One-body overlap functions, equations of motion, and phenomenological potentials

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(Received 2 July 2002; published 26 September 2002)

One-body overlap functions play an important role for the description of nuclear structure and nuclear reactions. Equations of motion for the one-body overlaps, based on particle-only, hole-only, and particle-hole approaches, are studied. A given overlap function is shown to satisfy four different Schrödinger-like equations, all of which can be derived in the framework of the Feshbach projection operator formalism. Approximating the relevant potential by a local potential is only valid in the particle-hole approach. Previously proposed one-body functions, which can be derived from the overlap functions, are also considered. It is argued that the latter do not satisfy a Schrödinger-like equation with an approximately local potential.

DOI: 10.1103/PhysRevC.66.034313 PACS number(s): 21.60.−n, 21.10.−k, 27.20.+n

I. INTRODUCTION

Overlap functions play an important role in the description of quantum-mechanical many-body systems. They are obtained by integrating a state of a many-particle system multiplied by a state of a subsystem with fewer particles over the coordinates of the latter. In the context of nuclear physics, where extensive experimental data shows that single-particle states correspond to physical reality, one-body overlap functions have been widely used and thoroughly studied [1]. One-body overlaps associated with bound many-body states are also called spectroscopic amplitudes and their norms are known as spectroscopic factors. The one-body overlap of a scattering state with a bound ground state of a smaller system can be identified with the Feshbach generalized optical-model wave function [2].

In their 1991 review [3], Mahaux and Sartor argue that it is the one-body overlap functions, rather than alternative functions such as the natural orbitals or the maximum-overlap orbitals, which provide a theoretical foundation for empirical single-particle states. Since analysis of direct one-nucleon transfer reactions indicate that the one-body overlap functions of low-lying single-particle excitations can be generated from a single-particle model, it becomes plausible to identify the corresponding potential with the nuclear mean field. Mahaux and Sartor investigate this point in some detail using the particle-hole formalism.

Other authors prefer to use alternative one-body functions which can, however, be derived from the one-body overlaps advocated by Mahaux and Sartor. In the context of the cluster model [4] and cluster radioactivity, *derived* functions are introduced which are nearly complete in the space of particle (or hole) states. One-body overlap functions, in contrast, require the full particle-plus-hole space for completeness [5]. This and normalization differences [4,6] suggest that it is the derived functions that satisfy Schrödinger-like equations with a (nearly) local potential rather than the one-body overlap functions themselves. Indeed, the equations for the one-body overlaps will take a very nonlocal form in particle-only models such as the cluster model or the Feshbach generalized optical model [2,7]. However, the situation is subtle as we show through a study of the properties of the various functions in the limit of a simple two-component model comprised of an A-body cluster plus a single nucleon. Irrespective of the question of whether the potentials involved in the equations are local or not, the alternative functions exhibit interesting properties. For example, they can be used to investigate the goodness of shell closures in even-even nuclei [8].

The dichotomy between the particle-hole and particle-only approaches to describing single-particle features of nuclear structure has motivated the work presented here. To sharpen the question under consideration we show in Fig. 1 a comparison of a spectroscopic amplitude obtained from a cluster-model calculation [9] with a single-particle wave function calculated in the framework of a simple potential model. The spectroscopic amplitude shown describes the overlap of the ^{7}Be$+p$ configuration with the ground state of

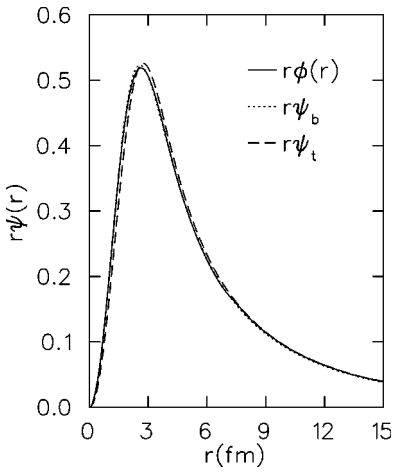

FIG. 1. Comparison of a one-body overlap function $\phi(r)$ calculated in a cluster model [9] with single-particle wave functions $\psi_b(r)$ and $\psi_t(r)$ obtained from simple potential-model approaches which employ Woods-Saxon potentials. The function ψ_b was calculated with the parametrization used by Barker [10] and ψ_t refers to the parameter set of Tombrello [11]. All three calculations are normalized to the spectroscopic factor obtained in the cluster-model approach.

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^{8}B (for channel spin $I=2$). The cluster model calculation is fully microscopic and uses a two-body potential. The potential-model calculation is macroscopic; a Woods-Saxon potential is used with parameters taken from Refs. [10] and [11], respectively. The normalization of the single-particle wave function was adjusted to agree with the norm of the spectroscopic amplitude, the spectroscopic factor. Note that the proper norm for the single-particle wave function cannot be calculated in the simple potential model and has to be taken from a microscopic approach [5], here provided by the cluster model. We find very good agreement between the two calculations. For the case shown here we can conclude that the spectroscopic amplitude does indeed satisfy a Schrödinger equation with a local potential. This is surprising since a local potential does not arise naturally in the cluster model.

It is the purpose of the present paper to elucidate the formalisms underlying these two approaches and their relationship to each other. In particular, we will address the question of why the nuclear structure features encapsulated in the functions shown in Fig. 1 agree so well with each other, despite some quite dramatic differences in the actual calculations. Is this agreement coincidental or can we identify some underlying physical mechanism for this similarity? We approach these issues by considering several sets of equations which the one-body overlap functions must satisfy. We specifically show that, in addition to a set of nonlocal equations originating from a particle-only or hole-only approach, one can derive equations which contain potentials that are approximately local. The latter set of equations requires a particle-hole approach. The various possible equations of motion for the one-body overlaps are discussed in Sec. II. In Sec. III we then explore properties of several auxiliary functions associated with one-body overlaps. We discuss realistic nuclear spectra in order to identify low-lying weak states which cannot be easily explained in a simple potential model. We argue that the *derived* functions associated with these states cannot satisfy a simple set of equations with local potentials. To illustrate the formalism we employ, we consider two simple models in Sec. IV: We discuss noninteracting particles in a potential well and the spatially uniform system. Our conclusions are presented in Sec. V. In Appendix A we show how the one-body overlap functions arise naturally when calculating expectation values of one-body operators and in Appendix B we explore the properties of the natural orbitals which play an important but hidden role throughout the paper. The Hamiltonians associated with the particle-only, hole-only, and particle-hole approaches studied here are related to each other in Appendix C.

II. ONE-BODY OVERLAP FUNCTIONS AND EQUATIONS OF MOTION

The simplest type of overlap function is a one-body overlap, which can be written as follows [1]:

$$\phi^A_{nm}(\mathbf{r}) = \sqrt{A-1}\int \prod_{i=1}^{A-1} d\mathbf{r}_i \Psi^{n*}_{A-1}(\mathbf{r}_1,\ldots,\mathbf{r}_{A-1}) \times \Psi^m_A(\mathbf{r}_1,\ldots,\mathbf{r}_{A-1},\mathbf{r}), \quad (1)$$

where Ψ^n_{A-1} and Ψ^m_A denote wave functions of nuclei with $A-1$ and A nucleons, respectively. In Dirac notation, the one-body overlap takes the following form:

$$\phi^A_{nm}(\mathbf{r}) = \langle \Psi^n_{A-1} | a(\mathbf{r}) | \Psi^m_A \rangle. \quad (2)$$

Here $a(\mathbf{r})$ $[a^\dagger(\mathbf{r})]$ is an annihilation (creation) operator which destroys (creates) a nucleon at position $\mathbf{r}$ and obeys the usual anticommutation relations. Often the reference state Ψ^m_A is understood and the superscript A and subscript m are dropped from the notation, i.e. $\phi^A_{nm}(\mathbf{r}) \to \phi_n(\mathbf{r})$. The spatial dependence of $\phi^A_{nm}(\mathbf{r})$ is related to the properties of the single-particle orbital of the Ath nucleon in the larger system. For a given A-body state, there are many one-body overlap functions, 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 one-body overlap functions completely determine the wave function Ψ^m_A. The one-body overlaps can also be used to evaluate matrix elements of one-body operators between different many-body wave functions (see Ref. [1] and Appendix A). When Ψ^n_{A-1} and Ψ^m_A refer to bound states, then the overlap $\phi^A_{nm}(\mathbf{r})$ is also called a spectroscopic amplitude, and the associated integral $S_{nm} = \int d\mathbf{r} |\phi_{nm}(\mathbf{r})|^2$ is the well-known and frequently used spectroscopic factor [12]. The quantity S_{nm} 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 one-body overlap functions $\phi_n(\mathbf{r})$ associated with the different excited states of the $(A-1)$-body system are not independent of each other. They are related by a model-independent sum rule [13] and, moreover, they satisfy a set of complicated coupled differential-integral equations [1,5,14–16]. For obtaining equations of motion which are decoupled, one has essentially two different methods available. One can employ the full particle-plus-hole space and study the combined particle-hole propagator. The resulting equations of motion contain a self-energy operator which has a complicated form and requires energy averaging before a relation to the nuclear mean field can be established. This approach will be outlined in the next subsection. Alternatively, it is possible to separate particle and hole states by projecting on either the particle or hole subspace. This yields separate sets of equations, one for each subspace. The latter approach was used in Feshbach's derivation of a generalized optical potential in the context of his theory for nuclear reactions [2,7]. It also plays an essential role in the cluster model [4]. We will discuss the projection-operator method in Sec. II B. By considering both approaches it is possible to set up four different, formally exact, equations for each one-body overlap. The question to be addressed is not ''which set of equations is correct?''—they all are. The question to be addressed is rather ''which formalism is most useful in a given context and which result corresponds most closely to a particular approximation scheme, for example, the nuclear mean field or the cluster model?''

A. Mass operator and equations of motion

The formally simplest approach to obtaining a decoupled equation of motion for the one-body overlap functions makes use of the propagator method. It involves the full particle-hole propagator and the self-energy or mass operator. We start with the time-ordered particle-hole Green's function, Fourier-transformed over the time component [3,17]

$$G(\mathbf{r},\mathbf{r}';E)=G_p(\mathbf{r},\mathbf{r}';E)+G_h(\mathbf{r},\mathbf{r}';E), \tag{3}$$

$$G_p(\mathbf{r},\mathbf{r}';E)=\langle\psi_A^0|a(\mathbf{r})\frac{1}{E-(\hat{H}-E_0^A)+i\epsilon}a^\dagger(\mathbf{r}')|\psi_A^0\rangle, \tag{4}$$

$$G_h(\mathbf{r},\mathbf{r}';E)=\langle\psi_A^0|a^\dagger(\mathbf{r}')\frac{1}{E+(\hat{H}-E_0^A)-i\epsilon}a(\mathbf{r})|\psi_A^0\rangle. \tag{5}$$

Here $|\psi_A^0\rangle$ is the (normalized) Heisenberg ground state for the A-particle system and E_0^A the corresponding eigenvalue, $a(\mathbf{r})$ $[a^\dagger(\mathbf{r})]$ is a nucleon annihilation (creation) operator, and $\hat{H}$ denotes the nuclear many-body Hamiltonian. The full Green's function $G(\mathbf{r},\mathbf{r}';E)$ represents both particle and hole propagation in the many-body system. Inserting a complete set of $(A+1)$ $[(A-1)]$-body eigenfunctions of the Hamiltonian $\hat{H}$ into Eq. (4) [Eq. (5)], we obtain the Lehmann representation of the particle-hole propagator

$$G_p(\mathbf{r},\mathbf{r}';E)=\sum_m \phi_{0m}^{A+1}(\mathbf{r})\frac{1}{E-(E_m^{A+1}-E_0^A)+i\epsilon}\phi_{0m}^{A+1}(\mathbf{r}')^*, \tag{6}$$

$$G_h(\mathbf{r},\mathbf{r}';E)=\sum_m \phi_{m0}^{A}(\mathbf{r}')^*\frac{1}{E-(E_0^A-E_m^{A-1})-i\epsilon}\phi_{m0}^{A}(\mathbf{r}). \tag{7}$$

The $\phi(\mathbf{r})$ are unambiguously identified by the requirement that the complete set inserted in Eq. (4) [Eq. (5)] be comprised of eigenfunctions of $\hat{H}$—they are the one-body overlap functions introduced in the preceding section.

