The hole spectral function and the relationship between overlap functions, natural orbitals and the one-body density matrix in nuclei *

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A method to calculate the hole spectral function in the discrete part of the spectrum is suggested within the natural orbital representation of the one-body density matrix of A-nucleon system using its relationship with the overlap functions of the eigenstates in the $(A-1)$-nucleon system.

The cross-section of direct nucleon removal processes is determined by the spectral function which contains the information on the nuclear structure and is interpreted as the probability for the removal of a nucleon with given momentum and energy from the target nucleus with A nucleons (e.g., [1–25]). In particular, in the plane-wave impulse approximation the cross-section for the direct knock-out process is proportional to the diagonal element $S(\mathbf{k}, \mathbf{k}, E) \equiv S(\mathbf{k}, E)$ of the hole spectral function (or matrix) in the momentum representation:

$$S(\mathbf{k}, \mathbf{k}'; E) = \left\langle \Psi_0 \left| a^+(\mathbf{k}')\delta(E + \widehat{H} - E_A^0)a(\mathbf{k}) \right| \Psi_0 \right\rangle, \tag{1}$$

where $|\Psi_0\rangle$ is the ground state wave function of the target nucleus with A nucleons, $a^+(\mathbf{k}')$ and $a(\mathbf{k})$ are creation and annihilation operators for a nucleon with momentum $\mathbf{k}'$ and $\mathbf{k}$, respectively, $\widehat{H}$ is the Hamiltonian of the system with $(A-1)$-nucleons and E_A^0 is the ground state energy of the target nucleus. If the latter has a total spin and parity $J^\pi = 0^+$, then introducing a complete set of eigenstates of $\widehat{H}$ for the system of $(A-1)$-nucleons $|\Psi_f\rangle$ (where the state $|\Psi_f\rangle$ is characterized by the energy E_f with both discrete and continuous values and by other discrete and continuous quantum numbers) the hole spectral function can be written in the form:

$$S(\mathbf{k}, \mathbf{k}', E) = \sum_f \langle \Psi_0 \left| a^+(\mathbf{k}') \right| \Psi_f \rangle \langle \Psi_f \left| a(\mathbf{k}) \right| \Psi_0 \rangle \delta(E + E_f - E_A^0) \tag{2}$$

$$\equiv \sum_f \Phi_f^*(\mathbf{k}')\Phi_f(\mathbf{k})\delta(E + E_f - E_A^0), \tag{3}$$

where

$$\Phi_f(\mathbf{k}) \equiv \langle \Psi_f \left| a(\mathbf{k}) \right| \Psi_0 \rangle \tag{4}$$

is the overlap function in the momentum representation [26–28].

The methods used to calculate the spectral function are reviewed, e.g. in [7, 14, 16]. The use of the independent-particle shell model (when the overlap function (4) is equal to the single-particle wave function of the occupied state) cannot explain the fragmentation or spreading of the hole strength. This is because, due to the residual interaction, the hole state in 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.

In this work we suggest a method to calculate the hole spectral functions using essentially the one-body density matrix (OBDM) of A-nucleon system in the natural orbital representation [29] and its relationships with the natural orbitals (which diagonalize the OBDM) and the overlap functions (4). An expansion of the latter in the basis of the natural orbitals is used. The following two reasons can justify the use of the method:

1) Recently the diagonalization of the realistic one-body density matrix of the correlated nuclear ground state obtained by various correlation methods [16], such as the Jastrow method [30–32], as well as the generator coordinate method [16, 33, 34] and the coherent density fluctuation model [16, 34, 35] gave reliable information on the natural orbitals and occupation numbers in nuclei. These quantities correspond to the realistic behaviour of nuclear characteristics which are sensitive to the short-range nucleon-nucleon correlations, such as the nucleon and cluster momentum distributions, the mean kinetic and removal energies, radii and others. The natural orbitals in nuclei, as well as those in other fermion systems, such as ^3He liquid drops [36], are strongly localized and quite different from the overlap functions and from the mean-field type orbitals [30, 34, 36, 37]. Thus, it is of importance to apply the natural orbitals corresponding to realistic OBDM obtained in correlation theoretical methods to calculate the hole spectral function $S(\mathbf{k}, \mathbf{k}', E)$.

