. The simplification occurs since the equations for the spectroscopic amplitudes are no longer coupled; instead, we have A independent equations. Since we still have A particles and A orbitals, we can construct an antisymmetric A-body wave function by taking it to be a Slater determinant. In this model, it is redundant to explicitly enforce antisymmetry, e.g., through projection operators. The quality of this approach depends on how well the single-particle potential is chosen and how well the single-particle wave functions reproduce the shape of the spectroscopic amplitudes.

The second one-body model presented here is usually derived within the generator-coordinate formalism. We obtained it by truncating a set of coupled integral equations. In this approach, antisymmetry is (approximately) imposed for each orbital separately through (approximate) projection operators. Unlike the first one-body approximation it can include many-particle correlations in the $(A-1)$-body subsystem. In principle, this approach is also simpler since we do not need to consider all the orbitals together. The price we pay is that the potential cannot be approximated as simply since it implicitly contains a projection into antisymmetric states. There is also an explicit projection operator that must be approximated. The quality of this approach depends on the choice of the $(A-1)$-body wave functions and the importance of the channel coupling.

It is important to realize that there is not one unique single-particle model. Different one-body approximations to the nuclear many-body problem exist and can be derived independently of each other. The resulting single-particle models may differ in subtle but crucial details and should therefore not be confused with each other. We have derived two such models and discussed their relation to each other and distinctions between them. In particular, the very different techniques for including antisymmetry should be noted.

The spectroscopic factor, in its simplest form, reflects the partition probability of the A-body system into smaller clusters with allowance for antisymmetry effects. In the present paper it is cast in a complimentary light. It presents itself as a manifestation of the distortion of the $(A-1)$-body system due to the presence of the Ath particle. This distortion is both dynamical due to the interactions and kinematical due to antisymmetry. Since these are pure many-body effects they are, by definition, absent from one-body approximations. When center-of-mass corrections are included, the spectroscopic factors can be greater than 1 without violating the Pauli principle. Otherwise they must be less than or equal to 1.

A full calculation must include both the one-body and

many-body effects. As the present paper emphasizes, this can be accomplished through the use of spectroscopic amplitudes. Obtaining these amplitudes, however, requires the full solution of the coupled equations presented here or a fully microscopic model. While this is still a distant goal, some recent fully microscopic approaches show promising results for low-mass systems [22]. Furthermore, models such as the shell model, the continuum shell model, or the cluster model include some many-nucleon correlations and provide reasonable approximations to the full problem. Since many-body effects are not contained in one-body models, cross sections calculated in this framework need to include the spectroscopic factor. For processes that are strongly peaked in the tail region, like the low-energy $^{7}\mathrm{Be}(p,\gamma)^{8}\mathrm{B}$ and $^{16}\mathrm{O}(p,\gamma)^{17}\mathrm{F}^*$ reactions, the one-body and many-body effects can be combined into a single parameter — the asymptotic normalization coefficient.

APPENDIX A: THE BASES

We begin by defining a basis $\{\Psi_{A-1}^n\}_{n=1,2,\ldots}$ for $\mathrm{H}_{A-1}^{\mathcal{A}}$, the space of completely antisymmetric $(A-1)$-body wave functions $\psi_{A-1}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1})$. The basis states are orthonormal,

$$\int \prod_{i=1}^{A-1} d\boldsymbol{r}_i \Psi_{A-1}^{n*}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1})\Psi_{A-1}^{n'}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1})$$
$$= \delta_{nn'}, \tag{A1}$$

and complete in $\mathrm{H}_{A-1}^{\mathcal{A}}$, that is,

$$\int \prod_{i=1}^{A-1} d\boldsymbol{r}_i' \sum_{n=1}^{\infty} \Psi_{A-1}^n(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1})$$
$$\times \Psi_{A-1}^{n*}(\boldsymbol{r}_1',\ldots,\boldsymbol{r}_{A-1}')\psi_{A-1}(\boldsymbol{r}_1',\ldots,\boldsymbol{r}_{A-1}')$$
$$= \psi_{A-1}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1}) \tag{A2}$$

holds for any $\psi_{A-1}\in \mathrm{H}_{A-1}^{\mathcal{A}}$. Specifically, for the sake of convenience, we choose Ψ_{A-1}^n which are eigenstates of the $(A-1)$-body Hamiltonian $H_{A-1}=-\Sigma_{i=1}^{A-1}(\nabla_{r_i}^2/2m_i) + \frac{1}{2}\Sigma_{i,j=1}^{A-1}V(|\boldsymbol{r}_i-\boldsymbol{r}_j|)$. To do so, we have to include both bound and scattering states. The superscript n labels the discrete as well as the continuous spectrum of H_{A-1}.

