Restoration of overlap functions and spectroscopic factors in nuclei

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An asymptotic restoration procedure is applied for analyzing bound-state overlap functions, separation energies, and single-nucleon spectroscopic factors by means of a model one-body density matrix emerging from the Jastrow correlation method in its lowest order approximation for ^{16}O and ^{40}Ca nuclei. Comparison is made with available experimental data and mean-field and natural orbital representation results.

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Both single-nucleon spectroscopic factors and the overlap functions have attracted much attention in questions concerning the interpretation of recent $(e,e'p)$, $(d,^3\mathrm{He})$, and (γ,p) experimental data (e.g., [1–15]). The growing interest is motivated in principle by the possibility to clarify the limitation of the nuclear mean-field picture. For instance, the relatively low values of the spectroscopic factors deduced from these experiments show clearly the importance of the short-range correlation effects in nuclei and the necessity of detailed investigations of the high-momentum components of the nucleon wave function which cannot be included within the mean-field approximation [16–21].

The underlying relationship between the differential cross section and the structure of the nuclear wave function is often empirically analyzed using the plane-wave impulse approximation (PWIA). For instance, in this approximation the $(e,e'p)$-reaction cross section for a transition to a specific state with quantum numbers α in the residual nucleus has the following form (see, e.g., [12,22])

$$\sigma_{(e,e'p)} \equiv \frac{d^5\sigma}{d\Omega_{e'}d\Omega_p dE_p} = \mathscr{K}\sigma_{ep}|\phi_\alpha(\mathbf{k})|^2. \tag{1}$$

The first term $\mathscr{K}$ is kinematical factor , σ_{ep} is the off-shell electron-proton scattering cross section [23], and the nuclear structure component $|\phi_\alpha(\mathbf{k})|^2$ is the squared Fourier transform of the overlap function between the ground state of the target nucleus $\Psi^{(A)}$ and the final state of the residual nucleus $\Psi^{(A-1)}$ [24,25,16]:

$$\phi_\alpha(\mathbf{r}) = \langle \Psi_\alpha^{(A-1)}|a(\mathbf{r})|\Psi^{(A)}\rangle, \tag{2}$$

$a(\mathbf{r})$ being an annihilation operator for a nucleon with spatial coordinate $\mathbf{r}$ (spin and isospin coordinates are not put in evidence). The overlap function (2) is not orthonormalized. Its norm defines the spectroscopic factor of the level α,

$$S_\alpha = \langle \phi_\alpha|\phi_\alpha\rangle, \tag{3}$$

and the normalized overlap function

$$\tilde{\phi}_\alpha(\mathbf{r}) = S_\alpha^{-1/2}\phi_\alpha(\mathbf{r}). \tag{4}$$

Usually, $\tilde{\phi}_\alpha(\mathbf{r})$ is calculated from an empirical Saxon-Woods potential with a distinct potential radius for each separate transition α. Quantitative estimates are then deduced by fitting both the potential radius and the spectroscopic factor S_α in order to obtain a good agreement between the experimentally measured cross sections $(d\sigma/d\Omega)_{\mathrm{expt}}$ and those predicted from appropriate calculations for the reaction process.

The full theoretical description of the experiments mentioned above has many components. We should like to mention among them the proper account of the reaction mechanism, of the distortion effects (including the distortion due to the final state interaction), of the meson exchange currents contributions, the study of the A dependence, and others (see, e.g., [22,12]). Obviously, however, the theoretical estimates of the overlap functions (2) and the spectroscopic factors (3) are of crucial importance for the adequate evaluation of recent $(e,e'p)$, $(d,^3\mathrm{He})$, and (γ,p) experiments. The problem is that the normalized overlap functions (4) cannot be identified with a phenomenological shell-model single-particle wave function especially for energies farther from the Fermi energy, sometimes even within the valence shell [16]. It is known that generally, the independent-particle shell model cannot explain the fragmentation or spreading of the hole strength [26,22,20]. This is because, due to the residual interaction, the hole state of the target nucleus is not an eigenstate of the $(A-1)$-nucleon system and its strength is distributed over several states of the final system. Possible modifications going beyond the uncorrelated shell-model approximation quickly become rather involved.

Recently, it has been shown [27] that the knowledge of the ground-state one-body density matrix of the target nucleus is sufficient to determine, at least in principle, the overlap functions, spectroscopic factors, and separation energies of the bound $(A-1)$-particle eigenstates. The aim of the present paper is to apply the procedure suggested in [27] using the model one-body density matrix [28–30] in which the short-range correlation terms of the Jastrow correlation method are taken into account. The resulting quantitative estimates allow us to make instructive conclusions for the properties of the overlap functions in comparison with the associated shell-model orbitals and the natural orbitals [31] which are of frequent interest in this context [16,19,20].