The equation of motion for the particle-hole propagator can be written as

$$\left(E+\frac{\hbar^2}{2m}\nabla_r^2\right)G(\mathbf{r},\mathbf{r}';E)-\int d\mathbf{r}''\Sigma(\mathbf{r},\mathbf{r}'';E)G(\mathbf{r}'',\mathbf{r}';E) =\delta(\mathbf{r}-\mathbf{r}'), \tag{8}$$

where $\Sigma(\mathbf{r},\mathbf{r}'';E)$ denotes the mass operator (or "self-energy"), which describes the interaction of the propagating particle or hole with all the other particles or holes in the medium. It is also related to the Green's function by Dyson's equation [3,17].

Inserting the Lehmann representation into Eq. (8), one obtains an equation of motion for the one-body overlap functions [3,18]. For the particle states it takes the form

$$\left((E_m^{A+1}-E_0^A)+\frac{\hbar^2}{2m}\nabla_r^2\right)\phi_{0m}^{A+1}(\mathbf{r}) -\int d\mathbf{r}'\Sigma(\mathbf{r},\mathbf{r}';E_m)\phi_{0m}^{A+1}(\mathbf{r}')=0, \tag{9}$$

and the corresponding equation for the hole states is obtained with the replacements $(E_m^{A+1}-E_0^A)\Rightarrow(E_0^A-E_m^{A-1})$ and $\phi_{0m}^{A+1}(\mathbf{r})\Rightarrow\phi_{m0}^{A}(\mathbf{r})^*$. The squared norm of a discrete particle or hole state $\phi_{0m}(\mathbf{r})$, the spectroscopic factor S_{0m}, can also be expressed in terms of the self-energy $\Sigma(\mathbf{r},\mathbf{r}';E_m)$ (see Refs. [3,18]). With the normalized one-body overlap function $\hat{\phi}_{nm}(\mathbf{r})\equiv\phi_{nm}(\mathbf{r})/\sqrt{S_{nm}}$ one obtains

$$\begin{aligned}S_{0m}&=\int d\mathbf{r}|\phi_{0m}^{A+1}(\mathbf{r})|^2\\&=\left[1-\frac{d}{dE}\int d\mathbf{r}d\mathbf{r}'\,\hat{\phi}_{0m}^{A+1}(\mathbf{r})^*\right.\\&\quad\left.\times\Sigma(\mathbf{r},\mathbf{r}';E)\hat{\phi}_{0m}^{A+1}(\mathbf{r}')\right]^{-1}_{E=E_m}\end{aligned} \tag{10}$$

for the particle states and analogously for the hole states. [For the hole states it is necessary to replace $(E_m^{A+1}-E_0^A)$ by $(E_0^A-E_m^{A-1})$ and $\phi_{0m}^{A+1}(\mathbf{r})$ by $\phi_{m0}^{A}(\mathbf{r})^*$.]

Introducing the modified mass operator $\mathcal{M}(\mathbf{r},\mathbf{r}';E)=\Sigma(\mathbf{r},\mathbf{r}';E+i\epsilon)$ (valid for real energy E) allows one to work with a quantity that can be analytically continued from the real axis into the upper plane of the complex energy plane. With this operator, the equation for the overlap functions becomes

$$\left(\mathcal{E}_m+\frac{\hbar^2}{2m}\nabla_r^2\right)\phi_m(\mathbf{r})-\int d\mathbf{r}''\mathcal{M}(\mathbf{r},\mathbf{r}';E_m)\phi_m(\mathbf{r}')=0, \tag{11}$$

where $\mathcal{E}_m=(E_m^{A+1}-E_0^A)$, $\phi_m(\mathbf{r})=\phi_{0m}^{A+1}(\mathbf{r})$ holds for particle states and $\mathcal{E}_m=(E_0^A-E_m^{A-1})$, $\phi_m(\mathbf{r})=\phi_{m0}^{A}(\mathbf{r})^*$ holds for hole states. The above equation of motion defines a Hamiltonian

$$\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}')=-\frac{\hbar^2}{2m}\nabla_r^2\delta(\mathbf{r}-\mathbf{r}')+\mathcal{M}(\mathbf{r},\mathbf{r}';E). \tag{12}$$

Thus, the modified mass operator plays a role similar to that of a potential in a single-particle problem. Equation (11) is an elegant, formally exact, one-body equation for the one-body overlap functions—the complexities of the many-body system are contained in $\mathcal{M}(\mathbf{r},\mathbf{r}';E)$: The influence of the nuclear medium leads to a nonlocal, energy-dependent, complex form for this operator. Usually, the mass operator is generated perturbatively, which yields—to lowest order—the Hartree-Fock approximation.

The above development treats the particle and the hole states which are built on a given A-body reference state $|\Psi_A\rangle$ on equal footing and yields bound as well as elastic scattering overlap functions. This is also what is required of the nuclear mean field—that it be able to simultaneously de-

scribe particle and hole states, bound and scattering states. Equations (11) and (12) above seem to imply that the modified mass operator $\mathcal{M}(\mathbf{r},\mathbf{r}';E)$ can be identified with the nuclear mean field. Such conclusion, however, is problematic, since the solutions of Eq. (11), which contains $\mathcal{M}(\mathbf{r},\mathbf{r}';E)$, include states that cannot be easily described in a mean-field approach. This applies in particular to certain low-lying states in the spectra of $(A\pm1)$-nucleon systems adjacent to nuclei for which the independent-particle model predicts a closed-shell structure. These states have the ''wrong'' quantum numbers, i.e., quantum numbers that are not compatible with a description of the state as a hole or particle with respect to the neighboring closed-shell A-body configuration. The associated spectroscopic factors for one-nucleon transfer to/from the A-body ground state are small. For example, the $5/2^+$ state at 5.270 MeV and the $1/2^+$ state at 5.299 MeV in ^{15}N and the $1/2^-$ state at 3.104 MeV in ^{17}F have associated overlaps that can be obtained from the mass operator approach but not from an independent particle model. In the independent particle model, the ground state of ^{16}O is a closed-shell configuration with the $0s_{1/2}$, $0p_{3/2}$, and $0p_{1/2}$ orbitals completely filled. In this picture, the ^{17}F $5/2^+$ ground state, the $1/2^+$ state at 0.495 MeV, and the $3/2^+$ state at 5.000 MeV can be easily understood as an additional proton placed in the $0d_{5/2}$, $1s_{1/2}$, or $0d_{3/2}$ orbitals, respectively. Similarly, the ^{15}N $1/2^-$ ground state and the $3/2^-$ state at 6.324 MeV can be explained as proton holes in the $0p_{1/2}$ and $0p_{3/2}$ orbitals of the ^{16}O ground state, respectively. Single-particle wave functions corresponding to these states can be easily generated in a potential model with a harmonic oscillator or Woods-Saxon shape plus a spin-orbit term. The $5/2^+$ and $1/2^+$ states in ^{15}N and the $1/2^-$ state in ^{17}F, however, do not have such a simple structure. While these states do not exist in the independent particle model in this energy range, they can be understood as hole or particle states with respect to the ^{16}O ground state provided the latter contains correlations beyond the simple mean field. Such many-body correlations result in partial occupancies of the single-particle orbitals, e.g., in ^{16}O one obtains weakly occupied $0d_{5/2}$ and $1s_{1/2}$ orbitals and a $0p_{1/2}$ orbit that is not quite full. Consequently, it is possible to remove (add) a nucleon from (to) a small component of the ^{16}O many-body wave function. The associated spectroscopic factors are small, but nonzero. The measured values are $S_{5/2^+}=0.019$, $S_{1/2^+}=0.018$ for the ^{15}N system [19]; the exact value of $S_{1/2-}$ for the ^{17}F case has not yet been determined experimentally, but is known to be small [20]. It then follows from Eq. (10) that in the vicinity of these levels $\mathcal{M}(\mathbf{r},\mathbf{r}';E)$ is rapidly varying with energy. This suggests that the nuclear mean field should be identified with an energy-averaged version of the mass operator rather than with the modified mass operator itself. This conclusion is in agreement with the definition of the mean field given by Mahaux and Sartor [3].

B. Projection operator formalism and equations of motion

An alternative method for deriving decoupled equations of motion for the one-body overlap functions makes use of the projection operator formalism, which was used by Feshbach in his work on the generalized optical potential [2]. In this approach, the total many-body wave function is partitioned into an ''open-channel'' segment, i.e., a part that is of interest for studying a particular phenomenon, and a ''closed-channel'' segment, the remaining part of the wave function. By eliminating the closed channels, a Schrödinger equation is obtained for the open channels, and an effective Hamiltonian can be derived, which in turn can be used to analyze various aspects of the nuclear many-body problem. The formalism is quite general. The resulting equations depend only on the existence of an appropriate projection operator, not on an explicit realization thereof. We make use of the flexibility of this technique and construct three different projection operators which allow us to derive three different, formally exact, equations of motion for one-body overlap functions—one describing particle states, one for hole states, and one which applies to both. The expressions we obtain clarify the relationships between the particle-only, hole-only, and particle-hole approaches, and they highlight the limitations of the former two. The fact that all three sets of equations can be derived in the projection operator formalism demonstrates that these limitations are defined by the chosen model space, not by the formalism employed.

We first derive equations of motion for one-body overlaps which correspond to particle states. We start with the Schrödinger equation for the $(A+1)$-body system

$$H|\Psi^m_{A+1}\rangle=E^{A+1}_m|\Psi^m_{A+1}\rangle, \tag{13}$$

and introduce the following projection operator:

$$P^p_n=\int d\mathbf{r}d\mathbf{r}'\,a^\dagger(\mathbf{r})|\Psi^n_A\rangle\mathcal{N}^A(n,\mathbf{r},n,\mathbf{r}')^{-1}\langle\Psi^n_A|a(\mathbf{r}'). \tag{14}$$

Here $\mathcal{N}(n,\mathbf{r},m,\mathbf{r}')=\langle\Psi^n_A|a(\mathbf{r})a^\dagger(\mathbf{r}')|\Psi^m_A\rangle$ plays an important role for the projection into the space of particle states: The operator $\int d\mathbf{r}a^\dagger(\mathbf{r})|\Psi^n_A\rangle\langle\Psi^n_A|a(\mathbf{r})$, without the $\mathcal{N}^{-1}$, is not a projection operator, although it has a simple completeness relation associated with it; $A^{-1}\Sigma_n\int d\mathbf{r}a^\dagger(\mathbf{r})|\Psi^n_A\rangle\langle\Psi^n_A|a(\mathbf{r})|\psi_{A+1}\rangle=|\psi_{A+1}\rangle$ holds for any completely antisymmetric $(A+1)$-body state $|\psi_{A+1}\rangle$. (See also Appendix A of Ref. [5].) Since $\mathcal{N}^A(n,\mathbf{r},m,\mathbf{r}')$ might be singular, caution is required when inverting this operator. For the present purposes we can simply exclude the space spanned by the eigenfunctions corresponding to zero eigenvalues. [For more information on the operator $\mathcal{N}(n,\mathbf{r},m,\mathbf{r}')$, see Appendix A and Refs. [2,4].] The state $P^p_n|\Psi^m_{A+1}\rangle$, which is obtained by projection from an eigenstate $|\Psi^m_{A+1}\rangle$ of the $(A+1)$-body Hamiltonian, has the same one-body overlap function $\phi^{A+1}_{nm}(\mathbf{r})=\langle\Psi^n_A|a(\mathbf{r})P^p_n|\Psi^m_{A+1}\rangle=\langle\Psi^n_A|a(\mathbf{r})|\Psi^m_{A+1}\rangle$, associated with it as the original (unprojected) state.