We now consider two different A-body spaces. The first, denoted by H_A, is spanned by

$$\Psi_A^{n,r}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)\equiv \Psi_{A-1}^n(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1})\delta(\boldsymbol{r}-\boldsymbol{r}_A), \tag{A3}$$

where $\boldsymbol{r}$ is a continuous parameter. The $\Psi_A^{n,r}$ are orthonormal with respect to both n and $\boldsymbol{r}$:

$$\int \prod_{i=1}^{A} d\boldsymbol{r}_i \Psi_A^{n,r*}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)\Psi_A^{n',r'}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)$$
$$= \delta_{nn'}\delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{A4}$$

and the completeness condition for this basis is given by

$$\int \prod_{i=1}^{A} d\boldsymbol{r}_i'$$
$$\times \left(\sum_{n=1}^{\infty}\int d\boldsymbol{r}\Psi_A^{n,r}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)\Psi_A^{n,r*}(\boldsymbol{r}_1',\ldots,\boldsymbol{r}_A')\right)$$
$$\times \psi_A(\boldsymbol{r}_1',\ldots,\boldsymbol{r}_A')$$
$$= \psi_A(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A), \tag{A5}$$

where $\psi_A\in H_A$. The space H_A is a direct sum of the subspaces $H_A^{\mathcal{A}}$ and $H_A^{\mathcal{M}}$ which contain, respectively, totally antisymmetric and mixed-symmetry A-body states. The latter are antisymmetric in the first $A-1$ coordinates and symmetric with respect to exchanges between the Ath nucleon and any other particle. For $A=2$, the space $H_{A=2}^{\mathcal{M}}$ is completely symmetric.

An arbitrary wave function $\psi_A\in H_A$ can thus be written as the sum of an antisymmetric and a mixed-symmetric component,

$$\psi_A(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)=\frac{\mathcal{A}}{\sqrt{A}}\psi_A(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)$$
$$+\left(1-\frac{\mathcal{A}}{\sqrt{A}}\right)\psi_A(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A) \tag{A6}$$
$$= \psi_A^{\mathcal{A}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)+\psi_A^{\mathcal{M}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A), \tag{A7}$$

where $\psi_A^{\mathcal{A}}\in H_A^{\mathcal{A}}$, $\psi_A^{\mathcal{M}}\in H_A^{\mathcal{M}}$, and $\mathcal{A}$ denotes an "intercluster" antisymmetrization operator, which antisymmetrizes between the Ath coordinate and the remaining $A-1$ coordinates. $\mathcal{A}$ is normalized by the condition $\mathcal{A}^2=\sqrt{A}\mathcal{A}$. Since $(\mathcal{A}/\sqrt{A})(1-\mathcal{A}/\sqrt{A})=0$, the two subspaces are orthogonal to each other, that is,

$$\int \prod_{i=1}^{A} d\boldsymbol{r}_i \psi_A^{\mathcal{A}*}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)\psi_A^{\mathcal{M}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)=0. \tag{A8}$$

Furthermore, a symmetric operator $\hat{\mathcal{O}}^{\mathcal{S}}$ cannot connect the two subspaces,

$$\int \prod_{i=1}^{A} d\boldsymbol{r}_i \psi_A^{\mathcal{A}*}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)\hat{\mathcal{O}}^{\mathcal{S}}\psi_A^{\mathcal{M}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)=0. \tag{A9}$$

This includes the case where $\hat{\mathcal{O}}^{\mathcal{S}}=H_A$, where H_A is the A-body Hamiltonian.

The space $H_A^{\mathcal{A}}$ is spanned by

$$_\mathcal{A}\Psi_A^{n,r}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) \equiv \mathcal{A}\Psi_A^{n,r}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

$$= \mathcal{A}[\Psi_{A-1}^n(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{A-1})\delta(\boldsymbol{r}-\boldsymbol{r}_A)] \tag{A10}$$

or, equivalently,

$$|_\mathcal{A}\Psi_A^{n,r}\rangle = a^\dagger(\boldsymbol{r})|\Psi_{A-1}^n\rangle, \tag{A11}$$

where $a^\dagger(\boldsymbol{r})$ creates a nucleon at position $\boldsymbol{r}$ and we have used the convention $\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = \langle \boldsymbol{r}_1, \ldots, \boldsymbol{r}_A | \psi_A \rangle$. The creation and annihilation operators $a^\dagger(\boldsymbol{r})$ and $a(\boldsymbol{r})$ obey the usual anticommutation relations, which ensure that the right-hand side of Eq. (A11) is totally antisymmetric. The completeness condition for the basis $\{_\mathcal{A}\Psi_A^{n,r}\}$ takes the form

$$\int \prod_{i=1}^A d\boldsymbol{r}_i' \left(\frac{1}{A} \sum_{n=1}^\infty \int d\boldsymbol{r} _\mathcal{A}\Psi_A^{n,r}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) \right.$$

$$\left. \times {}_\mathcal{A}\Psi_A^{n,r*}(\boldsymbol{r}_1', \ldots, \boldsymbol{r}_A') \right) \psi_A(\boldsymbol{r}_1', \ldots, \boldsymbol{r}_A') = \psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A),$$

