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THE HOLE SPECTRAL FUNCTION AND THE RELATIONSHIP BETWEEN OVERLAP FUNCTIONS, NATURAL ORBITALS AND THE ONE-BODY DENSITY MATRIX IN NUCLEI[1]

A.N.Antonov[2], *M.V.Stoitsov*[2], *M.K.Gaidarov*[2], *S.S.Dimitrova*[2], *P.E.Hodgson*[3]

A method to calculated 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.

[1] The investigation has been performed at INRNE (Bulgaria) in collaboration with Bogoliubov Laboratory of Theoretical Physics, JINR.

Дырочная спектральная функция и связь между функциями перекрытия, натуральными орбиталями и одночастичной матрицей плотности ядер

А.Н.Антонов и др.

Предложен метод для вычисления дырочной спектральной функции для дискретной части спектра. Используется представление натуральных орбиталей одночастичной матрицы плотности A-нуклонной системы и ее связь с функциями перекрытия для состояний $(A-1)$-нуклонного ядра.

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1. Introduction

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 [1—16]. 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:

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[2] Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia 1784, Bulgaria
[3] Nuclear Physics Laboratory, Department of Physics, University of Oxford, Oxford OX1-3RH, U.K.

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

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, $\hat{H}$ 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 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:

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

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

where

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

is the overlap function in the momentum representation [17—19].

The methods used to calculated 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. The structure of the spectral function has been studied in the framework of the Green function method [1,20]. The detailed analyses have been carried out by expanding the mass operator into a perturbation series [1,3,4, 20,21]. Calculations using continuum shell model with residual interactions were given in [5,22]. The nucleon-nucleon correlation effects on the spectral functions were studied with the Green function method in [23—27,13]. It was shown that the overlap functions can be determined by a Schrödinger type equation in the discrete [8,12] and continuous [12] spectrum of the Hamiltonian for the $(A-1)$-body residual nucleus. The deep-hole nuclear levels and their large widths established from (e, e', p) and $(p, 2p)$ reactions have been considered within the many-body field theory without any model approaches in [26]. The Hartree-Fock method using Skyrme forces has been applied to calculate the proton hole-spectral function in [28].

In this work we use the natural orbital representation of the one-body density matrix (OBDM) in A-nucleon system [29]. In this representation the OBDM is diagonalized by the so-called natural orbitals (NO) which form a complete orthonormal set of functions. An expansion of the overlap functions (4) in the basis of the natural orbitals is used. We suggest a method to calculate the hole spectral functions using essentially the NO and overlap functions and their relationship with the OBDM. 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 ^{3}He 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 (**k**, **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.

In Section 2 we introduce the necessary quantities which are used in the theoretical method to calculate the hole spectral function. The method is given in Section 3.

2. The Hole Spectral Function and the Natural Orbital Representation in Nuclei

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

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

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:

$$\rho(x, x') = \sum\!\!\!\!\!\!\int_f \Phi_f^*(x)\, \Phi_f(x'), \tag{7}$$

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:

$$S(\mathbf{k}, \mathbf{k}', E) = \sum_{a,b} \varphi_a^*(\mathbf{k}')\, \varphi_b(\mathbf{k}) \sum\!\!\!\!\!\!\int_f \langle \Phi_f | \varphi_a \rangle \langle \varphi_b | \Phi_f \rangle\, \delta(E + E_f - E_A^0) \equiv$$

$$\equiv \sum_{a,b} \varphi_a^*(\mathbf{k}')\, \varphi_b(\mathbf{k})\, S_{ab}(E), \tag{9}$$

where

$$S_{ab}(e) \equiv \sum\!\!\!\!\!\!\int_f \langle \Phi_f | \varphi_a \rangle \langle \varphi_b | \Phi_f \rangle\, \delta(E + E_f - E_A^0). \tag{10}$$

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

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

from (8) and (9) is the amplitude for 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 $|\Psi_f\rangle$ [19]

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

and the occupation probability of the orbital a:

$$N_a = \sum\!\!\!\!\!\!\int_f |\theta_{af}|^2 = \sum\!\!\!\!\!\!\int_f S_{af} = \sum\!\!\!\!\!\!\int_f |\langle \varphi_a | \Phi_f \rangle|^2. \tag{13}$$

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:

$$S_{ab}(E) = \sum_{\nu,\, \alpha} \langle \Phi_{\nu\alpha} | \varphi_a \rangle \langle \varphi_b | \Phi_{\nu\alpha} \rangle\, \delta(E + E_\nu - E_A^0) +$$

$$+ \sum_c \langle \Phi_{E_f = E_A^0 - E_c} | \varphi_a \rangle \langle \varphi_b | \Phi_{E_f = E_A^0 - E_c} \rangle \theta (E_A^0 - E_{A-1}^{thr} - E) \equiv$$

$$\equiv S_{ab}^{d.s}(E) + S_{ab}^{c.s.}(E), \tag{14}$$

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 $E \leq E_A^0 - E_{A-2}^0$.