We can now define a projection operator that is complementary to P^p_m, $Q^p_m=1-P^p_m$, and derive an exact equation of motion for the one-body overlap $\phi^{A+1}_{nm}(\mathbf{r})=\langle\Psi^n_A|a(\mathbf{r})|\Psi^m_{A+1}\rangle$. We proceed by partitioning the $(A+1)$-body wave function $|\Psi^m_{A+1}\rangle=P^p_n|\Psi^m_{A+1}\rangle+Q^p_n|\Psi^m_{A+1}\rangle$, and formally eliminating $Q^p_n|\Psi^m_{A+1}\rangle$. The pro-

cedure follows Feshbach's derivation of the generalized optical potential very closely and yields

$$E_m^{A+1}\phi_{nm}^{A+1}(\mathbf{r}) = \int d\mathbf{r}'d\mathbf{r}''\langle\Psi_A^n|a(\mathbf{r}) \times\left(H+HQ_n^p\frac{1}{E_m^{A+1}-Q_n^pHQ_n^p}Q_n^pH\right) \times a^\dagger(\mathbf{r}')|\Psi_A^n\rangle\mathcal{N}^A(n,\mathbf{r}',n,\mathbf{r}'')^{-1}\phi_{nm}^{A+1}(\mathbf{r}'') \tag{15}$$

$$= \int d\mathbf{r}'\mathcal{H}_n^p(\mathbf{r},\mathbf{r}';E_m^{A+1})\phi_{nm}^{A+1}(\mathbf{r}'), \tag{16}$$

where the Hamiltonian $\mathcal{H}_n^p(\mathbf{r},\mathbf{r}';E_m^{A+1})$ is defined by the last equality. A similar equation for the particle Green's function is given by Eq. (C5).

In analogy with the above treatment, one can derive equations of motion for overlap functions which correspond to hole states. This case was considered previously by Boffi *et al.* [21]. Here we start with the Schrödinger equation for an $(A-1)$-body state $|\Psi_{A-1}\rangle$, $H|\Psi_{A-1}^m\rangle = E_m^{A-1}|\Psi_{A-1}^m\rangle$, and introduce the hole projection operator

$$P_n^h = \int d\mathbf{r}d\mathbf{r}'\,a(\mathbf{r})|\Psi_A^n\rangle\rho^A(n,\mathbf{r},n,\mathbf{r}')^{-1}\langle\Psi_A^n|a^\dagger(\mathbf{r}'), \tag{17}$$

where $\rho^A(n,\mathbf{r},m,\mathbf{r}') = \langle\Psi_A^n|a^\dagger(\mathbf{r})a(\mathbf{r}')|\Psi_A^m\rangle$ denotes a density matrix element. The equation of motion for the one-body overlaps corresponding to hole states takes the following form:

$$E_m^{A-1}\phi_{mn}^A(\mathbf{r})^* = \int d\mathbf{r}'d\mathbf{r}''\langle\Psi_A^n|a(\mathbf{r}) \times\left(H+HQ_n^h\frac{1}{E_m^{A-1}-Q_n^hHQ_n^h}Q_n^hH\right) \times a^\dagger(\mathbf{r}')|\Psi_A^n\rangle\rho^A(n,\mathbf{r}',n,\mathbf{r}'')^{-1}\phi_{mn}^A(\mathbf{r}'')^* \tag{18}$$

$$= \int d\mathbf{r}'\mathcal{H}_n^h(\mathbf{r},\mathbf{r}';E_m^{A-1})\phi_{mn}^A(\mathbf{r}')^*. \tag{19}$$

This equation differs very clearly from Eq. (16); in particular, since we have restricted ourselves to the space of hole states, it applies to overlaps corresponding to hole states only. Also note that the inverse of the density matrix element $\rho^A(n,\mathbf{r}',n,\mathbf{r}'')$ occurs in the above expression, instead of $\mathcal{N}^A(n,\mathbf{r}',n,\mathbf{r}'')^{-1}$. A caveat similar to that relevant for $\mathcal{N}^A$ applies to ρ^A with respect to inverting the possibly singular operator.

The Feshbach projection operator formalism can also be used to derive the particle-hole Hamiltonian. We combine the Schrödinger equations for the particle and hole states into the form $\tilde{H}|\Psi_{A\pm1}^m\rangle = \mathcal{E}_m|\Psi_{A\pm1}^m\rangle$, with $\mathcal{E}_m$ as defined in Sec. II A [see the text following Eq. (11)], $\hat{A} = \int d\mathbf{r}a^\dagger(\mathbf{r})a(\mathbf{r})$ denoting the particle-number operator, and $\tilde{H} \equiv (H-E_0^A)(\hat{A}-A)$. We now introduce the particle-hole projection operator

$$P_n^{ph} = \int d\mathbf{r}d\mathbf{r}'[a(\mathbf{r})+a^\dagger(\mathbf{r})]|\Psi_A^n\rangle\mathcal{N}_{ph}^A(n,\mathbf{r},n,\mathbf{r}') \times\langle\Psi_A^n|[a(\mathbf{r}')+a^\dagger(\mathbf{r}')], \tag{20}$$

where $\mathcal{N}_{ph}^A(n,\mathbf{r},n',\mathbf{r}') \equiv \langle\Psi_A^n|[a(\mathbf{r})+a^\dagger(\mathbf{r})][a(\mathbf{r}')+a^\dagger(\mathbf{r}')]|\Psi_A^{n'}\rangle$. Note that this projection operator does not preserve the particle number. For time-reversal invariant A-body states, $|\Psi_A^n\rangle$, $\mathcal{N}_{ph}^A(n,\mathbf{r},n,\mathbf{r}')$ reduces to a delta function $\mathcal{N}_{ph}^A(n,\mathbf{r},n,\mathbf{r}') \to \delta(\mathbf{r}-\mathbf{r}')$. For the rest of this discussion we will restrict ourselves to such A-body states. With this projection operator we can carry out the usual Feshbach projection procedure to obtain the following equation of motion for the one-body overlap function

$$\mathcal{E}_m\phi_{nm}^{A+1}(\mathbf{r}) = \int d\mathbf{r}'\langle\Psi_A^n|[a(\mathbf{r})+a^\dagger(\mathbf{r})] \times\left(\tilde{H}+\tilde{H}Q_n^{ph}\frac{1}{\mathcal{E}_m-Q_n^{ph}\tilde{H}Q_n^{ph}}Q_n^{ph}\tilde{H}\right) \times[a(\mathbf{r}')+a^\dagger(\mathbf{r}')]|\Psi_A^n\rangle\phi_{nm}^{A+1}(\mathbf{r}') = \int d\mathbf{r}'\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}',\mathcal{E}_m)\phi_{nm}^{A+1}(\mathbf{r}'). \tag{21}$$

The fact that $\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}';\mathcal{E}_m)$, as defined here, is indeed the particle-hole Hamiltonian is demonstrated explicitly in Appendix C by calculating the Green's functions. The above equation is written for particle overlaps, but it applies equally well to hole states. In the latter case, $\phi_{nm}^{A+1}(\mathbf{r})$ needs to be replaced by $\phi_{mn}^A(\mathbf{r})^*$.

The particle-only ($\mathcal{H}^p$), hole-only ($\mathcal{H}^h$), and particle-hole ($\mathcal{H}_{\mathcal{M}}$) Hamiltonians above can be related to each other by applying the projection operator formalism to the associated Green's functions. This is done in Appendix C. We find that the particle-only Hamiltonian, which occurs in the denominator of the particle Green's function, is the optical-model Hamiltonian used by Feshbach. The analogous Hamiltonian for the hole case appears in the denominator of the single-hole propagator. Since the particle-hole Green's function is simply the sum of the particle and hole contributions, and is related to the particle-hole Hamiltonian $\mathcal{H}_{\mathcal{M}}$ by the equation

$$\check{G}(E) = \frac{1}{E-\check{\mathcal{H}}_{\mathcal{M}}}, \tag{22}$$

the three Hamiltonians are connected to each other through

$$\frac{1}{E-\check{\mathcal{H}}_{\mathcal{M}}}=\frac{1}{E-[\check{\mathcal{H}}^{p}_{n}(E)-E^{A}_{n}]+i\epsilon}\check{\mathcal{N}}^{A}+\frac{1}{E+[\check{\mathcal{H}}^{h}_{n}(E)-E^{A}_{n}]-i\epsilon}\check{\rho}^{A}. \tag{23}$$

Here $\check{O}$ denotes the integral operator which acts as follows: $\check{\mathcal{O}}f(\mathbf{r})=\int d\mathbf{r}'\,\mathcal{O}(\mathbf{r},\mathbf{r}')f(\mathbf{r}')$. We observe that in the limit of completely empty (full) single-particle orbitals, the particle-hole Hamiltonian $\mathcal{H}_M(\mathbf{r},\mathbf{r}';E)$ reduces to $\mathcal{H}^{p}_{m}(\mathbf{r},\mathbf{r}';E)$ $[\mathcal{H}^{h}_{m}(\mathbf{r},\mathbf{r}';E)]$. Equation (23) can be inverted to give $\check{\mathcal{H}}_{\mathcal{M}}$ in terms of $\check{\mathcal{H}}^{p}_{n}$ and $\check{\mathcal{H}}^{h}_{n}$, but the resulting expression is very complicated (see Appendix C).

To illustrate the differences between the Hamiltonians $\mathcal{H}^{p}$, $\mathcal{H}^{h}$, and $\mathcal{H}_{\mathcal{M}}$, we consider Eqs. (16), (19), and (21). We take into account only the leading terms in the parantheses of each equation (i.e. we ignore contributions from those terms that contain Q^{p}, Q^{h}, or Q^{ph}) and take the Hamiltonian to be of the form $H=\int d\mathbf{r}d\mathbf{r}'H^{1}(\mathbf{r},\mathbf{r}')a^{\dagger}(\mathbf{r})a(\mathbf{r}')+\frac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1-\mathbf{r}_2)a^{\dagger}(\mathbf{r}_1)a^{\dagger}(\mathbf{r}_2)a(\mathbf{r}_1)a(\mathbf{r}_2)$, where $H^{1}(\mathbf{r},\mathbf{r}')$ denotes a one-body Hamiltonian, which in the simplest case reduces to a kinetic energy term, and V refers to a two-body potential. A straightforward calculation then yields

$$\begin{aligned}\mathcal{H}^{p}_{n}-E^{A}_{n}\approx&\int H^{1}(\mathbf{r},\mathbf{r}'')\mathcal{P}^{p}(\mathbf{r}'',\mathbf{r}')d\mathbf{r}''\\&+\int d\mathbf{r}'''\langle\Psi^{n}_{A}|\int d\mathbf{r}''V(\mathbf{r}-\mathbf{r}'')\\&\times a^{\dagger}(\mathbf{r}'')a(\mathbf{r}'')a(\mathbf{r})a^{\dagger}(\mathbf{r}''')|\Psi^{n}_{A}\rangle\\&\times\mathcal{N}^{A}(n,\mathbf{r}''',n,\mathbf{r}')^{-1},\end{aligned} \tag{24}$$

$$\begin{aligned}E^{A}_{n}-\mathcal{H}^{h}_{n}\approx&\int H^{1}(\mathbf{r},\mathbf{r}'')\mathcal{P}^{h}(\mathbf{r}'',\mathbf{r}')d\mathbf{r}''\\&+\int d\mathbf{r}'''\langle\Psi^{n}_{A}|\int d\mathbf{r}''V(\mathbf{r}-\mathbf{r}'')\\&\times a^{\dagger}(\mathbf{r}'')a(\mathbf{r}'')a^{\dagger}(\mathbf{r})a(\mathbf{r}''')|\Psi^{n}_{A}\rangle\\&\times\rho^{A}(n,\mathbf{r}''',n,\mathbf{r}')^{-1},\end{aligned} \tag{25}$$

$$\mathcal{H}_{M}\approx H^{1}(\mathbf{r},\mathbf{r}')+\langle\Psi^{n}_{A}|\delta(\mathbf{r}-\mathbf{r}')\int V(\mathbf{r}-\mathbf{r}'')a^{\dagger}(\mathbf{r}'')a(\mathbf{r}'')d\mathbf{r}''-V(\mathbf{r}-\mathbf{r}')a^{\dagger}(\mathbf{r})a(\mathbf{r}')|\Psi^{n}_{A}\rangle. \tag{26}$$