$$\tag{A12}$$

where ψ_A is a fully antisymmetric A-body wave function from H_A^A. When ψ_A in Eq. (A12) is replaced by a state from $H_A^\mathcal{M}$, the right-hand side of the equation vanishes. Thus $\mathcal{P}_\mathcal{A} \equiv 1/A \sum_{n=1}^\infty \int d\boldsymbol{r} |_\mathcal{A}\Psi_A^{n,r}\rangle\langle_\mathcal{A}\Psi_A^{n,r}|$ is a projection operator which projects states $\psi_A \in H_A$ onto their antisymmetric component $\psi_A^A \in H_A^A$. That $\mathcal{P}_\mathcal{A}^2 = \mathcal{P}_\mathcal{A}$ holds can be shown by using Eq. (A14) below.

The advantages of using totally antisymmetric basis states are obvious. The disadvantages of employing this basis lies in the fact that the states are no longer orthonormal. Instead, we have

$$\int \prod_{i=1}^A d\boldsymbol{r}_i {}_\mathcal{A}\Psi_A^{n,r*}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) {}_\mathcal{A}\Psi_A^{n',r'}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

$$= \mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}'). \tag{A13}$$

The norm operator, $\hat{\mathcal{N}}$, and its kernel, $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$, have various interesting properties and are discussed in Appendix B.

The basis states $_\mathcal{A}\Psi_A^{n,r}$ are not linearly independent, but are related to each other through the norm operator, $\hat{\mathcal{N}}$, as follows:

$$_\mathcal{A}\Psi_A^{n,r}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

$$= \frac{1}{A} \sum_{n'=1}^\infty \int d\boldsymbol{r}' \mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}') {}_\mathcal{A}\Psi_A^{n',r'}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A).$$

$$\tag{A14}$$

In fact, the $\{_\mathcal{A}\Psi_A^{n,r}\}$ basis is overcomplete and, at least in the case where the Ψ_{A-1}^n are Slater determinants, spans the space H_A^A A times. This accounts for the factor $1/A$ in the first line of Eq. (2.1), and in the completeness relation, Eq. (A12).

An arbitrary antisymmetric A-body wave function $\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$ can now be expanded in one of the above bases. Using the set $\{\Psi_A^{n,r}\}$, we have

$$\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = \frac{1}{\sqrt{A}} \sum_{n=1}^\infty \int d\boldsymbol{r}\Psi_A^{n,r}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)\phi_n(\boldsymbol{r}),$$

$$\tag{A15}$$

with expansion coefficients

$$\phi_n(\boldsymbol{r}) = \sqrt{A} \int \prod_{i=1}^A d\boldsymbol{r}_i \Psi_A^{n,r*}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A).$$

$$\tag{A16}$$

Alternatively, we can use the antisymmetric basis, $\{_\mathcal{A}\Psi_A^{n,r}\}$, to write

$$\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = \frac{1}{A} \sum_{n=1}^\infty \int d\boldsymbol{r} {}_\mathcal{A}\Psi_A^{n,r}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)\phi_n(\boldsymbol{r}),$$

$$\tag{A17}$$

where

$$\phi_n(\boldsymbol{r}) = \int \prod_{i=1}^A d\boldsymbol{r}_i {}_\mathcal{A}\Psi_A^{n,r*}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A).$$

$$\tag{A18}$$

Equation (A17) follows by applying the antisymmetrization operator to Eq. (A15) and Eq. (A18) can be derived from Eq. (A16) by using the identity $\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = (\mathcal{A}/\sqrt{A})\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$, which holds for totally antisymmetric A-body states, and the Hermitian properties of $\mathcal{A}$. Thus, the coefficients are the same in both expansions.

From Eq. (A15), it follows that is also possible to write the wave function ψ_A as

$$\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = \frac{1}{\sqrt{A}} \sum_{n=1}^\infty \Psi_{A-1}^n(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{A-1})\phi_n(\boldsymbol{r}_A).$$

$$\tag{A19}$$

The coefficients $\phi_n(\boldsymbol{r})$ are identical to those in the previous expansions. From Eqs. (A11) and (A18), one infers that they take the following form:

$$\phi_n(\boldsymbol{r}_A) = \langle \Psi_{A-1}^n | a(\boldsymbol{r}) | \psi_A \rangle. \tag{A20}$$

When $\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$ denotes a bound state and the Ψ_{A-1}^n, which occur in the definitions of both $\Psi_A^{n,r}$ and $_\mathcal{A}\Psi_A^{n,r}$, are eigenstates of the $(A-1)$-body system, then the $\phi_n(\boldsymbol{r})$ are the *spectroscopic amplitudes* and the associated integrals $S_n \equiv \int d\boldsymbol{r} |\phi_n(\boldsymbol{r})|^2$ are the *spectroscopic factors*. The A-dependent normalization factors in the above equations are included so that $\int \prod_{i=1}^A d\boldsymbol{r}_i |\psi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)|^2 = 1$ holds, as well as

$$\sum_{n=1}^\infty \int d\boldsymbol{r} |\phi_n(\boldsymbol{r})|^2 = A, \tag{A21}$$

in accordance with the conventional normalization of the spectroscopic factors. This last equation follows by squaring Eq. (A15), integrating over the coordinates, and using the completeness of the $\Psi_A^{n,r}$.