The exact one-body density matrix associated with the ground state $\Psi^{(A)}$ of the target nucleus with A nucleons is defined as

$$\rho(\mathbf{r},\mathbf{r}') = \langle \Psi^{(A)}|a^\dagger(\mathbf{r})a(\mathbf{r}')|\Psi^{(A)}\rangle. \tag{5}$$

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Inserting the complete set of eigenstates $\Psi_\alpha^{(A-1)}$ of the residual $(A-1)$ nucleus, Eq. (5) reads

$$\rho(\mathbf{r},\mathbf{r}')=\sum_\alpha \phi_\alpha^*(\mathbf{r})\phi_\alpha(\mathbf{r}')=\sum_\alpha S_\alpha\tilde{\phi}_\alpha^*(\mathbf{r})\tilde{\phi}_\alpha(\mathbf{r}'), \quad (6)$$

where ϕ_α and $\tilde{\phi}_\alpha$ are the overlap functions (2) and (4), respectively, S_α is the spectroscopic factor (3), and the summation implicitly includes also the continuum states associated with all scattering channels of the $(A-1)$ system.

The one-body density matrix has a quite similar form in its natural orbital representation [31]

$$\rho(\mathbf{r},\mathbf{r}')=\sum_\alpha N_\alpha\psi_\alpha^*(\mathbf{r})\psi_\alpha(\mathbf{r}'), \quad (7)$$

where the natural orbitals ψ_α are defined as a complete orthonormal set of functions which diagonalize the one-body density matrix (5) with eigenvalues N_α called natural occupation numbers. Properties of the overlap functions and the natural orbitals are considered for various many-body systems, such as atomic nuclei [16,28,29,19,20,32–34] and liquid drops of ^{3}He [35].

In the case of a spherical ground state $\Psi^{(A)}$ with 0^+ angular momentum and parity, each eigenstate $\Psi_\alpha^{(A-1)}$ is characterized by the "single-particle" quantum numbers ljm, i.e., $\alpha\equiv nljm$, with n being the number of the ljm state. The overlap functions and the natural orbitals then factorize into radial and spin-angular parts

$$\begin{aligned}\phi_\alpha(\mathbf{r})&=\phi_{nlj}(r)Y_{ljm}(\Omega,\sigma),\\ \psi_\alpha(\mathbf{r})&=\psi_{nlj}(r)Y_{ljm}(\Omega,\sigma),\end{aligned} \quad (8)$$

where $Y_{ljm}(\Omega,\sigma)=[Y_l(\Omega)\times\chi^{1/2}(\sigma)]_m^j$ and σ is the spin variable. Using Eq. (8), the one-body density matrix reads

$$\rho(\mathbf{r},\mathbf{r}')=\sum_{lj}\rho_{lj}(r,r')\sum_{m\sigma}Y_{ljm}^*(\Omega,\sigma)Y_{ljm}(\Omega',\sigma). \quad (9)$$

Because of the spherical symmetry, S_{nlj}, N_{nlj}, and the radial contributions $\rho_{lj}(r,r')$ entering the one-body density matrix (9) do not depend on the magnetic quantum number m. From Eqs. (6) and (7) it then follows that in each lj subspace the spectroscopic factor S_{nlj} is smaller than the largest natural occupation number $N_{nlj}^{\max}$ with the same lj, i.e.,

$$S_{nlj}\leqslant N_{nlj}^{\max}. \quad (10)$$

The procedure of [27] is based on the generally accepted asymptotic behavior of the neutron overlap functions associated with the bound states of the $(A-1)$ system,

$$\phi_{nlj}(r)\rightarrow C_{nlj}\exp(-k_{nlj}r)/r, \quad (11)$$

where

$$k_{nlj}=\hbar^{-1}\sqrt{2m(E_{nlj}^{(A-1)}-E_0^{(A)})} \quad (12)$$

depends on the separation energy $\epsilon_\alpha=E_{nlj}^{(A-1)}-E_0^{(A)}$. Obviously, the higher excited states have faster decay. Therefore, for large values $r'=a\rightarrow\infty$, Eqs. (6) and (9) lead to the asymptotic relation

$$\rho_{lj}(r,a)\rightarrow\phi_{n_0lj}(r)C_{n_0lj}\exp(-k_{n_0lj}a)/a, \quad (13)$$

where $\phi_{n_0lj}(r)$ is the radial part of the lowest overlap function in the lj subspace considered. The unknown constant C_{n_0lj} can be derived from the asymptotic behavior of the diagonal part $\rho_{lj}(r,r)$ since

$$\rho_{lj}(a,a)\rightarrow|C_{n_0lj}|^2\exp(-2k_{n_0lj}a)/a^2. \quad (14)$$

By means of Eqs. (13) and (14) one can derive the lowest (bound-state) overlap function with quantum numbers lj and radial part