3. The Theoretical Method

The hole spectral function (Eqs. (9) and (14)) is essentially connected with the natural orbitals $\{\varphi_a\}$ and the overlap functions Φ_f and their relationship with the OBDM. Firstly, we shall outline briefly this relationship.

In the case of spherical symmetry the overlap functions have the form:

$$\Phi_f^{(q)}(x) = \Phi_f^{(qlj)}(r)\, Y_{ljm}(\Omega, \sigma), \tag{15}$$

where $\Phi_f^{(qlj)}(r)$ is the radial part, $Y_{ljm}(\Omega, \sigma)$ 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. Substituting Eq. (15) in Eq. (7), the OBDM can be written as:

$$\rho(x, x') = \sum_{qlj} \rho^{(qlj)}(r, r') \sum_m Y_{ljm}^*(\Omega, \sigma)\, Y_{ljm}(\Omega', \sigma'), \tag{16}$$

where the radial part of the OBDM is:

$$\rho^{(qlj)}(r, r') = \sum_f \Phi_f^{(qlj)}(r)\, \Phi_f^{(qlj)}(r'). \tag{17}$$

It is known [19] 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 $\nu = 0, 1, \ldots$ with increasing energy) of the $(A - 1)$-nucleon system is given by [17,18,37]:

$$\Phi_\nu^{(qlj)}(r) \to C_\nu^{(qlj)} \exp(-k_\nu^{(qlj)} r)/r, \tag{18}$$

where

$$k_\nu^{(qlj)} = \frac{1}{\hbar} [2m_q (E_\nu^{(qlj)} - E_A^0)]^{1/2}. \tag{19}$$

For protons some mathematical complications arise due to an additional long-range part originating from the Coulomb interaction [18], though everything from the neutron case remains valid. It is assumed in [37] that Eq. (18) is also valid for the overlap functions corresponding to the $(A-1)$ continuum.

The asymptotic form of the overlap functions (Eqs. (18) and (19)) determines the asymptotic behaviour of the radial part of the OBDM [37]. Since higher excited states have faster decay, at large values of $r' \equiv a \to \infty$ one gets:

$$\rho^{(qlj)}(r, a) \to \Phi_0^{(qlj)}(r)\, C_0^{(qlj)} \exp(-k_0^{(qlj)} a)/a. \tag{20}$$

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

$$\rho^{(qlj)}(a, a) \to |C_0^{(qlj)}|^2 \exp(-2k_0^{(qlj)} a)/a^2. \tag{21}$$

By means of Eqs. (20) and (21) one can derive the lowest bound state overlap function

$$\Phi_0^{(qlj)}(r) = \frac{\rho^{(qlj)}(r, a)}{C_0^{(qlj)} \exp(-k_0^{(qlj)} a)/a}, \tag{22}$$

as well as the separation energy

$$\varepsilon_0^{(qlj)} = \hbar^2 k_0^{(qlj)^2} / 2m_q \tag{23}$$

and the spectroscopic factor

$$S_0^{(qlj)} = \langle \Phi_0^{(qlj)} | \Phi_0^{(qlj)} \rangle. \tag{24}$$

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:

$$\Phi_1^{(qlj)}(r) = \frac{\rho^{(qlj)}(r, a) - \Phi_0^{(qlj)}(r)\, \Phi_0^{(qlj)}(a)}{C_1^{(qlj)} \exp(-k_1^{(qlj)} a)/a}. \tag{25}$$

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):

$$S^{d.s.}(\mathbf{k}, \mathbf{k}', E) = \sum_{a,b} \varphi_a^*(\mathbf{k}')\, \varphi_b(\mathbf{k}) \sum_\nu \langle \Phi_\nu | \varphi_a \rangle \langle \varphi_b | \Phi_\nu \rangle\, \delta(E + E_\nu - E_A^0) \tag{26}$$

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.(20)—(25)).

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.(26).

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

$$\int_{-\infty}^{E_F^-} dES(\mathbf{k}, \mathbf{k}', E) = \rho(\mathbf{k}, \mathbf{k}'), \tag{27}$$

where E_F^- is a negative quantity whose absolute value is equal to the separation energy of the A-nucleon system [19].

We emphasize that the method described above enables one to obtain the hole spectral function in the discrete part of the spectrtum (i.e., the integrand of the left-hand side of Eq.(27) 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 the left-hand side of Eq.(27), 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.