APPENDIX B: THE NORM OPERATOR

The norm operator for the antisymmetric basis $\{_A\Psi_A^{n,r}\}$, $\hat{\mathcal{N}}$, and its kernel, $\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')$, have many interesting properties. To start with, the kernel can be written in several equivalent forms:

$$\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')$$

$$= \int \prod_{i=1}^{A} d\mathbf{r}_i \, _A\Psi_A^{n,r*}(\mathbf{r}_1, \ldots, \mathbf{r}_A) \, _A\Psi_A^{n',r'}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$

$$\text{(B1)}$$

$$= \sqrt{A} \int \prod_{i=1}^{A} d\mathbf{r}_i \Psi_A^{n,r*}(\mathbf{r}_1, \ldots, \mathbf{r}_A) \, _A\Psi_A^{n',r'}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$

$$\text{(B2)}$$

$$= \sqrt{A} \int \prod_{i=1}^{A} d\mathbf{r}_i \Psi_A^{n,r*}(\mathbf{r}_1, \ldots, \mathbf{r}_A) \mathcal{A} \Psi_A^{n',r'}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$

$$\text{(B3)}$$

$$= A \int \prod_{i=1}^{A} d\mathbf{r}_i \Psi_A^{n,r*}(\mathbf{r}_1, \ldots, \mathbf{r}_A) \frac{\mathcal{A}}{\sqrt{A}} \Psi_A^{n',r'}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$

$$\text{(B4)}$$

$$= \langle \Psi_{A-1}^{n} | a(\mathbf{r}) a^{\dagger}(\mathbf{r}') | \Psi_{A-1}^{n'} \rangle. \quad \text{(B5)}$$

We see that $\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')$ is not only the kernel of the norm operator for $\{_A\Psi_A^{n,r}\}$, Eq. (B1), but is also proportional to the overlap of an element from $\{_A\Psi_A^{n,r}\}$ with an element from the nonantisymmetrized basis $\{\Psi_A^{n,r}\}$, Eq. (B2). Furthermore, $\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')/\sqrt{A}$ is the matrix element of the "intercluster" antisymmetrization operator, $\mathcal{A}$, in the basis $\{\Psi_A^{n,r}\}$, Eq. (B3), or—equivalently—$\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')/A$ is the matrix element of the projection operator $\mathcal{A}/\sqrt{A}$ in that same basis, Eq. (B4). Finally, we can write $\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')$ as the matrix element of $a(\mathbf{r})a^{\dagger}(\mathbf{r}')$ in the $(A-1)$-body basis, Eq. (B5), where $a^{\dagger}(\mathbf{r})$ and $a(\mathbf{r})$ create and annihilate, respectively, a nucleon at position $\mathbf{r}$.

Since $\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')$ is proportional to a projection operator, it has no inverse. However, its square root—in the sense of a matrix operation—can be given. It is simply the matrix element of the antisymmetrization operator $\mathcal{A}$,

$$\sqrt{\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')}$$

$$= \int \prod_{i=1}^{A} d\mathbf{r}_i \Psi_A^{n,r*}(\mathbf{r}_1, \ldots, \mathbf{r}_A) \mathcal{A} \Psi_A^{n',r'}(\mathbf{r}_1, \ldots, \mathbf{r}_A).$$

$$\text{(B6)}$$

To see the projection operator nature of $\hat{\mathcal{N}}$ more directly, one can multiply Eq. (A15) by $_A\Psi_A^{n',r'}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$ and integrate over the coordinates. If ψ_A is completely antisymmetric, we obtain the following equation for the expansion coefficients:

$$\phi_n(\mathbf{r}) = \frac{1}{A} \sum_{n'=1}^{\infty} \int d\mathbf{r}' \mathcal{N}(n,\mathbf{r},n',\mathbf{r}') \phi_{n'}(\mathbf{r}'). \quad \text{(B7)}$$

For a mixed-symmetric state ψ_A, on the other hand, we find

$$0 = \frac{1}{A} \sum_{n'=1}^{\infty} \int d\mathbf{r}' \mathcal{N}(n,\mathbf{r},n',\mathbf{r}') \phi_{n'}(\mathbf{r}'), \quad \text{(B8)}$$

i.e., $\hat{\mathcal{N}}/A$, when acting on a set of expansion coefficients $\phi_n(\mathbf{r})$, behaves like a projection operator: It returns the coefficients $\phi_n(\mathbf{r})$ of an antisymmetric state and yields zero when the $\phi_n(\mathbf{r})$ correspond to a mixed-symmetric state. It follows immediately that in a restricted space of coefficients which originate from a completely antisymmetric wave function, $\hat{\mathcal{N}}/A$ becomes the identity matrix. In this restricted subspace, the functions $_A\Psi_A^{n',r'}/\sqrt{A}$ act in many ways as if they were orthonormal.