Here $\mathcal{P}^{p}(\mathbf{r}'',\mathbf{r}')$ and $\mathcal{P}^{h}(\mathbf{r}'',\mathbf{r}')$ are projection operators which eliminate the totally empty and completely filled orbitals, respectively. We find that the particle-hole Hamiltonian reduces to a familiar form—it contains a one-body contribution and two-body Hartree-plus-Fock terms. Its form is much simpler than that for the other Hamiltonians, since using the particle-only (hole-only) Hamiltonian requires that the hole (particle) states be eliminated from consideration. It is possible to recover the Hartree term in the particle-only or hole-only approaches if one inserts $|\Psi^{n}_{A}\rangle\langle\Psi^{n}_{A}|$ between $a(\mathbf{r}'')$ and $a(\mathbf{r})$ in Eq. (24) or between $a(\mathbf{r}'')$ and $a^{\dagger}(\mathbf{r})$ in Eq. (25), i.e., if one limits the intermediate states to one possibility, namely, Ψ^{n}_{A}. But even in this approximation the projection operator $\mathcal{P}^{p}(\mathbf{r}'',\mathbf{r}')$ or $\mathcal{P}^{h}(\mathbf{r}'',\mathbf{r}')$ remains present. In the limit of a pure one-body problem these projection operators suffice to eliminate the hole (particle) states, the inverse of $\mathcal{N}^{A}$ or ρ^{A} is not required. In the opposite limit, in the presence of strong two-body forces, the projection operators, which only remove orbitals with occupancy 0 or 1, become largely ineffective. In this situation, they eliminate only states very far from the Fermi surface and the removal of the remaining hole (particle) contributions requires the more complicated potential term and the higher order terms, which have been neglected here.

The one-body overlap function $\langle\Psi^{n}_{A-1}|a(\mathbf{r})|\Psi^{m}_{A}\rangle$ can be considered as a particle state with respect to the $(A-1)$-body state Ψ^{n}_{A-1} or as a hole state with respect to the A-body state Ψ^{m}_{A}. In the former case, the overlap function satisfies both Eq. (16) and Eq. (21); in the latter case it satisfies Eq. (19) and Eq. (21). Thus, a given one-body overlap function is the solution of the four different, formally exact, equations, Eq. (16), Eq. (19), and two versions of Eq. (21).

Despite this formal equivalence, the particle-hole and particle-only approaches lead to different physical interpretations, as the following example illustrates. If we consider an *s*-wave proton scattering from the ^{7}Be ground state, we find that the relative-motion wave function has a node. There are two different possibilities for explaining the origin of the this node. In the particle-hole picture the potential has an *s*-wave bound state and the scattering state must have a node in order to be orthogonal to the bound state. In the particle-only picture there is an occupied *s*-wave orbital to which the scattering state must be orthogonal in order to respect the Pauli exclusion principle. Both of these explanations, although basically correct, have shortcomings. In the particle-hole picture, the potential is energy dependent so the single-particle states are not strictly orthogonal to each other. Similarly, in the particle-only picture, the scattering state does not need to be completely orthogonal to the bound *s*-wave orbital, since the latter might not be fully occupied. These two shortcomings are related to each other since the energy dependence of the mean-field (mass operator) is related to the occupancy of the orbitals, as is made explicit in Eq. (10).

The nuclear mean field is the energy average of the mass operator that arises in the particle-hole formalism. In contrast, the cluster model is based on a particle-only approach. Thus it would be difficult to derive the nuclear mean field in the particle-only formalism or the cluster model in the particle-hole formalism. However, both approaches—if correctly implemented—yield the same one-body overlap functions. This is the lesson of Fig. 1.

III. THE ROLE OF AUXILIARY FUNCTIONS

Equation (15) has previously been considered in the context of cluster-model calculations. Since the cluster model is based on a particle-only approach, Eq. (15) emerges natu-

rally as the relevant differential equation for the one-body overlap functions. However, due to the presence of $(\mathcal{N}^A)^{-1}$, this equation is quite ''asymmetric;'' $\mathcal{H}^p$ is non-Hermitean and cannot be easily related to a phenomenological Hamiltonian with a local potential. In the preceeding section, we have shown that this problem appears since the hole states have been explicitly excluded from the model space. In order to recover a more symmetric equation of motion one has to employ the particle-hole formalism, which also enables one to make a connection to a phenomenological Hamiltonian with a local potential, namely, by using the energy-averaged mass operator.

Cluster models describe the dynamics of simple configurations, such as the single nucleon-plus-core system considered here, as well as more complicated processes involving two (or more) composite nuclear fragments. In general it becomes quite problematic to incorporate the relevant hole space and thus other possibilities for arriving at a practical and esthetically more satisfying equation of motion need to be explored. Alternative one-body functions, which lead to Schrödinger equations with more symmetric Hamiltonians, have been derived from the one-body overlaps used in the preceeding sections. For example, the auxiliary functions $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ and $\overline{\phi}^{A}_{nm}(\mathbf{r})$, defined by

$$\phi^{A+1}_{nm}(\mathbf{r}) = \int d\mathbf{r}'\, \mathcal{N}^A(n,\mathbf{r},n,\mathbf{r}')\, \tilde{\phi}^{A+1}_{nm}(\mathbf{r}') \tag{27}$$

and

$$\overline{\phi}^{A}_{nm}(\mathbf{r}) = \int d\mathbf{r}'\, \mathcal{N}(n,\mathbf{r},n,\mathbf{r}')^{-1/2} \phi^{A}_{nm}(\mathbf{r}'), \tag{28}$$

respectively, have been studied in Refs. [4,22]. The power (-1/2), to which $\mathcal{N}^A$ is raised in the latter equation, is to be understood in an operator sense in $\mathbf{r}$ space. In practice, powers of $\mathcal{N}^A$ can be easily calculated by using the eigenfunctions of $\mathcal{N}^A$, the so-called natural orbitals [3,23,24]. Note that the function $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ is not uniquely defined by Eq. (27), since $\mathcal{N}^A$ can be singular. This is, however, not very relevant, since those components of $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ which are nonunique, are projected out by $\mathcal{N}^A(n,\mathbf{r},n,\mathbf{r}')$ and $a^\dagger(\mathbf{r}')|\Psi^n_A\rangle$ in the associated equation of motion

$$E^{A+1}_m \int d\mathbf{r}'\, \mathcal{N}^A(n,\mathbf{r},n,\mathbf{r}')\, \tilde{\phi}^{A+1}_{nm}(\mathbf{r}')$$

$$= \int d\mathbf{r}' \langle \Psi^n_A | a(\mathbf{r}) \left(H + HQ^p_n \frac{1}{E^{A+1}_m - Q^p_n H Q^p_n} Q^p_n H \right) \times a^\dagger(\mathbf{r}') |\Psi^n_A\rangle \tilde{\phi}^{A+1}_{nm}(\mathbf{r}') \tag{29}$$

$$= \int d\mathbf{r}'\, \tilde{\mathcal{H}}^p_n(\mathbf{r},\mathbf{r}';E^{A+1}_m)\, \tilde{\phi}^{A+1}_{nm}(\mathbf{r}')^*. \tag{30}$$

While the above equation contains a Hamiltonian $(\tilde{\mathcal{H}}^p)$ which is more symmetric than $\mathcal{H}^p$ [see Eq. (15)], the operator $\mathcal{N}^A$ is still present on the left-hand side of Eq. (30) [27]. The presence of this projection operator makes it difficult to establish a connection to a Schrödinger equation with a phenomenological potential.

Using the function $\overline{\phi}^{A}_{nm}(\mathbf{r})$, defined by Eq. (28), allows one to absorb the projection operator $\mathcal{N}^A$ into the definition of the associated Hamiltonian $\overline{\mathcal{H}}^p_n(\mathbf{r},\mathbf{r}';E^{A+1}_m)$:

$$E^{A+1}_m \overline{\phi}^{A+1}_{nm}(\mathbf{r}) = \int d\mathbf{r}'\, d\mathbf{r}''\, d\mathbf{r}''\, \mathcal{N}^A(n,\mathbf{r},n,\mathbf{r}')^{-1/2} \langle \Psi^n_A | a(\mathbf{r}') \times \left(H + HQ^p_n \frac{1}{E^{A+1}_m - Q^p_n H Q^p_n} Q^p_n H \right) \times a^\dagger(\mathbf{r}'') |\Psi^n_A\rangle \mathcal{N}^A(n,\mathbf{r}'',n,\mathbf{r}''')^{-1/2} \overline{\phi}^{A+1}_{nm}(\mathbf{r}''') \tag{31}$$

$$= \int d\mathbf{r}'\, \overline{\mathcal{H}}^p_n(\mathbf{r},\mathbf{r}';E^{A+1}_m)\, \overline{\phi}^{A+1}_{nm}(\mathbf{r}')^*. \tag{32}$$

The function $\overline{\phi}^{A}_{nm}(\mathbf{r})$ and the Hamiltonian $\overline{\mathcal{H}}^p_n(\mathbf{r},\mathbf{r}';E^{A+1}_m)$ play a prominent role in the nuclear cluster model. Arguments in support of employing the barred quantities are, among others, the claims that $\overline{\mathcal{H}}^p$ can be well approximated by a local Hamiltonian and that the Perey effect is minimal for this Hamiltonian [4]. The Perey effect is the difference between the wave functions generated by nonlocal and local equivalent Hamiltonians [16]. The latter argument, however, is misleading, as Fig. 1 clearly demonstrates. The function $\phi(\mathbf{r})$ shown here has been calculated in a cluster-model approach [9], i.e., it satisfies a nonlocal equation of the form given in Eq. (15). We observe that $\phi(\mathbf{r})$ agrees well with $\psi_t(\mathbf{r})$ and $\psi_b(\mathbf{r})$, two single-particle functions generated in a phenomenological approach with a local potential. Nevertheless, the Hamiltonian $\mathcal{H}^p$ can, in general, not be approximated by a local function. The reason for the excellent agreement seen in Fig. 1 is the fact that $\phi(\mathbf{r})$ *also* satisfies an equation of the form given in Eq. (21), and the Hamiltonian $\mathcal{H}_\mathcal{M}$, which occurs in the latter equation, can be approximated by a local function, namely, the energy-averaged mass operator.

Furthermore, if one studies the functions $\overline{\phi}_m(\mathbf{r})$, which can be generated in a microscopic model, such as the nuclear shell model, one has to conclude that these functions cannot be the solutions of a one-body Schrödinger equation with a simple local potential. To see this, we compare the squared norm

$$\overline{S}^A_{nm} = \int d\mathbf{r} |\overline{\phi}^A_{nm}(\mathbf{r})|^2, \tag{33}$$

of the function $\overline{\phi}^{A}_{nm}(\mathbf{r})$, with the squared norm S^A_{nm} of the overlap $\phi^A_{nm}(\mathbf{r})$, from which $\overline{\phi}^{A}_{nm}(\mathbf{r})$ has been derived, for the low-lying states of the ^{15}N and ^{17}F systems, see Fig. 2. All calculations were carried out using the OXBASH shell

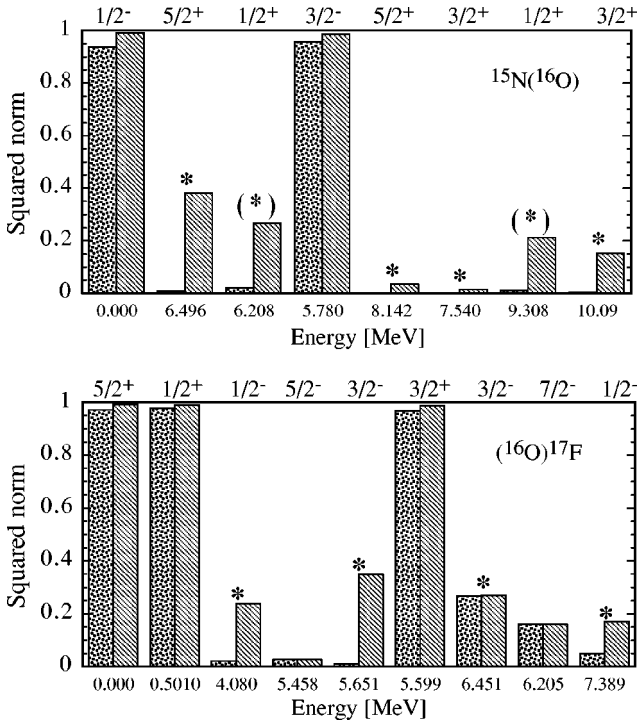

FIG. 2. Comparison of the spectroscopic factors S (shown as dotted bars) and the normalizations of the barred amplitudes $\overline{S}$ (shown as striped bars), for low-lying states in ^{15}N and ^{17}F. All values are those calculated with OXBASH with the WBP interaction in a $2\hbar\omega$ space [25]. The states marked with an asterisk are not present in a simple one-particle model.

model code with the WBP [25] interaction in a $2\hbar\omega$ model space. The ^{16}O ground state was chosen as the $(A=16)$-body reference state.