References

1. Gross D.H.E., Lipperheide R. — Nucl. Phys., 1970, A150, p.449.
2. Jacob G., Maris Th.A.J. — Rev. Mod. Phys., 1973, 45, p.6.
3. Wille U., Gross D.H.E., Lipperheide R. — Phys. Rev., 1971, C4, p.1070.
4. Wille U., Lipperheide R. — Nucl. Phys., 1972, A189, p.113.

5. Fritsch W., Lipperheide R., Wille U. — Nucl. Phys., 1972, A198, p.515.
6. Hodgson P.E. — Rep. on Progr. in Physics, 1975, 38, p.847.
7. Dieperink A.E.L., T. de Forest Jr. — Ann. Rev. Nucl. Sci., 1975, 25, p.1.
8. Boffi S., Capuzzi F. — Lett. Nuovo Cim., 1979, 25, p.209.
9. Boffi S., Giusti C., Pacati F.D., Frullani S. — Nucl. Phys., 1979, A319, p.461.
10. Ciofi degli Atti C. — Progr. in Part. and Nucl. Phys., 1980, 3, p.163.
11. Boffi S., Molinari A. — In: Proceedings of the International School of Physics «Enrico Fermi», Course LXXIX, Varenna 1980, North-Holland Publ. Company, Amsterdan — New York — Oxford, 1981, p.373.
12. Boffi S., Capuzzi F. — Nucl. Phys., 1981, A351, p.219.
13. Antonov A.N., Nikolaev V.A., Petkov I.Zh. — Z. Phys., 1982, A304, p.239.
14. Frullani S., Mougey J. — Adv. Nucl. Phys., 14, Plenum Press, New York, 1984, p.1.
15. Dean G.W.R., Brussaard P.J. — Z. Phys., 1986, A323, p.351.
16. Antonov A.N., Hodgson P.E., Petkov I.Zh. — Nucleon Correlations in Nuclei, Springer-Verlag, Berlin — Heidelberg — New York, 1993, p.1.
17. Berggren T. — Nucl. Phys., 1965, 72, p.337.
18. Bang J.M., Gareev F.A., Pinkston W.T., Vaagen J.S. — Phys. Rep., 1985, 125, p.253.
19. Mahaux C., Sartor R. — Adv. Nucl. Phys., 20, Plenum Press, New York, 1991, p.1.
20. Engelbrecht C.A., Weidenmuller H.A. — Nucl. Phys., 1972 , A184, p.385.
21. Faessler A., Kusuno S., Strobel G.L. — Nucl. Phys., 1973, A203, p.513.
22. Fritsch W., Lipperheide R., Wille U. — Phys. Lett., 1973, 45B, p.103.
23. Orland H., Schaeffer R. — Nucl. Phys., 1978, A299, p.442.
24. Ramos A., Polls A., Dickhoff W.H. — In: The Nuclear Equation of State, Part A, ed. by W.Greiner and H.Stocker, Plenum Press, New York, 1989.
25. Sartor R. — Nucl. Phys., 1976, A267, p.29; 1977, A289, p.329.
26. Vagradov G.M., Gorchakov V.V. — Particles and Nuclei, 1974, 5, p.308; Vagradov G.M., Gareev F.A., Bang J. — Nucl. Phys., 1977, A278, p.319.
27. Sartor R., Mahaux C. — Phys. Rev., 1980, C21, p.2613.
28. Van Neck D., Waroquier M., Ryckebusch J. — Phys. Lett., 1990, 249B, p.157.
29. Lowdin P.-O. — Phys. Rev., 1955, 97, p.1474.
30. Stoitsov M.V., Antonov A.N., Dimitrova S.S. — Phys. Rev., 1993, C47, p.R455; Phys. Rev. 1993, C48, p.74.
31. Stoitsov M.V., Antonov A.N. — Z. Phys., 1993, A345, p.259.
32. Stoitsov M.V., Antonov A.N., Dimitrova S.S. — Z. Phys., 1993, A345, p.359.
33. Antonov A.N., Bonev I.S., Christov C.V., Nikolov E.N., Petkov I.Zh. — Nuovo Cim., 1990, A103, p.1287.
34. Antonov A.N., Kadrev D.N., Hodgson P.E. — Phys. Rev., 1994, C50, p.164.
35. Antonov A.N., Christov C.V., Nikolov E.N., Petkov I.Zh., Hodgson P.E. — Nuovo Cim., 1989, A102, p.1701.
36. Lewart D.S., Pandharipande V.R., Pieper S.C. — Phys. Rev., 1988, B37, p.4950.
37. Van Neck D., Waroquier M., Heyde K. — Phys. Lett., 1993, B314, p.255.

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