If we expand an excited state of the A-body system, $\Psi_A^{k}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$, as in Eq. (2.1), we obtain expansion coefficients $\phi_n^{A,k}(\mathbf{r}) \equiv \langle \Psi_{A-1}^{n} | a(\mathbf{r}) | \Psi_A^{k} \rangle$. For $k=1$, $\Psi_A^{k=1}$ describes the ground state of the A-nucleon system and the $\phi_n^{A,k=1}(\mathbf{r})$ reduce to the usual spectroscopic amplitudes. For a fixed n, on the other hand, the $\phi_n^{A,k}(\mathbf{r})$ correspond to particle states built on $|\Psi_{A-1}^{n}\rangle$. Similarly, one can expand an $(A-1)$-body state, Ψ_{A-1}^{n}, in terms of $(A-2)$-body basis states, Ψ_{A-2}^{m}, and obtain expansion coefficients $\phi_m^{A-1,n}(\mathbf{r}) \equiv \langle \Psi_{A-2}^{m} | a(\mathbf{r}) | \Psi_{A-1}^{n} \rangle$. With respect to the $(A-1)$-body system, the $(A-2)$-body functions represent hole states and the A-body functions are particle states. The expansion coefficients $\phi_m^{A-1,n}(\mathbf{r})$ can be used to rewrite the equations of motions [Eq. (2.5)],

$$(E_A - E_{A-1}^{n}) \phi_n(\mathbf{r}) = -\frac{\nabla_r^2}{2m} \phi_n(\mathbf{r}) + \sum_{n'=1}^{\infty} \sum_{m=1}^{\infty}$$

$$\times \int d\mathbf{r}' \phi_m^{A-1,n*}(\mathbf{r}') \phi_m^{A-1,n'}(\mathbf{r}')$$

$$\times V(|\mathbf{r}' - \mathbf{r}|) \phi_{n'}(\mathbf{r}). \quad \text{(B9)}$$

The kernel of the norm operator can also be written in terms of the particle or hole states. For the particle states, we insert a complete set of intermediate A-body states, $\Psi_A^{k}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$, in Eq. (B5) to obtain

$$\mathcal{N}(n,\mathbf{r},n',\mathbf{r}') = \sum_{k=1}^{\infty} \phi_n^{A,k}(\mathbf{r}) \phi_{n'}^{A,k*}(\mathbf{r}'). \quad \text{(B10)}$$

On the other hand, using Eq. (A3), the kernel of the norm operator can be expressed in terms of the $(A-1)$-body wave functions:

$$\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}') = \delta_{nn'}\,\delta(\boldsymbol{r}-\boldsymbol{r}') - (A-1)$$

$$\times \int \prod_{i=1}^{A-2} d\boldsymbol{r}_i \Psi_{A-1}^{n*}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-2},\boldsymbol{r}')$$

$$\times \Psi_{A-1}^{n'}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-2},\boldsymbol{r}). \qquad \text{(B11)}$$

This is not diagonal, in either n or $\boldsymbol{r}$, even for the simplest systems. From the last expression we derive the hole-state form

$$\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}') = \delta_{nn'}\,\delta(\boldsymbol{r}-\boldsymbol{r}') - \sum_{m=1}^{\infty} \phi_m^{A-1,n*}(\boldsymbol{r}')\,\phi_m^{A-1,n'}(\boldsymbol{r}). \qquad \text{(B12)}$$

Combining Eqs. (B10) and (B12), we obtain a completeness relation for the spectroscopic amplitudes corresponding to the set of particle and hole states:

$$\delta_{nn'}\,\delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_{m=1}^{\infty} \phi_m^{A-1,n*}(\boldsymbol{r}')\,\phi_m^{A-1,n'}(\boldsymbol{r})$$

$$+ \sum_{k=1}^{\infty} \phi_n^{A,k}(\boldsymbol{r})\,\phi_{n'}^{A,k*}(\boldsymbol{r}'). \qquad \text{(B13)}$$

The sum over m runs over all states of the $(A-2)$-body system [the hole states of the $(A-1)$-body system] while the sum over k runs over the states of the A-body system [the particle states of the $(A-1)$-body system]. The spectroscopic amplitudes for the particle states are not complete by themselves since they lack the contributions that are Pauli blocked, namely, those contributions corresponding to hole states. Contrary to the impression that this equation may give, the ϕ's are neither orthogonal nor normalized to one.