2) The basic quantity which is necessary to calculate the spectral function (3) is the overlap function (4). We show in this paper that the hole spectral function in the discrete part of the spectrum can be calculated by using the general relationship [37] which connects the asymptotic behaviour of the one-body density matrix with the overlap functions of the $(A-1)$-particle system eigenstates. This relationship is of general importance because it enables one to obtain quantities connected with the bound eigenstates of the $(A-1)$-particle system (such as overlap functions, spectroscopic factors and separation energies) by means of the exact OBDM (or by a realistic one obtained in a given correlation method) of the ground state of the A-particle system. In this way, the hole spectral function in the discrete part of the spectrum can be, in principle, calculated on the basis of the OBDM of the A-particle system.

Now we introduce the necessary quantities which are used in the theoretical method to calculate the hole spectral function.

The one-body density matrix of the ground state $|\Psi_0\rangle$ of the A-nucleon system has the form

$$\rho(x, x') = \langle \Psi_0 \left| a^+(x)a(x') \right| \Psi_0 \rangle, \tag{5}$$

where $x \equiv \{\mathbf{r}\sigma\tau\}$ labels spatial, spin and isospin coordinates and $a^+(x), a(x')$ are the creation and annihilation operators.

The natural orbitals (NO) $\varphi_a(x)$ are defined [29] as the complete orthonormal set of single-particle wave functions which diagonalize the OBDM:

$$\rho(x, x') = \sum_a N_a \varphi_a^*(x) \varphi_a(x'). \tag{6}$$

The eigenvalues N_a $(0 \le N_a \le 1, \sum_a N_a = A)$ are the natural occupation numbers. We note that the sum (6) is over the discrete states determined by the finite-range NO $\varphi_a(\mathbf{k})$.

The OBDM (5) can be presented also in the form:

$$\rho(x, x') = \sum_f \!\!\!\!\!\!\diagup \; \Phi_f^*(x)\Phi_f(x'), \tag{7}$$

where $\Phi_f(x) = \langle \Psi_f |a(x)| \Psi_0 \rangle$ is the overlap function in the coordinate representation.

The overlap functions can be expanded in the basis of the natural orbitals (e.g., in momentum space):

$$\Phi_f(\mathbf{k}) = \sum_a \langle \varphi_a | \Phi_f \rangle \varphi_a(\mathbf{k}) \tag{8}$$

The hole spectral function is then given by the expression:

$$
\begin{aligned}
S(\mathbf{k}, \mathbf{k}', E) &= \sum_{a,b} \varphi_a^*(\mathbf{k}')\varphi_b(\mathbf{k}) \sum_f \!\!\!\!\!\!\diagup \; \langle \Phi_f | \varphi_a \rangle \langle \varphi_b | \Phi_f \rangle \delta(E + E_f - E_A^0) \\
&\equiv \sum_{a,b} \varphi_a^*(\mathbf{k}')\varphi_b(\mathbf{k}) S_{ab}(E),
\end{aligned} \tag{9}
$$

where

$$S_{ab}(E) \equiv \sum_f \!\!\!\!\!\!\diagup \; \langle \Phi_f | \varphi_a \rangle \langle \varphi_b | \Phi_f \rangle \delta(E + E_f - E_A^0). \tag{10}$$

The quantity (for which different notations exist, e.g. [14, 15]):

$$\theta_{a,f} \equiv S_{a,f}^{1/2} \equiv \langle \varphi_a | \Phi_f \rangle \tag{11}$$

from (8) and (9) is the amplitude of the contribution of the orbital a to the overlap function for the eigenstate $|\Psi_f\rangle$. We mention that the quantity (11) determines both the spectroscopic factor of the state $|\Psi_f\rangle$ [28]

$$S_f^{A-1} \equiv \langle \Phi_f | \Phi_f \rangle = \sum_a |\theta_{a,f}|^2 = \sum_a S_{a,f} = \sum_a |\langle \varphi_a | \Phi_f \rangle|^2 \tag{12}$$

and the occupation probability of the orbital a:

$$N_a = \sum_f \!\!\!\!\!\!\diagup \; |\theta_{a,f}|^2 = \sum_f \!\!\!\!\!\!\diagup \; S_{a,f} = \sum_f \!\!\!\!\!\!\diagup \; |\langle \varphi_a | \Phi_f \rangle|^2 . \tag{13}$$

In general, for a given orbital a, only a limited subset of states f of the residual nucleus contribute to the sums (10) and (13).