$$\phi_{n_0lj}(r)=\frac{\rho_{lj}(r,a)}{C_{n_0lj}\exp(-k_{n_0lj}a)/a}, \quad (15)$$

as well as the associated separation energy

$$\epsilon_{n_0lj}=\hbar^2k_{n_0lj}^2/2m \quad (16)$$

and the spectroscopic factor

$$S_{n_0lj}=\langle\phi_{n_0lj}|\phi_{n_0lj}\rangle. \quad (17)$$

One can repeat the above procedure for the second bound state with the same multipolarity (if it exists) after subtracting the contribution of the lowest eigenstate. The result is

$$\phi_{n_1lj}(r)=\frac{\rho_{lj}(r,a)-\phi_{n_0lj}(r)\phi_{n_0lj}(a)}{C_{n_1lj}\exp(-k_{n_1lj}a)/a}, \quad (18)$$

with expressions similar to (16) and (17) for the separation energy ϵ_{n_1lj} and the spectroscopic factor S_{n_1lj}, respectively. The restoration procedure can be continued and one is able to analyze all bound states of the $(A-1)$-particle system once the one-body density matrix of the A-particle ground state is known. In the case of proton bound states some modifications due to the Coulomb asymptotic behavior of the overlap functions have to be taken into account.

The present calculations of the bound-state overlap functions, separation energies, and spectroscopic factors have been performed applying the recipe (13)–(18) to a model one-body matrix [28–30] obtained within the Jastrow correlation method in its low-order approximation for ^{16}O and ^{40}Ca nuclei. The model is based on harmonic oscillator single Slater determinant and Gaussian-like state-independent correlation factor. Although the resulting density matrix has a simple analytical form, it is physically significant that the short-range correlations are incorporated in it to a large extent. In addition, its natural orbital representation is well investigated [28–30].

Here we should like to mention that the procedure suggested in [27] requires accurate values of the one-body density matrix at large r. In principle this limits the practical application of the method. In our opinion, however, the analytical expressions of the one-body density matrix obtained

TABLE I. Separation energies ϵ_α and spectroscopic factors S_α calculated on the basis of the one-body density matrix [28–30] for ^{16}O and ^{40}Ca. Comparison is made with the Hartree-Fock (HF) single-particle energies (set SkI from [36]), natural occupation numbers N_α [29], and experimental data (Expt.). The energies are in MeV and only the states with $j+1/2$ are displayed.

	nl	$\epsilon_\alpha^{\rm HF}$	ϵ_α	Expt.	$S_\alpha^{\rm HF}$	S_α	N_α	Expt.
^{16}O	$1s$	32.96	35.82	47.0 [a]	1	0.940	0.95	
	$1p$	20.81	17.48	21.8 [b]	1	0.953	0.965	
	$1d$	5.31	12.76	4.14 [b]	0	0.004	0.006	
^{40}Ca	$1s$	41.04	32.85	56.0 [a]	1	0.763	0.89	0.75 [d]
	$1p$	32.17	29.54	40.0 [a]	1	0.89	0.938	0.72 [d]
	$1d$	22.16	24.75	22.38 [c]	1	0.907	0.946	0.74 [d]
	$2s$	15.67	13.07	18.2 [c]	1	0.953	0.958	0.64 [d]
	$1f$	11.25	8.69	8.36 [c]	0	0.01	0.013	0.11 [d]

[a]From [37].
[b]From [38].
[c]From [39].
[d]From [6].

within some correlation methods give a basis for an easier numerical application of the procedure. This is the case in the present work. Using the model one-body density matrix from [28–30] we have to avoid, however, another difficulty arising from its Gaussian asymptotic behavior. This is achieved by applying the recipe (13)–(18) not for a single asymptotic point a but within an asymptotic region (a_L, a_U) bracketing the point a and sustained after the point where the diagonal element $\rho_{lj}(r,r)$ is less than 10% from its maximal value. We are looking for such a radial contribution $\rho_{n_0lj}(r,r')=\phi_{n_0lj}(r)\phi_{n_0lj}(r')$ whose diagonal part is less than or equal to $\rho_{lj}(r,r)$ at each point r and which minimizes the trace $\mathrm{Tr}[(\rho_{lj}-\rho_{n_0lj})^2]$. Then a_L, a, and a_U as well as the unknown C_{n_0lj} and k_{n_0lj} are uniquely determined by the requirement that the overlap function (15) satisfy Eqs. (13) and (14) simultaneously with minimal least-squared deviation within the region (a_L, a_U). We should mention that the procedure suggested is not a unique one, but this problem does not exist when a realistic one-body density matrix with a correct exponential asymptotic behavior is considered.