The S^A_{nm}, shown as dotted bars in Fig. 2, display a pattern that one would expect near a closed-shell nucleus such as ^{16}O: They are large (≈ 1) for those states which can be described as a proton-hole configuration (e.g., the $1/2^-$ ground state and $3/2^-$ excited state of ^{15}N) or single-proton configurations (e.g., the $5/2^+$, $1/2^+$, and $3/2^+$ states of ^{17}F) with respect to the ^{16}O reference state; they are small ($\approx$ few percent) for those ^{15}N and ^{17}F states which have a more complicated ($2h$-$1p$ or $1h$-$2p$) structure. The $\overline{S}^A_{nm}$ values (shown as striped bars in Fig. 2), on the other hand, agree with the S^A_{nm} only for those states which have a closed shell-plus-particle or hole-in-a-closed shell structure. Unlike the spectroscopic factors S^A_{nm}, they are *not* small for the states with the more complicated structure—those low-lying states that have the wrong quantum numbers and cannot be easily generated by a mean-field approach, as has been discussed at the end of Sec. II A. For example, the $\overline{S}^A_{nm}$ value for the $1/2^-$ state at 4.080 MeV in ^{17}F is 23.7%, and for the $3/2^-$ state at 5.651 MeV it is 34.9%.

To generate a spectrum and strength distributions such as those displayed by the $\overline{S}^A_{nm}$ shown in the bottom (top) part of Fig. 2 is nontrivial in a particle-only (hole-only) approach. It is very unlikely that the relevant particle-only (hole-only) Hamiltonian $\overline{\mathcal{H}}^p_n$ ($\overline{\mathcal{H}}^h_n$) could be approximated by a phenomenological form with a local potential. In the particle-only case the potential model would have to generate a single-particle spectrum in which, e.g., the $1/2^-$ and $3/2^-$ orbitals occured at energies higher than the $5/2^+$ and $1/2^+$ orbitals. In other words, the spectrum would have to contain the usual sd-shell orbitals, fp-shell orbitals, etc., and, superposed on that, states which lie below the Fermi surface in more commonly employed Woods-Saxon type potential models. These additional orbitals would have to occur at positive energies and would appear to have been ''reflected at the Fermi surface,'' from negative to positive energy values. Analogously, the hole-only case exhibits a spectrum which contains also ''reflected states'' superposed onto the usual set of orbitals. The structure displayed in Fig. 2 is not special to the ^{16}O region. Similar features occur near many other nuclei for which the standard independent particle model predicts a closed shell or subshell structure, e.g., ^{12}C, ^{28}Si, ^{32}S, ^{36}S, ^{48}Ca, etc.

The three functions discussed here have rather different physical interpretations: The one-body overlap $\phi^{A+1}_{nm}(\mathbf{r}) = \langle \Psi^n_A | a(\mathbf{r}) | \Psi^m_{A+1} \rangle$ gives the probability amplitude for finding the $(A+1)$-body system in the state m when a nucleon is added to the A-body system (in state n) at point $\mathbf{r}$. Pauli blocking limits the possibilities for adding particles to the system and reduces the associated spectroscopic factor accordingly. The effect of Pauli blocking is formally eliminated for the auxiliary function $\overline{\phi}^{A+1}_{nm}(\mathbf{r})$. The norm $\overline{S}^{A+1}_{nm}$ of the function $\overline{\phi}^{A+1}_{nm}(\mathbf{r})$ gives the ratio of the norm S^{A+1}_{nm} of the overlap $\phi^{A+1}_{nm}(\mathbf{r})$ to the maximum norm allowed by the Pauli principle. In other words, $\overline{S}^{A+1}_{nm}$ measures the similarity of the $(A+1)$-body system and the configuration that is obtained by adding a nucleon to the Pauli-allowed component of the A-body state. Thus, the values of S^{A+1}_{nm} and $\overline{S}^{A+1}_{nm}$ that are shown in the bottom portion of Fig. 2 can be understood as follows: The $p_{1/2}$ orbital is mostly Pauli blocked (i.e., occupied) in the ^{16}O ground state; hence the spectroscopic factor associated with the $1/2^-$ state in ^{17}F (at 4.080 MeV) is small. The value of $\overline{S}^{A+1}_{nm}$ for this state, in contrast, is sizable, thus indicating that the $1/2^-$ state is structurally similar to the configuration that is obtained by adding a $p_{1/2}$ proton to the small component of the ^{16}O wave function which has an unoccupied $p_{1/2}$ single-proton orbital. The ^{15}N spectrum can be understood analogously: The $d_{5/2}$ orbital has a small occupancy in ^{16}O, so the spectroscopic factor associated with the $5/2^+$ state in ^{15}N (at 6.496 MeV) is small. Nevertheless, the relevant $\overline{S}^{A+1}_{nm}$ value is large, which indicates that the $5/2^+$ state is structurally similar to the configuration that is obtained by removing a $d_{5/2}$ proton from the small component of the ^{16}O wave function which has an occupied $d_{5/2}$ proton orbital.

The auxiliary function $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ contains information on the projected $(A+1)$-body state $P^p_n | \Psi^m_{A+1} \rangle = \int d\mathbf{r} a^\dagger(\mathbf{r}) | \Psi^n_A \rangle \tilde{\phi}^{A+1}_{nm}(\mathbf{r})$, with P^p_n given by Eq. (14). Note that $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ occurs behind an antisymmetrization operator which eliminates those components of $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ that do not lead to a completely antisymmetric $(A+1)$-body state. Thus

$\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ is not unique and its norm is not well defined. However, the components of $\tilde{\phi}^{A+1}_{nm}(\mathbf{r})$ that remain after antisymmetrization is enforced define the projected state completely.

Although all three one-body functions discussed here contain valuable information on the structure of the many-body system, only the one-body overlap $\phi^{A+1}_{nm}(\mathbf{r})$ can be identified with the phenomenological single-particle wave function. The agreement between the microscopically calculated function $\phi^{A+1}_{nm}(\mathbf{r})$ and the Woods-Saxon eigenfunction shown in Fig. 1 confirms this. Given the complicated form of Eqs. (15) and (18), which contain the equations of motion for $\phi^{A+1}_{nm}(\mathbf{r})$, this is—at first glance—a surprising result. Equation (21) is the key to understanding this point: The one-body overlap function does not only satisfy the complicated equation of motion that was derived in a particle-only (or hole-only) approach and has a nonlocal potential, it also obeys Eq. (21). The latter equation is based on a particle-hole approach and contains the nuclear mean field as the relevant potential. It is this field that can be approximated by a local potential. The complications in Eqs. (15) and (18) arise because part of the space (hole states or particle states) have been eliminated from consideration. Introducing alternative Hamiltonians, such as $\overline{\mathcal{H}}$ and $\tilde{\mathcal{H}}$ discussed here, does not remedy the problem. These Hamiltonians are too complex to allow for an approximation by local functions. For example, the kinetic energy term takes on a more complicated form in $\overline{\mathcal{H}}^p_n(\mathbf{r},\mathbf{r}';E^{A+1}_n)$, namely, $\hat{\mathcal{N}}^{-1/2}\hat{T}\hat{\mathcal{N}}^{1/2}$, than in $\mathcal{H}^p_n(\mathbf{r},\mathbf{r}';E^{A+1}_n)$, where it is given by $\hat{T}\mathcal{P}^p$, see Eq. (24). Moreover, as we have demonstrated here, the strength distributions that are obtained with these alternative Hamiltonians are neither in agreement with the predictions of a potential model nor with experimental observations.

IV. LIMITING CASES

In order to illustrate the formalism employed in this work, we discuss applications to two simple limiting cases of (nuclear) many-body systems. We explore both noninteracting fermions in a one-body potential and spatially uniform systems. We focus in particular on clarifying the role of the projection operator which eliminates the hole or particle states from consideration.

A. Non-interacting particles in a one-body potential

We consider a set of A noninteracting fermions in a one-body potential $U(\mathbf{r})$. The relevant A-body Hamiltonian can be written as

$$H^A=\sum_{i=1}^{A} H_i\,, \tag{34}$$

where $H_i=-\nabla_i^2/(2m)+U(\mathbf{r}_i)$. (Note that we employ a local potential for convenience only; a nonlocal version does not significantly alter our findings.) The A-body wave functions that describe this system are Slater determinants constructed from A occupied single-particle orbitals. In particular, for the ground state the A lowest orbitals are filled. The particle and hole contributions to the full Green's function are given by

$$G_p(\mathbf{r},\mathbf{r}';E)=\sum_{m=A+1}^{\infty}\psi_m(\mathbf{r})\frac{1}{E-E_m+i\epsilon}\psi_m(\mathbf{r})^*, \tag{35}$$

$$G_h(\mathbf{r},\mathbf{r}';E)=\sum_{m=1}^{A}\psi_m(\mathbf{r})^*\frac{1}{E-E_m-i\epsilon}\psi_m(\mathbf{r}), \tag{36}$$

where $\psi_m(\mathbf{r})$ denotes a single-particle orbital and E_m is the corresponding single-particle energy. The modified mass operator reduces to the one-body potential $\mathcal{M}(\mathbf{r},\mathbf{r}';E)=U(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$. The operator P^p_n of Eq. (14), which projects into the space of particle states, reduces to a very simple expression—a step function. Since the A-body wave function considered here is a Slater determinant, i.e., the occupancies of the single-particle orbitals are restricted to the values one and zero only, the role of P^p_n is simply to eliminate the filled orbitals from active consideration. Thus, the equation of motion takes the following form in the particle-only space:

$$E_m\phi^{A+1}_{0m}(\mathbf{r}_i)=H_i\theta(H_i-E_f)\phi^{A+1}_{0m}(\mathbf{r}_i), \tag{37}$$

where E_f denotes the Fermi energy [compare also Eq. (15)] and θ is the Heaviside step function. The effective Hamiltonian is $H_i\theta(H_i-E_f)$, i.e., even for this simple system one obtains a Hamiltonian which is nonlocal and not (manifestly) symmetric. The effect of the projection operator is formally present, albeit in the form of a simple step function, which can be easily implemented in the formalism. The operator $\mathcal{N}$ reduces to this simple form and commutes with the Hamiltonian if and only if the relevant A-body wave function is a Slater determinant. Rewriting Eq. (37) as $E_m\theta(H_i-E_f)\phi^{A+1}_{0m}(\mathbf{r}_i)=H_i\phi^{A+1}_{0m}(\mathbf{r}_i)$, with the step function included on the left side of the equation, allows for a comparison with Eq. (29). Introducing correlations beyond antisymmetry effects and those included in the central potential causes a smearing of the step function and makes it necessary to include the full norm operator. Arguments analogously to those presented here apply to the hole-only space. Naturally, a step function which projects out the *unoccupied* states has to be introduced and all other quantities have to be modified accordingly.