To illustrate the formalism, we consider a two-particle system. In this case, the $\Psi_{A-1}^n(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1}) \equiv \Psi_1^n(\boldsymbol{r})$ are one-body wave functions and the kernel of the norm operator is given by

$$\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}') = \delta_{nn'}\,\delta(\boldsymbol{r}-\boldsymbol{r}') - \Psi_1^{n*}(\boldsymbol{r}')\Psi_1^{n'}(\boldsymbol{r}). \qquad \text{(B14)}$$

The terms diagonal in n are projection operators onto states orthogonal to $\Psi_1^n(\boldsymbol{r})$. This is also true for larger particle numbers if the $\Psi_{A-1}^n(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{A-1})$ are single Slater determinants [in that case $\mathcal{N}(n,\boldsymbol{r},n,\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') - \sum_{s=1}^{A} \phi_s^{n*}(\boldsymbol{r}')\phi_s^n(\boldsymbol{r})$, where the sum is over occupied single-particle orbitals $\phi_s^n(\boldsymbol{r}')$]. While the matrix elements diagonal in n are projection operators by themselves, one needs to divide the full norm operator by A in order to obtain a projection operator.

APPENDIX C: A BOUND FOR THE SPECTROSCOPIC FACTOR

In this appendix, we show that S_n can be written as the product of two factors, which express antisymmetry and dynamic distortion effects, respectively. When recoil and center-of-mass corrections are neglected, both factors have to be less than or equal to 1, yielding an upper limit of 1 for the spectroscopic factor.

We start by defining a normalized spectroscopic amplitude $\tilde{\phi}_n(\boldsymbol{r}) = \phi_n(\boldsymbol{r})/\sqrt{S_n}$ and express $\sqrt{S_n}$ as follows:

$$\sqrt{S_n} = \int d\boldsymbol{r}\,\tilde{\phi}_n^*(\boldsymbol{r})\,\phi_n(\boldsymbol{r}) = \langle \mathcal{A}[\tilde{\phi}_n \Psi_{A-1}^n]|\psi_A\rangle. \qquad \text{(C1)}$$

Next, we introduce a projection operator

$$P_n \equiv \frac{|\mathcal{A}[\tilde{\phi}_n \Psi_{A-1}^n]\rangle\langle \mathcal{A}[\tilde{\phi}_n \Psi_{A-1}^n]|}{N_n}, \qquad \text{(C2)}$$

where $N_n = \langle \mathcal{A}[\tilde{\phi}_n \Psi_{A-1}^n]|\mathcal{A}[\tilde{\phi}_n \Psi_{A-1}^n]\rangle$. An arbitrary state $|\psi_A\rangle$ can then be broken into two orthogonal parts:

$$|\psi_A\rangle = P_n|\psi_A\rangle + (1-P_n)|\psi_A\rangle \equiv |\psi_A^{\|,n}\rangle + |\psi_A^{\perp,n}\rangle, \qquad \text{(C3)}$$

where $|\psi_A^{\|,n}\rangle$ and $|\psi_A^{\perp,n}\rangle$ are the components of $|\psi_A\rangle$ which are parallel and orthogonal, respectively, to the state $|\mathcal{A}[\tilde{\phi}_n \Psi_{A-1}^n]\rangle$. We can then write the spectroscopic factor as

$$S_n = N_n\langle \psi_A^{\|,n}|\psi_A^{\|,n}\rangle = N_n(\langle \psi_A|\psi_A\rangle - \langle \psi_A^{\perp,n}|\psi_A^{\perp,n}\rangle). \qquad \text{(C4)}$$

The expression in brackets is less than or equal to one since $\langle \psi_A|\psi_A\rangle = 1$ and both $\langle \psi_A^{\|,n}|\psi_A^{\|,n}\rangle$ and $\langle \psi_A^{\perp,n}|\psi_A^{\perp,n}\rangle$ are positive semidefinite. When the $(A-1)$-body system is completely described by the wave function Ψ_{A-1}^n, i.e. when there are no distortions due to the potential of the Ath nucleon, $\langle \psi_A^{\perp,n}|\psi_A^{\perp,n}\rangle$ vanishes and $\langle \psi_A^{\|,n}|\psi_A^{\|,n}\rangle = 1$. Thus $\langle \psi_A^{\|,n}|\psi_A^{\|,n}\rangle$, and therefore S_n, provides a measure of the dynamic distortions induced by the presence of the extra particle.

Since the factor N_n can be expressed as

$$N_n = 1 - \sum_{m=1}^{\infty} \left(\int d\boldsymbol{r}\,\phi_m^{A-1,n*}(\boldsymbol{r})\,\tilde{\phi}_n(\boldsymbol{r}) \right)^2, \qquad \text{(C5)}$$

where the sum is explicitly non-negative and less than or equal to one, it is also restricted, $N_n \leq 1$. N_n carries the effect of the antisymmetrization and equals one only when $\phi_n(\boldsymbol{r})$ is orthogonal to $\phi_m^{A-1,n}(\boldsymbol{r})$ for all m.