The function $S_{ab}(E)$ (given by Eq.(10) and often called also "spectral function") can be rewritten [5] introducing the different states $|\Psi_f\rangle$ of the residual nucleus: i) the bound states $|\Psi_{E_\nu, \alpha}\rangle$ with energy E_ν and degeneracy quantum number α, and ii) the continuum states $|\Psi_{E_f, c}\rangle$ with energy E_f and the channel index c which specifies the channel where there is an incoming wave (all other channels contain

only outgoing waves), as well as all degeneracies like spin projections etc. Then Eq.(10) becomes:

$$
\begin{aligned}
S_{ab}(E) &= \sum_{\nu,\alpha} \langle \Phi_{\nu\alpha} | \varphi_a \rangle \langle \varphi_b | \Phi_{\nu\alpha} \rangle \delta(E + E_\nu - E_A^0) \\
&+ \sum_c \langle \Phi_{E_f = E_A^0 - E, c} | \varphi_a \rangle \langle \varphi_b | \Phi_{E_f = E_A^0 - E, c} \rangle \theta(E_A^0 - E_{A-1}^{thr.} - E) \\
&\equiv S_{ab}^{d.s.}(E) + S_{ab}^{c.s.}(E),
\end{aligned}
\tag{14}
$$

where $\Phi_{\nu\alpha}$ and $\Phi_{E_f,c}$ are the overlap functions associated with the bound and continuum eigenstates of the residual nucleus and $E_{A-1}^{thr.}$ is the threshold for particle decay of this nucleus. If the latter is a nucleon threshold, then $E_{A-1}^{thr.} = E_{A-2}^0$, where E_{A-2}^0 is the ground-state energy of the nucleus with $A-2$ nucleons [5]. The hole-spectral function (14) contains two parts: i) the spectral function in the discrete part of the spectrum $S_{ab}^{d.s.}(E)$, and ii) the spectral function in the continuum of the hole spectrum $S_{ab}^{c.s.}(E)$ with $E \le E_A^0 - E_{A-2}^0$.

As can be seen from Eqs.(9) and (14) the hole spectral function is essentially connected with the natural orbitals $\{\varphi_a\}$ and the overlap functions Φ_f and their relationship with the OBDM. Now we shall outline briefly this relationship.

In the case of spherical symmetry the OBDM can be written in the form:

$$
\rho(x, x') = \sum_{qlj} \rho^{(qlj)}(r, r') \sum_m Y_{ljm}^*(\Omega, \sigma) Y_{ljm}(\Omega', \sigma'),
\tag{15}
$$

where the radial part of the OBDM is:

$$
\rho^{(qlj)}(r, r') = \sum_f^f \Phi_f^{(qlj)}(r) \Phi_f^{(qlj)}(r').
\tag{16}
$$

In the above equations $\Phi_f^{(qlj)}(r)$ is the radial part of the overlap function, $Y_{ljm}(\Omega, \sigma)$ is the spin-angular function, q denotes the nature (proton and neutron) of the overlap function and l, j are angular and total momentum quantum numbers.

It is known [28] that the overlap functions associated with the bound states of the $(A-1)$- and $(A+1)$-nucleon systems are eigenstates of a single-particle Schrödinger equation in which the mass operator plays the role of a potential. Due to the finite range of the mass operator, the asymptotic behaviour of the radial part of the neutron overlap functions for bound states ν (labeled by ν=0, 1, ... with increasing energy) of the $(A-1)$-nucleon system is given by [26, 27, 37]:

$$
\Phi_\nu^{(qlj)}(r) \to C_\nu^{(qlj)} exp(-k_\nu^{(qlj)} r)/r,
\tag{17}
$$

where

$$
k_\nu^{(qlj)} = \frac{1}{\hbar} [2m_q(E_\nu^{(qlj)} - E_A^0)]^{1/2}.
\tag{18}
$$

For protons some mathematical complications arise due to an additional long-range part originating from the Coulomb interaction [27], though everything from the neutron case remains valid. It is assumed in [37] that Eq.(17) is also valid for the overlap functions corresponding to the $(A-1)$ continuum.

The asymptotic form of the overlap functions (Eqs.(17) and (18)) determines the asymptotic behaviour of the radial part of the OBDM $\rho^{(qlj)}(r, r')$ [37]. It is shown in [37] that at large values of $r' \equiv a \to \infty$ one can derive the lowest bound state overlap function by means of the radial part of the OBDM:

$$
\Phi_0^{(qlj)}(r) = \frac{\rho^{(qlj)}(r, a)}{C_0^{(qlj)} exp(-k_0^{(qlj)} a)/a},
\tag{19}
$$

as well as the separation energy

$$\varepsilon_0^{(qlj)} = \hbar^2 k_0^{(qlj)2}/2m_q \qquad (20)$$

and the spectroscopic factor

$$S_0^{(qlj)} = \langle \Phi_0^{(qlj)} | \Phi_0^{(qlj)} \rangle. \qquad (21)$$

The normalization coefficient $C_0^{(qlj)}$ can be obtained from the asymptotic form of the diagonal part of the radial OBDM:

$$\rho^{(qlj)}(a,a) \to \left| C_0^{(qlj)} \right|^2 exp(-2k_0^{(qlj)}a)/a^2. \qquad (22)$$