The simple example discussed here illustrates an important point: the fact that the mean field can in general not be recovered in an approach that is based on an incomplete (particle-only or hole-only) space. If we view the one-body potential $U(\mathbf{r})$ as an approximation to the nuclear mean field, we find that the step function prevents us from determining the function $U(\mathbf{r})$ from either the particle-only or the hole-only equations of motion—both sets of equations are required. Moreover, only in simple cases, such as the one presented here, is the mean field Hamiltonian $\mathcal{H}_{\mathcal{M}}$ given by the sum of the particle-only and hole-only Hamiltonians; more generally, the Hamiltonians are related by Eq. (23), which poses a much greater challenge.

B. Spatially uniform Fermi systems

The investigation of spatially uniform Fermi systems is instructive and allows for important simplifications. For nuclear matter, a hypothetical uniform medium with an equal number of protons and neutrons, and with the Coulomb interaction turned off, we have the following situation: All relevant physical quantities are smooth functions of energy, and averages need not be taken. This holds in particular for the mass operator and the single-particle energies. Translational invariance implies that the spatial nonlocality of the modified mass operator is simple, $\mathcal{M}(\mathbf{r},\mathbf{r}';E)=\mathcal{M}(|\mathbf{r}-\mathbf{r}'|;E)$, and the one-body overlap functions are represented by plane waves. Similarly, the $\mathcal{N}^A$ operator and the density matrix depend on the difference $|\mathbf{r}-\mathbf{r}'|$ only, $\mathcal{N}^A(n,\mathbf{r},n,\mathbf{r}')=\mathcal{N}^A_n(|\mathbf{r}-\mathbf{r}'|)$, $\rho^A(n,\mathbf{r},n,\mathbf{r}')=\rho^A_n(|\mathbf{r}-\mathbf{r}'|)$. Consequently, the one-body overlaps are eigenfunctions of $\rho^A_n(|\mathbf{r}-\mathbf{r}'|)$, i.e., overlap functions and natural orbitals coincide for nuclear matter (see also Appendix B). The Fourier transform of the $\mathcal{N}^A$ operator has the simple form $\mathcal{N}^A_n(\mathbf{k},\mathbf{k}')=(2\pi)^{3/2}\mathcal{N}^A_n(\mathbf{k})\,\delta(\mathbf{k}-\mathbf{k}')=[1-\eta_n(\mathbf{k})]\delta(\mathbf{k}-\mathbf{k}')$ and the spectroscopic factors reduce to occupancies $\eta_n(\mathbf{k})=\langle\Psi^n_A|a^\dagger(\mathbf{k})a(\mathbf{k})|\Psi^n_A\rangle=1-\langle\Psi^n_A|a(\mathbf{k})a^\dagger(\mathbf{k})|\Psi^n_A\rangle$, which give the average number of nucleons with momentum k in the state $|\Psi^n_A\rangle$. The projection operator P^p_n takes the form

$$P^p_n=\int d\mathbf{k}a^\dagger(\mathbf{k})|\Psi^n_A\rangle[1-\eta_n(\mathbf{k})]^{-1}\langle\Psi^n_A|a(\mathbf{k}), \quad (38)$$

and the equation of motion, Eq. (15), becomes

$$\begin{aligned}E^{A+1}_m\phi^{A+1}_{nm}(\mathbf{k})=&\int d\mathbf{k}'\langle\Psi^n_A|a(\mathbf{k})\\&\times\left(H+HQ^p_n\frac{1}{E^{A+1}_m-Q^p_nHQ^p_n}Q^p_nH\right)\\&\times a^\dagger(\mathbf{k}')|\Psi^n_A\rangle[1-\eta_n(\mathbf{k}')]^{-1}\phi^{A+1}_{nm}(\mathbf{k}'),\end{aligned} \quad (39)$$

where $a(\mathbf{k})$, $a^\dagger(\mathbf{k})$, and $\phi^{A+1}_{nm}(\mathbf{k})=\langle\Psi^n_A|a(\mathbf{k})|\Psi^m_{A+1}\rangle$ denote the Fourier transforms of $a(\mathbf{r})$, $a^\dagger(\mathbf{r})$, and $\phi^{A+1}_{nm}(\mathbf{r})$, respectively. As can be seen by comparing these expressions to Eqs. (14) and (15), eliminating the hole states from consideration reduces in the nuclear matter case to simply including the occupancies of the momentum eigenstates, i.e., the effect of the $\mathcal{N}^A$ operator is incorporated in a simple multiplicative factor. In particular, when n refers to a translationally invariant ground state of an A-body system and m refers to a system with momentum $\mathbf{k}_m$, we find

$$\begin{aligned}&E^{A+1}_m[1-\eta_0(\mathbf{k})]\delta(\mathbf{k}-\mathbf{k}_m)\\&\quad=E^{A+1}_m\langle\Psi^0_A|a(\mathbf{k})a^\dagger(\mathbf{k}_m)|\Psi^0_A\rangle\\&\quad=\langle\Psi^0_A|a(\mathbf{k})\left(H+HQ^p_0\frac{1}{E^{A+1}_m-Q^p_0HQ^p_0}Q^p_0H\right)\\&\qquad\times a^\dagger(\mathbf{k}_m)|\Psi^0_A\rangle,\end{aligned} \quad (40)$$

since in that case $\phi^{A+1}_{nm}(\mathbf{k})\propto\delta(\mathbf{k}-\mathbf{k}_m)$.

Furthermore, in this limiting case of spatially uniform systems there exist simple relationships between the auxiliary functions introduced in Sec. III and the one-body overlap functions. We find

$$\phi^{A+1}_{nm}(\mathbf{k})=[1-\eta_n(\mathbf{k})]\tilde{\phi}^{A+1}_{nm}(\mathbf{k}) \quad (41)$$

and

$$\overline{\phi}^A_{nm}(\mathbf{k})=[1-\eta_n(\mathbf{k})]^{-1/2}\phi^A_{nm}(\mathbf{k}). \quad (42)$$

The hole-only case can be treated analogously.

V. CONCLUSIONS

One-body overlap functions play an important role for the description of nuclear structure and nuclear reactions. They contain both single-particle and many-nucleon aspects of the nuclear many-body problem and can, in principle, be obtained from a fully microscopic model or as the solution of a set of coupled-channels equations. Since for most cases it is not possible to obtain exact solutions, one has to resort to approximations and/or employ truncated model spaces. Various one-body approximations, e.g., were discussed in Ref. [5] and their relationships to phenomenological potential models was demonstrated. In the present work, we have focused on the effects of restricting the model space to particle-only or hole-only states. Using the Feshbach projection operator formalism, we have derived equations of motion for the one-body overlaps in the particle-only, hole-only, and particle-hole spaces. When treated properly, all three approaches will give the same result. We have shown for a simple example that this is indeed the case—we compared the overlap obtained from a cluster-model (particle-only) calculation with a single-particle wave function calculated in a potential model, which serves as an approximation to the full particle-hole approach, and we found excellent agreement between the two functions.

Approximating the relevant (particle-only, hole-only, or particle-hole) Hamiltonians by one that contains a simple kinetic energy term and a local potential is only valid in the particle-hole approach, as we have demonstrated here. Only the full particle-hole space is able to accommodate the mass operator (self-energy term) and it is the energy average of this operator that can be identified with the nuclear mean field and thus be approximated by a phenomenological potential, such as those used by the optical model and the shell model.

Hamiltonians which are derived in particle-only or hole-only approaches are valid in their respective frameworks. Normally, however, they have a very complicated form and cannot be approximated by a function which includes a simple local potential. The complications arise since part of the space, namely all hole states or all particle states, have been eliminated from consideration. Introducing auxiliary functions, such as the $\overline{\phi}(\mathbf{r})$ and $\tilde{\phi}(\mathbf{r})$ functions discussed here, might lead to simpler and more symmetric forms for the Hamiltonians, but does not solve the problem. The

single-particle strength distributions that result from these Hamiltonians do not agree with the predictions of a potential model, nor do they ressemble the experimental findings. Nevertheless, the particle-only and hole-only approaches provide useful insights into the nuclear many-body problem as, e.g., the success of the cluster model illustrates. The usefulness of such an approach relies on the proper interpretation of the relevant physical quantities. In particular, the auxiliary functions $\bar{\phi}(\mathbf{r})$ and $\tilde{\phi}(\mathbf{r})$ discussed here should *not* be identified with standard phenomenological single-particle functions. The function $\bar{\phi}(\mathbf{r})$, e.g., contains nuclear structure information that is complementary to, but different from, the information encapsulated in the one-body overlap. It is indeed useful for exploring the spectroscopic properties of low-lying states, such as signatures for nuclear shell closures. Work on this aspect is in progress [8].

In the present study, we have focused on one-body overlaps. One can also consider more general overlap functions, such as those employed in cluster model approaches, and their associated equations of motion. In alpha decay calculations, e.g., a four-body analog of the function $\bar{\phi}(\mathbf{r})$ studied here is introduced [4,6]. In that context, the function is assumed to satisfy a local differential equation. Given the findings presented here, we recommend that this assumption be reexamined. To adequately address the issue, the present study needs to be extended to accommodate configurations involving two composite nuclear fragments.

ACKNOWLEDGMENTS

The authors thank H. Sherif for valuable discussions and comments on drafts of the paper. Financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC) is appreciated.

APPENDIX A: ONE-BODY OPERATORS

We consider a one-body operator $\mathcal{F}=\int d\mathbf{r}d\mathbf{r}'a^{\dagger}(\mathbf{r})a(\mathbf{r}')F(\mathbf{r},\mathbf{r}')$. The operator $\mathcal{F}$ is Hermitean when $F(\mathbf{r},\mathbf{r}')=F^{*}(\mathbf{r}',\mathbf{r})$ holds. Matrix elements of such a Hermitean operator, with respect to many-body states, take the form

$$\langle\psi_A^n|\mathcal{F}|\psi_A^{n'}\rangle=\int d\mathbf{r}\,d\mathbf{r}'F(\mathbf{r},\mathbf{r}')\langle\psi_A^n|a^{\dagger}(\mathbf{r})a(\mathbf{r}')|\psi_A^{n'}\rangle. \tag{A1}$$

Thus, information on the operator is contained in $F(\mathbf{r},\mathbf{r}')$, while the structure of the many-body states is contained in the density matrix

$$\rho(n,\mathbf{r},n',\mathbf{r}')=\langle\psi_A^n|a^{\dagger}(\mathbf{r})a(\mathbf{r}')|\psi_A^{n'}\rangle, \tag{A2}$$

which contains diagonal as well as off-diagonal matrix elements. Closely related to the density matrix is the operator

$$\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')=\langle\psi_A^n|a(\mathbf{r})a^{\dagger}(\mathbf{r}')|\psi_A^{n'}\rangle, \tag{A3}$$

which, in the framework of cluster models, takes the role of a norm operator. From the anticommutation relations for $a(\mathbf{r})$ and $a^{\dagger}(\mathbf{r})$ it follows that the functions $\rho(n,\mathbf{r},n',\mathbf{r}')$ and $\mathcal{N}(n,r,n',r')$ are related to each other via

$$\rho(n,\mathbf{r},n',\mathbf{r}')+\mathcal{N}(n,\mathbf{r}',n',\mathbf{r})=\delta_{nn'}\delta(\mathbf{r},\mathbf{r}'). \tag{A4}$$

Here we will concentrate on $\rho(n,\mathbf{r},n',\mathbf{r}')$, but a parallel development follows for $\mathcal{N}(n,\mathbf{r},n',\mathbf{r}')$, with $(A-1)$ replaced by $(A+1)$.