From the above considerations it follows that $S_n \leq 1$. If antisymmetry was neglected, the spectroscopic factor could be as large as A, since the sum rule given in Eq. (A21) would be the only restriction on S_n. When center-of-mass corrections are incorporated, Eq. (C4) still holds, but Eq. (C5) has to be modified and N_n can become larger than one. The influence of center-of-mass corrections is discussed in the next Appendix.

APPENDIX D: CENTER-OF-MASS CORRECTIONS AND INTRINSIC SPECTROSCOPIC AMPLITUDES

When dealing with the center-of-mass problem it is useful to introduce the Jacobi coordinates $\boldsymbol{\rho}_j = \boldsymbol{R}_j - \boldsymbol{r}_{j+1}$, where $\boldsymbol{R}_j$ is the center-of-mass coordinate of the j-body system defined by particles 1 through j. Taking into account the center-of-

mass motion, the A and $(A-1)$-body wave functions are written as

$$\psi_A(r_1,\ldots,r_A)=\frac{\exp[ik_A\cdot R_A]}{\sqrt{\mathcal{V}}}\psi_A^I(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-1})$$

$$\text{(D1)}$$

and

$$\Psi^{n,k_{A-1}}(r_1,\ldots,r_{A-1})$$

$$=\frac{\exp[ik_{A-1}\cdot R_{A-1}]}{\sqrt{\mathcal{V}}}\Psi_I^n(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-2}),$$

$$\text{(D2)}$$

respectively. Here k_A and k_{A-1} are the center-of-mass momenta of the A and $(A-1)$-body systems, respectively. We have used box normalization with volume $\mathcal{V}$. The spectroscopic amplitude is written as

$$\phi_{n,k_{A-1}}(r)=\sqrt{A}\int\prod_{i=1}^{A}dr_i\,\delta(r-r_A)\Psi^{n,k_{A-1}^*}(r_1,\ldots,r_{A-1})$$

$$\times\psi_A(r_1,\ldots,r_A)$$

$$=\frac{\exp[ir\cdot(k_A-k_{A-1})]}{\sqrt{\mathcal{V}}}\sqrt{A}$$

$$\times\int\prod_{i=1}^{A-1}d\boldsymbol{\rho}_i\frac{\exp\left[i\boldsymbol{\rho}_{A-1}\cdot\left(\dfrac{A-1}{A}k_A-k_{A-1}\right)\right]}{\sqrt{\mathcal{V}}}$$

$$\text{(D3)}$$

$$\times\Psi_I^{n*}(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-2})\psi_A^I(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-1})$$

$$\text{(D4)}$$

$$=\frac{\exp[ir\cdot(k_A-k_{A-1})]}{\sqrt{\mathcal{V}}}\tilde{\phi}_n^I\left(\frac{A-1}{A}k_A-k_{A-1}\right).$$

$$\text{(D5)}$$

This equation is unexpected and requires some comments. Formally it is correct: the spatial dependence of the spectroscopic amplitude is given by a plane wave and the spectroscopic factor is $|\tilde{\phi}_n^I([(A-1)/A]k_A-k_{A-1})|^2$. Since $\tilde{\phi}_n(k)$ is on the order of $1/\sqrt{\mathcal{V}}$, it is small and the condition that the spectroscopic factor must be less then or equal to one is easily satisfied. The plane wave behavior of the spectroscopic amplitude arises from translational invariance. The combination $([(A-1)/A]k_A-k_{A-1})$ is Galilean invariant. By taking both the $(A-1)$-body and the A-body systems to be in states of good momentum we have forced the Ath particle to also be in a state of good momentum; $\tilde{\phi}_n^I(k)$ is then the probability amplitude for finding the Ath particle with relative momentum k when the $(A-1)$-body system is in state n. Its Fourier transform, which we identify as the intrinsic spectroscopic amplitude, is given by [compare Eq. (A16)]

$$\phi_n^I(\boldsymbol{\rho})=\int dk_{A-1}\frac{\exp[i\boldsymbol{\rho}\cdot k_{A-1}]}{\sqrt{\mathcal{V}}}\tilde{\phi}_n^I(k_{A-1})$$

$$=\int dk_{A-1}\phi_{n,k_{A-1}}(\boldsymbol{\rho})|_{k_A=0}\qquad\text{(D6)}$$

$$=\sqrt{A}\int\prod_{i=1}^{A-1}d\boldsymbol{\rho}_i\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_{A-1})$$

$$\times\Psi_I^{n*}(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-2})\psi_A^I(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-1}).\quad\text{(D7)}$$

In analogy with $\tilde{\phi}_n^I(k)$, $\phi_n^I(\boldsymbol{\rho})$ is the probability amplitude for finding the Ath particle at the distance $\boldsymbol{\rho}$ from the center of mass of the $(A-1)$-body system when that system is in the state n. The intrinsic A-body wave function can be written in terms of the intrinsic spectroscopic amplitudes as [compare Eq. (2.1)]

$$\psi_A^I(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-1})=\frac{1}{\sqrt{A}}\sum_{n=1}^{\infty}\phi_n^I(\boldsymbol{\rho}_{A-1})\Psi_I^n(\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_{A-2}).$$

$$\text{(D8)}$$

As we show in the next paragraph, the intrinsic spectroscopic amplitude is also the quantity that is needed to calculate physical observables.