As shown in [37], the overlap functions for all bound states of the $(A-1)$-nucleon system can be constructed from the OBDM repeating the above procedure. For instance, the overlap function for the next bound state is:

$$\Phi_1^{(qlj)}(r) = \frac{\rho^{(qlj)}(r,a) - \Phi_0^{(qlj)}(r)\Phi_0^{(qlj)}(a)}{C_1^{(qlj)}exp(-k_1^{(qlj)}a)/a}. \qquad (23)$$

In the case of the continuum contributions to the OBDM one can calculate the particular sum over the scattering channels c: $\sum_c [\Phi_c^{(qlj)}(r,E)C_c(E)]$, but not the overlap function for each channel [37].

The method for calculating of the hole spectral function in the discrete part of the spectrum (for non-degenerate states ν):

$$S^{d.s.}(\mathbf{k}, \mathbf{k'}, E) = \sum_{a,b} \varphi_a^*(\mathbf{k'})\varphi_b(\mathbf{k}) \sum_\nu \langle \Phi_\nu | \varphi_a \rangle \langle \varphi_b | \Phi_\nu \rangle \delta(E + E_\nu - E_A^0) \qquad (24)$$

from a given theoretical correlation method consists in the following procedure:
1) By diagonalizing the one-body density matrix of the A-particle system ground state one obtains the natural orbitals $\{\varphi_a(\mathbf{k})\}$ (e.g., as in [30–35,16]); 2) The bound-state overlap functions Φ_ν and separation energies ε_ν are calculated on the basis of the one-body density matrix following the approximate method described above (Eqs.(19)-(23)). 3) The amplitudes of the contribution of the natural orbital a to the overlap function $\langle \varphi_a | \Phi_\nu \rangle$ are calculated and the results substituted in Eq.(24). The overlap functions of the discrete states indeed allow the corresponding part of the spectral function to be calculated directly from Eq.(3). However, the third step of the procedure also makes it possible to calculate simultaneously on the same footing the amplitudes (11) and some particular terms of the sums in Eqs.(12), (13) and (24). The spectroscopic amplitudes (11) can then be calculated with shell model single-particle wave functions and compared with those obtained from natural orbitals. It can be seen from Eqs.(1) and (5) that the energy integral of the hole spectral function (1) defines the one-body density matrix in the momentum representation

$$\int_{-\infty}^{E_F^-} dES(\mathbf{k}, \mathbf{k'}, E) = \rho(\mathbf{k}, \mathbf{k'}), \qquad (25)$$

where E_F^- is a negative quantity whose absolute value is equal to the separation energy of the A-nucleon system [28].

We emphasize that the method described above enables one to obtain the hole spectral function in the discrete part of the spectrum (i.e. the integrand of the left-hand side of Eq.(25) in the energy interval between $E_A^0 - E_{A-2}^0$ and E_F^-) on the basis of the one-body density matrix calculated in a given correlation method. The knowledge of $\rho(\mathbf{k}, \mathbf{k'})$ can give some information on the remaining part of the integrand in

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the left-hand side of Eq.(25), namely the hole spectral function in the continuum part of the spectrum in the energy interval between $-\infty$ and $E_A^0 - E_{A-2}^0$.

In this paper we suggest a new theoretical method to obtain the hole spectral function in the discrete part of the spectrum. The method is based on the natural orbital representation in nuclear theory and uses essentially both the natural orbitals and overlap functions as well as their relationship with the OBDM. Thus the theoretical point of the method consists in the possibility of using the OBDM which is related to the properties of the A-nucleon system to calculate the hole spectral function which determines the cross-section of the nucleon removal processes and gives information on the structure of the $(A-1)$-nucleon system. The applications of the method can serve also as a test of the predictions of the correlated methods concerning the OBDM of the correlated ground state of the A-nucleon system.

Our program to apply the suggested method includes two stages: i) calculations of overlap functions on the basis of realistic OBDM from a given correlation method and studies of their properties, and ii) calculations of hole spectral functions in the discrete part of the spectrum and comparison with available experimental data. The results from the fulfilment of this program will be given elsewhere.

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