We insert a complete set of orthonormal $(A-1)$-body wave functions in the expression for the density matrix and obtain

$$\rho(n,\mathbf{r},n',\mathbf{r}')=\sum_m\langle\psi_A^n|a^{\dagger}(\mathbf{r})|\Psi_{A-1}^m\rangle\langle\Psi_{A-1}^m|a(\mathbf{r}')|\psi_A^{n'}\rangle \tag{A5}$$

$$=\sum_m\phi_{mn}^{*A}(\mathbf{r})\phi_{mn}^{A}(\mathbf{r}'). \tag{A6}$$

This equation is very general; it only requires that the many-body functions $|\Psi_{A-1}^m\rangle$ form a complete orthonormal set. Given such a set, a second set can be generated through a unitary transformation $|\check{\Psi}_{A-1}^m\rangle=\Sigma_{m'}U_{mm'}|\Psi_{A-1}^{m'}\rangle$, where $U_{mm'}=\langle\Psi_{A-1}^{m'}|\check{\Psi}_{A-1}^m\rangle$ denotes a matrix elements of a unitary matrix. The corresponding transformation for the functions $\phi_{mn}^A(\mathbf{r})$ is given by

$$\check{\phi}_{mn}^A(\mathbf{r})=\sum_{m'}U_{mm'}\phi_{m'n}^A(\mathbf{r}'). \tag{A7}$$

This transformation differs from the usual transformation of wave functions since neither the $\phi_{m'n}^A(\mathbf{r}')$ nor the $\check{\phi}_{mn}^A(\mathbf{r})$ form an orthonormal set. Note that the $\phi_{mn}^A(\mathbf{r}')$ coincide with the one-body overlap functions introduced in Sec. II if and only if the associated many-body functions Ψ_{A-1}^m are eigenfunctions of the relevant Hamiltonian.

APPENDIX B: NATURAL ORBITALS

We now consider the density matrix $\rho(\mathbf{r},n,\mathbf{r}',n')=\langle\psi_A^n|a^{\dagger}(\mathbf{r})a(\mathbf{r}')|\psi_A^{n'}\rangle$ for fixed $n=n'$. For simplicity we suppress the index n in what follows. The natural orbitals $\hat{\varphi}_m(\mathbf{r}')$ are defined as the set of single-particle wave functions which diagonalize the density matrix $\rho(\mathbf{r},\mathbf{r}')$:

$$\int d\mathbf{r}'\rho(\mathbf{r},\mathbf{r}')\hat{\varphi}_m(\mathbf{r}')=\lambda_m\hat{\varphi}_m(\mathbf{r}). \tag{B1}$$

Since $\rho(\mathbf{r},\mathbf{r}')$ is Hermitian, the natural orbitals form a complete set and can be taken to be orthonormal. The natural orbitals are not uniquely defined if one or more of the eigenvalues λ_n are degenerate. This situation arises when $\lambda_m=0$ or 1, which occurs when there are completely empty or completely filled single-particle orbitals in the many-body wave function $|\psi_A^n\rangle$. The density matrix can be expressed in terms of natural orbitals

$$\rho(\mathbf{r},\mathbf{r}') = \sum_m \lambda_m \hat{\varphi}_m(\mathbf{r}) \hat{\varphi}_m^*(\mathbf{r}'). \tag{B2}$$

Note that the natural orbitals, unlike the one-body overlap functions, are completely defined by the structure of the A-body state.

Inserting Eq. (A6) into the eigenvalue equation, Eq. (B1), we obtain

$$\hat{\varphi}_m(\mathbf{r}) = \frac{1}{\lambda_m} \sum_{m'} \phi_{m'}^*(\mathbf{r}) \int d\mathbf{r}' \phi_{m'}(\mathbf{r}') \hat{\varphi}_m(\mathbf{r}'), \tag{B3}$$

i.e., natural orbitals with nonzero eigenvalues can be expanded in terms of the overlap functions from any basis $|\Psi_{A-1}^m\rangle$. The remaining natural orbitals, associated with $\lambda_m = 0$, can be chosen arbitrarily, provided they are orthogonal to those given by Eq. (B3). The combination of both collections, the natural orbitals with zero eigenvalues plus those with nonzero eigenvalues, forms a complete set. Thus Eq. (B3) can be inverted:

$$\phi_m(\mathbf{r}) = \sum_{m'} \hat{\varphi}_{m'}^*(\mathbf{r}) \int d\mathbf{r}' \hat{\varphi}_{m'}(\mathbf{r}') \phi_m(\mathbf{r}'). \tag{B4}$$

We can associate natural amplitudes $\varphi_m(\mathbf{r})$ with the natural orbitals by defining $\varphi_m(\mathbf{r}) = \sqrt{\lambda_m}\hat{\varphi}_m^*(\mathbf{r})$. (This expression holds for hole states, in the particle case the complex conjugation is not present.) Equation (B3) implies that the orthonormal set of $(A-1)$-body states given by

$$|{}_N\Psi_{A-1}^m\rangle = \frac{1}{\lambda_m} \sum_{m'} \int d\mathbf{r}' \phi_{m'}(\mathbf{r}') \varphi_m^*(\mathbf{r}') |\Psi_{A-1}^{m'}\rangle \tag{B5}$$

provides the basis for generating the natural amplitudes $\varphi_m(\mathbf{r})$ with $\lambda_m \neq 0$. The set $\{|{}_N\Psi_{A-1}^m\rangle\}$ is not complete. The remaining states $|{}_N^R\Psi_{A-1}^m\rangle$ which are required to make the set complete can be generated arbitrarily, provided they are orthogonal to the $|{}_N\Psi_{A-1}^m\rangle$ and to each other. The resulting set $\{|{}_N^C\Psi_{A-1}^m\rangle\} = \{|{}_N\Psi_{A-1}^m\rangle\} \cup \{|{}_N^R\Psi_{A-1}^m\rangle\}$ of $(A-1)$-body states is orthonormal and complete by construction.

When $\lambda_m \neq 0$, the matrix elements $U_{mm'} = \langle \Psi_{A-1}^{m'} | {}_N^C\Psi_{A-1}^m \rangle$ of the unitary transformation relating the two bases are given by

$$U_{mm'} = \frac{1}{\lambda_m} \int d\mathbf{r}' \phi_{m'}(\mathbf{r}') \varphi_m^*(\mathbf{r}'). \tag{B6}$$

This discussion shows that the natural amplitudes simply correspond to a particular choice for the $(A-1)$-body basis $\{|{}_N^C\Psi_{A-1}^m\rangle\}$. They have the same properties as the one-body overlap functions discussed in Ref. [5], with the exception of properties associated with the equations of motion. [The unusual placement of the complex conjugation in this discussion is due to the use of hole states, which transform as the complex conjugates of particle states. Using the norm operator, $\mathcal{N}(r,r')$, results in equations that look more familiar.]

Since the wave functions of the set $\{|{}_N^R\Psi_{A-1}^m\rangle\}$ correspond to states which are unoccupied $(\lambda = 0)$, it follows that $a(\mathbf{r})|\psi_A\rangle = \Sigma_m \varphi_m(\mathbf{r})|{}_N\Psi_{A-1}^m\rangle$. Thus any state orthogonal to $a(\mathbf{r})|\psi_A\rangle$, for all $\mathbf{r}$, is also orthogonal to all the functions $|{}_N\Psi_{A-1}^m\rangle$ generated by Eq. (B5). It also follows that $|{}_N\Psi_{A-1}^m\rangle = (1/\lambda_m)\int d\mathbf{r}\varphi_m^*(\mathbf{r})a(\mathbf{r})|\psi_A\rangle$ and that the states $|{}_N^C\Psi_{A-1}^m\rangle$ are eigenfunctions of the operator $\int d\mathbf{r} a(\mathbf{r})|\psi_A\rangle\langle\psi_A|a^\dagger(\mathbf{r})$.

The eigenvalues λ_m are restricted to lie in the interval $[0,1]$. The upper limit follows from the fact that a spectroscopic factor cannot be greater than one (when center-of-mass effects are neglected). The lower limit follows from the quadratic form of Eq. (A6). When an eigenvalue λ_m equals one, the state $|\psi_A\rangle$ is a pure product state $|\psi_A\rangle = \int d\mathbf{r}\varphi_m^*(\mathbf{r})a^\dagger(\mathbf{r})|{}_N\Psi_{A-1}^m\rangle$ with $\int d\mathbf{r}\varphi_m(\mathbf{r})a(\mathbf{r})|{}_N\Psi_{A-1}^m\rangle = 0$. If for any state $|\Psi_{A-1}^m\rangle$ the corresponding spectroscopic factor is 1, it then follows from Eq. (A6) that the corresponding amplitude is a natural amplitude with eigenvalue 1.

The natural orbitals provide the extrema $\chi(\mathbf{r}) = \varphi_m(\mathbf{r})$ of

$$\int d\mathbf{r}d\mathbf{r}' |\rho(\mathbf{r},\mathbf{r}') - \chi(\mathbf{r})\chi^*(\mathbf{r}')|^2 \tag{B7}$$

as can be easily verified by variation with respect to $\chi(\mathbf{r})$. Similarly, the overlap $\int d\mathbf{r}|\langle\psi_A|a^\dagger(\mathbf{r})|\chi_{A-1}\rangle|^2$ is maximized (for $\langle\chi_{A-1}|\chi_{A-1}\rangle = 1$) when $|\chi_{A-1}\rangle = |{}_N\Psi_{A-1}^m\rangle$.

The natural orbitals for ^{16}O and ^{40}Ca have been calculated by Fabrocini and Co' in Ref. [26]. The authors find that the shape of the natural orbitals is well reproduced by the single-particle wave functions from an independent particle model approach; deviations are only visible for the lowest orbitals. The occupancy of the lowest $1s$ orbital is found to be about 85% for either nucleus.

In general, the states $|\Psi_{A-1}^m\rangle$ and $|\Psi_{A+1}^m\rangle$ and the corresponding amplitudes are not related since the two sets of states belong to different spaces. However, since ρ and $\mathcal{N}$ are related by Eq. (A4), both operators are diagonalized by the same set of natural orbitals $\hat{\varphi}_m(\mathbf{r})$ with different eigenvalues, though, $\lambda_m^{\mathcal{N}} = 1 - \lambda_m$. The completeness relation (A4) can be expressed in terms of the natural orbitals

$$\sum_m (1-\lambda_m)\hat{\varphi}_m(\mathbf{r})\hat{\varphi}_m^*(\mathbf{r}') + \sum_m \lambda_m \hat{\varphi}_m(\mathbf{r})\hat{\varphi}_m^*(\mathbf{r}') = \delta(\mathbf{r},\mathbf{r}'). \tag{B8}$$

The first sum gives the particle contribution while the second sum gives the hole contribution. The effect of Pauli blocking on the particle states manifests itself in the factor $(1-\lambda_m)$.

A Caveat. Equation (B4) can be rewritten as

$$\phi_m(\mathbf{r}) = \sum_{m'} U_{m'm}\sqrt{\lambda_m}\hat{\varphi}_{m'}^*(\mathbf{r}). \tag{B9}$$

Since $U_{m'm}$ is a unitary matrix one might assume that the collection of functions $\phi_m(r)$ can be transformed into an orthonormal set by acting with $\rho(\mathbf{r},\mathbf{r}')^{-1/2}$ on the original set. Formally this would give

$$\hat{\phi}_m(\mathbf{r}) = \sum_{m'} U_{m'm}\hat{\varphi}_{m'}^*(\mathbf{r}). \tag{B10}$$

Since the $\hat{\varphi}^*_{m'}(\mathbf{r})$ are orthonormal and $U_{m'm}$ is unitary, one would expect the $\hat{\phi}_m(\mathbf{r})$ to be orthonormal. Unfortunately, this only works when $\rho(\mathbf{r},\mathbf{r}')$ has no zero eigenvalues. It is not sufficient to restrict the sum over m' to the subspace with nonzero eigenvalues, since $U_{m'm}$ is not necessarily unitary in this subspace. Similar considerations apply to the set of particle states, in which case the function $\rho(\mathbf{r},\mathbf{r}')^{-1/2}$ needs to be replaced $\mathcal{N}(\mathbf{r},\mathbf{r}')^{-1/2}$.

APPENDIX C: THE GREEN'S FUNCTION

Here we relate the particle-only ($\mathcal{H}^p$), hole-only ($\mathcal{H}^h$), and particle-hole ($\mathcal{H}_\mathcal{M}$) Hamiltonians to each other by applying the projection operator formalism to the associated Green's functions. We demonstrate explicitly that $\mathcal{H}_\mathcal{M}$, as defined in Eq. (21), is indeed the relevant particle-hole Hamiltonian.