We have performed the above numerical procedure separately for each set of quantum numbers nl (the model does not split the states with respect to $j=l\pm1/2$). It leads to predictions for the neutron separation energies ϵ_α, spectroscopic factors S_α, and the overlap functions $\tilde{\phi}_\alpha$ which are given in Table I and Fig. 1, respectively.

It is seen from Table I that the calculated separation energies ϵ_α are in acceptable agreement with the self-consistent Hartree-Fock (HF) results [36] and the available experimental data. The calculated spectroscopic factors S_α, however, differ significantly from their mean-field values. Because of the short-range correlations, a depletion of the states below and a filling of the states above the Fermi level results. At the same time the calculated values of S_α are consistent with experimentally deduced spectroscopic factors [6]. In general,

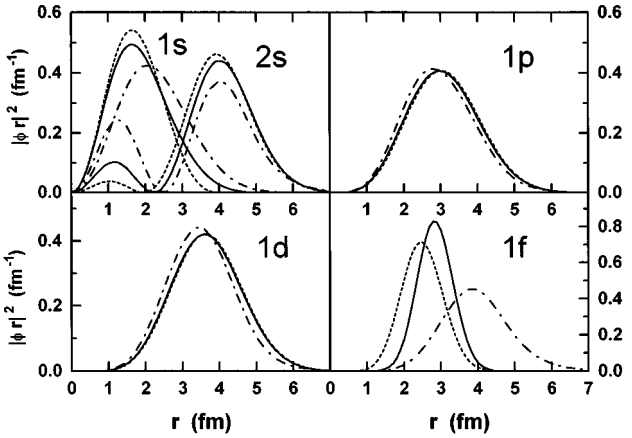

FIG. 1. Overlap functions (solid line), self-consistent Hartree-Fock single-particle wave functions (dot-dashed line), and natural orbitals (dashed line) for the nucleus ^{40}Ca.

the values of S_α emerging from the present restoration procedure are larger than the experimental ones. This fact is most probably related to the crude approximation for the density matrix used. The reason is the same for the larger value of $S_{2s1/2}$ in comparison with the spectroscopic factor of the lower $1s$ state in ^{40}Ca.

In Table I we compare S_α also with the natural occupation numbers N_α derived after diagonalyzing the same model one-body density matrix [28–30]. The comparison shows that our numerical procedure satisfies the general requirement (10). The trend of the calculated spectroscopic factors S_α follows that of the natural occupation numbers. This result becomes more transparent realizing that the overlap functions $\tilde{\phi}_\alpha$ are rather close to the natural orbitals ψ_α as is seen from Fig. 1.

From Fig. 1 it can be also seen that all three functions, the overlap, mean-field, and natural orbital wave functions, are quite similar for the hole states in nuclei. This justifies the use of shell-model orbitals instead of overlap functions within PWIA calculations (1) for such kind of nuclear states. This approximation, however, is no longer valid for the particle nuclear states where the mean-field wave functions significantly differ from the overlap functions (see the $1f$ state in Fig. 1). The latter take some intermediate position between the natural orbitals and the HF wave functions. It should be stressed that our model one-body density matrix is completely different from the Hartree-Fock one. It has been demonstrated in [28,29,35] that due to the short-range correlations (SRC's) the correlated particle-state orbitals are much more localized than the particle-state mean-field single-particle wave functions. This is the reason why the HF orbitals associated with the particle states go farther out than the overlap functions (or the natural orbitals) associated with the correlated one-body density matrix. The place of the correlated particle-state asymptotic region is affected by the SRC's while the HF particle-state orbitals have a larger spread although the orbit is more strongly bound.

The instructive conclusion is that neither natural orbitals nor shell-model wave functions can be used as particle-state overlap functions in the theoretical analysis of the experimental data. The present restoration procedure gives a pos-

sible solution of the problem if it is applied to some realistic ground-state one-body density matrices.

Concluding, we have demonstrated in this paper the possibility for restoring the separation energies, spectroscopic factors, and overlap functions for bound $(A-1)$-particle eigenstates on the basis of the ground-state one-body density matrix of the target A-particle system. Although we have used a quite crude approximation for the one-body density matrix [28–30], the asymptotic restoring procedure [27] leads to acceptable quantitative results. Thus one obtains a method for estimating such important quantities as spectroscopic factors and overlap functions which is supplemental to the more involved approaches [16]. For this purpose, one has simply to apply the present restoring procedure to more sophisticated one-body density matrices as, for example, the ones emerging from Brueckner-Hartree-Fock [40,41], variational Monte Carlo [35,42], or simplectic model calculations [43]. The resulting bound-state spectroscopic factors and overlap functions will have more realistic properties and can be used for reliable description of the characteristics of the $(e,e'p)$, $(d,{}^3\mathrm{He})$, (γ,p), and other one-nucleon removal nuclear processes.

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