We now write the transition matrix element, Eq. (4.2), in terms of the intrinsic spectroscopic amplitude as follows:

$$\langle\psi_A|\sum_{i=1}^{A}\exp[-ik\cdot r_i]|\psi_A^K\rangle$$

$$=\sum_{n,k_{A-1}}^{\infty}\int dr\,\phi_{n,k_{A-1}}^*(r)\exp[-ik\cdot r]\phi_{n,k_{A-1}}^K(r)$$

$$\text{(D9)}$$

$$=\sum_{n=1}^{\infty}\int d\boldsymbol{\rho}\,\phi_n^{I*}(\boldsymbol{\rho})\exp[-ik\cdot\boldsymbol{\rho}(A-1)/A]\phi_n^{KI}(\boldsymbol{\rho})$$

$$\times\delta(k_K+k-k_A),\qquad\text{(D10)}$$

where the transition operator has been taken to be a plane wave as is appropriate for radiative capture and the spin and isospin dependencies have been suppressed for simplicity. The functions $\phi_n^{KI}(\boldsymbol{\rho})$ and $\phi_n^I(\boldsymbol{\rho})$ are intrinsic spectroscopic amplitudes for the scattering and bound states, respectively. The delta function ensures overall momentum conservation. The $(A-1)/A$ factor in the exponential takes care of the laboratory to center-of-mass transformation.

The equations of motion for the intrinsic spectroscopic amplitudes are easily derived by substituting Eq. (D5) in Eq. (B9). This gives

$$(E_A^B - E_{A-1}^n)\phi_n^I(\boldsymbol{\rho}) = -\frac{\nabla_{\boldsymbol{\rho}}^2}{2\mu}\phi_n^I(\boldsymbol{\rho}) + \sum_{n'=1}^{\infty}\sum_{n'=1}^{\infty}$$

$$\times \int d\boldsymbol{\rho}' \rho_{nn'}(\boldsymbol{\rho}') V(|\boldsymbol{\rho}' - \boldsymbol{\rho}|)\phi_{n'}^I(\boldsymbol{\rho}),$$

(D11)

where μ is the reduced mass and

$$\rho_{nn'}(\boldsymbol{\rho}) = \left(\frac{A-1}{A-2}\right)^3 \phi_m^{In*}[\boldsymbol{\rho}(A-1)/(A-2)]$$

$$\times \phi_m^{In'}[\boldsymbol{\rho}(A-1)/(A-2)] \qquad (D12)$$

is the transition density for the $(A-1)$-body system. The $(A-1)/(A-2)$ factors originate in the conversion from the $\boldsymbol{R}_{A-2} - \boldsymbol{r}_{A-1}$ coordinate to the $\boldsymbol{R}_{A-1} - \boldsymbol{r}_{A-1}$ coordinate. The diagonal transition density is the usual density and is normalized to $A-1$.

The remaining quantity to consider is the norm operator, $\hat{\mathcal{N}}$. This is most easily done starting with Eq. (B12). We

obtain the following expression for the kernel $\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}')$:

$$\mathcal{N}(n,\boldsymbol{r},n',\boldsymbol{r}') = \delta_{nn'}\delta(\boldsymbol{r}-\boldsymbol{r}') - \left(\frac{(A-1)^2}{A(A-2)}\right)^3$$

$$\times \sum_{m=1}^{\infty} \tilde{\phi}_m^{n*}\left[\frac{(A-1)^2}{A(A-2)}\left(\boldsymbol{r}' + \frac{\boldsymbol{r}}{(A-1)}\right)\right]$$

$$\times \tilde{\phi}_m^{n'}\left[\frac{(A-1)^2}{A(A-2)}\left(\boldsymbol{r} + \frac{\boldsymbol{r}'}{(A-1)}\right)\right]. \qquad (D13)$$

In contrast to the situation where the center-of-mass corrections are neglected, the amplitudes in the sum given here depend on both coordinates. Consequently, the intrinsic spectroscopic factors $S_n^I = \int d\boldsymbol{\rho}|\phi_n^I(\boldsymbol{\rho})|^2$ no longer have to be less than 1. This is illustrated in Ref. [15] for the harmonic oscillator model. The completeness relation for the particle and hole states, Eq. (B13), is also modified, since this last equation must be used instead of Eq. (B12). The spectroscopic amplitudes corresponding to the particle states are just replaced by their intrinsic counterparts.

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