The particle propagator is given by

$$G_p(\mathbf{r},\mathbf{r}';E)=\langle\psi_A^0|a(\mathbf{r})\frac{1}{E-(H-E_0^A)+i\epsilon}a^\dagger(\mathbf{r}')|\psi_A^0\rangle$$
$$=\langle\psi_A^0|a(\mathbf{r})G(E)a^\dagger(\mathbf{r}')|\psi_A^0\rangle, \tag{C1}$$

where

$$G(E)=\frac{1}{E-(H-E_0^A)+i\epsilon}. \tag{C2}$$

An equation of motion for $G_p(\mathbf{r},\mathbf{r}';E)$ can be obtained through the use of projection operators. We introduce operators P_0^p and Q_0^p, such that $P_0^p a^\dagger(\mathbf{r})|\psi_A^0\rangle=a^\dagger(\mathbf{r})|\psi_A^0\rangle$ and $Q_0^p a^\dagger(\mathbf{r})|\psi_A^0\rangle=0$, and rewrite Eq. (C2) as

$$(E+E_0^A-P_0^pHP_0^p-Q_0^pHP_0^p-P_0^pHQ_0^p-Q_0^pHQ_0^p)(P_0^pGP_0^p$$
$$+Q_0^pGP_0^p+P_0^pGQ_0^p+Q_0^pGQ_0^p)=P_0^p+Q_0^p. \tag{C3}$$

Using the fact that $P_0^p(P_0^p+Q_0^p)P_0^p=P_0^p$ and $Q_0^p(P_0^p+Q_0^p)P_0^p=0$, we find

$$\left(E+E_0^A-P_0^pHP_0^p-P_0^pHQ_0^p\frac{1}{E+E_0^A-Q_0^pHQ_0^p}Q_0^pHP_0^p\right)$$
$$\times P_0^pGP_0^p=P_0^p. \tag{C4}$$

We now multiply this equation by $\langle\psi_A^0|a(\mathbf{r})$ from the left and $a^\dagger(\mathbf{r}')|\psi_A^0\rangle$ from the right and carry out the relevant integrations. The right-hand side of the resulting equation equals $\langle\psi_A^0|a(\mathbf{r})a^\dagger(\mathbf{r}')|\psi_A^0\rangle=\mathcal{N}_0(\mathbf{r},\mathbf{r}')$. To obtain a useful expression for the left-hand side, we use the explicit form of P_0^p, given in Eq. (14). We derive the following result:

$$(E+E_0^A)G_p(\mathbf{r},\mathbf{r}',E)-\int d\mathbf{r}''d\mathbf{r}'''\langle\psi_A^0|a(\mathbf{r})$$
$$\times\left(H+HQ_0^p\frac{1}{E+E_0^A-Q_0^pHQ_0^p}Q_0^pH\right)a^\dagger(\mathbf{r}'')|\psi_A^0\rangle$$
$$\times\mathcal{N}_0(\mathbf{r}'',\mathbf{r}''')^{-1}G_p(\mathbf{r}''',\mathbf{r}',E)=\mathcal{N}_0(\mathbf{r},\mathbf{r}'), \tag{C5}$$

which can also be written as

$$(E+E_0^A)G_p(\mathbf{r},\mathbf{r}',E)-\int d\mathbf{r}'''\mathcal{H}_0^p(\mathbf{r},\mathbf{r}''')G_p(\mathbf{r}''',\mathbf{r}',E)$$
$$=\mathcal{N}_0(\mathbf{r},\mathbf{r}'), \tag{C6}$$

where

$$\mathcal{H}_0^p(\mathbf{r},\mathbf{r}''')=\int d\mathbf{r}''\langle\psi_A^0|a(\mathbf{r})\left(H+HQ_0^p\right.$$
$$\left.\times\frac{1}{E+E_0^A-Q_0^pHQ_0^p}Q_0^pH\right)$$
$$\times a^\dagger(\mathbf{r}'')|\psi_A^0\rangle\mathcal{N}_0(\mathbf{r}'',\mathbf{r}''')^{-1} \tag{C7}$$

[compare also Eqs. (15),(16)].

Introducing operator notation $\check{\mathcal{O}}f(\mathbf{r})=\int d\mathbf{r}'\mathcal{O}(\mathbf{r},\mathbf{r}')f(\mathbf{r}')$, allows us to write Eq. (C5) in a very compact form

$$(E+E_0^A-\check{\mathcal{H}}_0^p)\check{G}_p(E)=\check{\mathcal{N}}_0, \tag{C8}$$

which can be formally solved for $\check{G}_p(E)$

$$\check{G}_p(E)=\frac{1}{E-(\check{\mathcal{H}}_0^p-E_0^A)+i\epsilon}\check{\mathcal{N}}_0^A \tag{C9}$$

$$=(\check{\mathcal{N}}_0^A)^{1/2}\frac{1}{E-(\tilde{\check{\mathcal{H}}}_0^p-E_0^A)+i\epsilon}(\check{\mathcal{N}}_0^A)^{1/2}. \tag{C10}$$

We observe that the particle-only Hamiltonian, which occurs in the denominator of the particle propagator, is the optical-model Hamiltonian used by Feshbach.

Expressions analogous to the ones given above can be derived for the hole propagator. Since the full particle-hole Green's function, which is connected to the particle-hole Hamiltonian $\mathcal{H}_\mathcal{M}$ through $\check{G}(E)=(E-\check{\mathcal{H}}_\mathcal{M})^{-1}$, is simply the sum of the particle and hole contributions, we can relate the three Hamiltonians $\mathcal{H}_\mathcal{M}$, $\mathcal{H}^p$ and $\mathcal{H}^h$ to each other:

$$\check{G}(E)=\frac{1}{E-\check{\mathcal{H}}_\mathcal{M}}=\frac{1}{E-(\check{\mathcal{H}}^p-E_n^A)+i\epsilon}\check{\mathcal{N}}_0^A$$
$$+\frac{1}{E+(\check{\mathcal{H}}^h-E_n^A)-i\epsilon}\check{\rho}_0^A. \tag{C11}$$

Although this equation can be formally solved for $\check{\mathcal{H}}_{\mathcal{M}}$ in various different ways, the resulting expressions are neither elegant nor very instructive, as the following example illustrates:

$$\check{\mathcal{H}}_{\mathcal{M}}=\left[\frac{1}{1-[(\check{\mathcal{H}}^p-E_0^A)+(\check{\mathcal{H}}^h-E_0^A)]\dfrac{1}{E+(\check{\mathcal{H}}^h-E_0^A)}\check{\rho}_0}\right]\times\left[(\check{\mathcal{H}}^p-E_0^A)-[(\check{\mathcal{H}}^p-E_0^A)+(\check{\mathcal{H}}^h-E_0^A)]\times\frac{E}{E+(\check{\mathcal{H}}^h-E_0^A)}\check{\rho}_0\right]. \tag{C12}$$

(A similar equation, with $\check{\mathcal{H}}^p$ and $\check{\mathcal{H}}^h$ interchanged and ρ_0 replaced by $\mathcal{N}_0$, can be derived as well.)

In order to demonstrate that the particle-hole Hamiltonian has the form given in Eq. (21), we derive an equation of motion for the full particle-hole propagator $G(\mathbf{r},\mathbf{r}';E)$, introduced in Eqs. (3) –(5). We begin by writing $G(\mathbf{r},\mathbf{r}';E)$ as

$$G(\mathbf{r},\mathbf{r}';E)=\langle\psi_A^0|[a(\mathbf{r})+a^\dagger(\mathbf{r})]\frac{1}{E-(H-E_0^A-i\epsilon)(\hat{A}-A)}\times[a(\mathbf{r}')+a^\dagger(\mathbf{r}')]|\psi_A^0\rangle \tag{C13}$$

and introducing the notation $\tilde{H}=(H-E_0^A)(\hat{A}-A)$, where $\hat{A}=\int d\mathbf{r}a^\dagger(\mathbf{r})a(\mathbf{r})$, the particle number operator, commutes with the Hamiltonian. We employ the following particle-hole projection operator:

$$P^{ph}=\int d\mathbf{r}d\mathbf{r}'[a(\mathbf{r})+a^\dagger(\mathbf{r})]|\psi_A^0\rangle\mathcal{N}_{ph}^A(\mathbf{r},\mathbf{r}')\langle\psi_A^0|[a(\mathbf{r}')+a^\dagger(\mathbf{r}')], \tag{C14}$$

where $\mathcal{N}_{ph}^A(\mathbf{r},\mathbf{r}')=\langle\psi_A^0|[a(\mathbf{r})+a^\dagger(\mathbf{r})][a(\mathbf{r}')+a^\dagger(\mathbf{r}')]|\psi_A^0\rangle$. For the remainder of this discussion we restrict ourselves to time-reversal invariant states. In this case $\mathcal{N}_{ph}^A$ reduces to $\mathcal{N}_{ph}^A(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')$ and we obtain

$$\left[E-\langle\psi_A^0|(a+a^\dagger)\left(\tilde{H}+\tilde{H}Q_0^{ph}\frac{1}{E-Q_0^{ph}\tilde{H}Q_0^{ph}}Q_0^{ph}\tilde{H}\right)\times(a+a^\dagger)|\psi_A^0\rangle\right]\check{G}(E)=[E-\check{\mathcal{H}}_{\mathcal{M}}(E_m^{A+1})]\check{G}(E)=1. \tag{C15}$$

From this expression we identify the particle-hole Hamiltonian as

$$\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}')=\langle\psi_A^0|[a(\mathbf{r})+a^\dagger(\mathbf{r})]\times\left(\tilde{H}+\tilde{H}Q_0^{ph}\frac{1}{E-Q_0^{ph}\tilde{H}Q_0^{ph}}Q_0^{ph}\tilde{H}\right)\times[a(\mathbf{r}')+a^\dagger(\mathbf{r}')]|\psi_A^0\rangle. \tag{C16}$$

Since Q_0^{ph} mixes particle and hole states it is not possible to cleanly separate the particle and the hole contributions.

Using the Hamiltonian $\tilde{H}$, the particle and the hole Hamiltonians can now be written as

$$\mathcal{H}_n^p(\mathbf{r},\mathbf{r}';E)-E_n^A\delta(\mathbf{r}-\mathbf{r}')=\int d\mathbf{r}''\langle\Psi_A^n|a(\mathbf{r})\left(\tilde{H}+\tilde{H}Q_n^p\frac{1}{E-E_n^A-Q_n^p\tilde{H}Q_n^p}Q_n^p\tilde{H}\right)\times a^\dagger(\mathbf{r}'')|\Psi_A^n\rangle\mathcal{N}^A(n,\mathbf{r}'',n,\mathbf{r}')^{-1} \tag{C17}$$

and

$$E_n^A\delta(\mathbf{r}-\mathbf{r}')-\mathcal{H}_n^h(\mathbf{r},\mathbf{r}';E)=\int d\mathbf{r}''\langle\Psi_A^n|a^\dagger(\mathbf{r})\left(\tilde{H}+\tilde{H}Q_n^h\frac{1}{E_n^A-E-Q_n^h\tilde{H}Q_n^h}Q_n^h\tilde{H}\right)\times a(\mathbf{r}'')|\Psi_A^n\rangle\rho^A(n,\mathbf{r}'',n,\mathbf{r}')^{-1}, \tag{C18}$$

respectively. The last three expressions highlight both the similarity and the differences between the three Hamiltonians $\mathcal{H}_{\mathcal{M}}$, $\mathcal{H}^p$, and $\mathcal{H}^h$.

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[27] This equation reduces to the form derived in Ref. [5] if the coupling term is neglected (i.e., the term containing Q_n). In the derivation of that reference there was some ambiguity about how the one-body overlap function could be recovered. Here we see that $\phi_{nm}^{A+1}(r)$ is uniquely given by Eq. (27).