Relationships between two–particle overlap functions and the two–body density matrix for many–fermion systems

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Relationships are obtained connecting the two–nucleon overlap function of the eigenstates in the $(A–2)$ particle system with the asymptotic behavior of the two–body density matrix for the ground state of the $A$–particle system. This makes it possible to calculate the two–body overlap functions, spectroscopic factors and separation energies on the basis of a realistic two–body density matrix. The procedure can be used in describing the $(e,e'NN)$ and $(\gamma,NN)$ reactions where the two–body overlap functions are a key ingredient in the analysis.

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I. INTRODUCTION

In this paper we examine the two–particle overlap functions in interacting many–body systems and derive general relationships connecting them with the ground state two–body density matrix. The procedure is based on the asymptotic properties of the overlap functions in coordinate space, when the distance between two of the particles and the center–of–mass of the remaining ones becomes very large. This work can be considered as an extension of the analysis presented in \cite{1} where the asymptotic behavior of the one–body density matrix and the single–particle overlap functions was examined. Such an extension to the two–body sector is of considerable interest in view of present–day experimental possibilities in electromagnetically induced two–body knock–out reactions like $(e,e'NN)$ and $(\gamma,NN)$.

The effects of ground–state NN correlations on two–nucleon knock–out reactions have been intensively studied and discussed. This includes the cases of the $(e,e'pp)$ and $(e,e'pn)$ reactions on $^{16}O$ and $^{12}C$ \cite{13,14,15,16} and their contributions (for $^{12}C$) to the semi–exclusive $(e,e'p)$ reaction \cite{11}, as well as of electroinduced \cite{12} and of photonuclear processes \cite{13,14}. It has been shown in \cite{14,15} that while for $(e,e'p)$ reactions the central short–ranged correlations (SRC) play only a marginal role, the two–proton knock–out in $(e,e'pp)$ processes exhibits a sizeable sensitivity to the ground–state correlation effects. It was pointed out in \cite{10} that the most promising extraction of SRC effect shows up in the longitudinal structure function which may be studied in the super–parallel kinematics. It was found \cite{1} that the knock–out of $^1S_0$ $pp$–pair dominates the $^{16}O(e,e'pp)$ reaction and this gives good perspectives for extracting information on SRC in nuclei from such processes. It has been shown also \cite{11} that the two–hadron knock–out is a substantial contribution to the $(e,e')$ reaction mechanism above the quasielastic peak. The correlation effects on $^4He(e,e'd)$ reaction cross–section have been studied in \cite{13}. The important role of the tensor correlations on the photonuclear cross–sections has been pointed out in \cite{13,14}. It was concluded in \cite{10} that combined analysis of $(\gamma,p)$ and $(e,e'p)$ reactions, together with new data from $(\gamma,NN)$ and $(e,e'NN)$ processes will lead to better understanding in electromagnetically induced knock–out and that namely the $pp$–channel is more sensitive to the SRC \cite{10,15}.

The two–nucleon overlap functions and their properties are reviewed widely e.g. in \cite{20}. They have been used in \cite{10} as one of the components of the charge–current density, containing the information on the nuclear structure in studies of two–nucleon knock–out and transitions to the low–lying discrete final states of the residual nucleus. The overlap functions used in \cite{8} are constructed using phenomenological single–particle wave functions and a correlation function from \cite{21}. As mentioned in \cite{8} a more sophisticated treatment should be given in principle on the basis of full calculations of the two–nucleon spectral function where both long– and short–range correlations are consistently considered and hence spectroscopic factors are automatically included. In \cite{22} first calculations of the two–nucleon spectral function of $^{16}O$ have been performed. Long–range correlations are treated by a Dressed RPA and SRC are included in the pair removal amplitude by adding defect functions obtained from solutions of the Bethe–Goldstone equation for the finite nucleus.

The aim of the present paper is to study to what extent observables important for two–particle emission, such as the two–nucleon overlap function, can be derived on the basis of the nuclear ground state two–body density matrix. Our attempt is inspired by the possibility to extract one–nucleon overlap functions from the one–body density matrix of the nuclear ground state that has been proved in \cite{8} and successfully applied for calculating the overlap functions, spectroscopic factors and separation energies associated with the bound states of the $(A−1)$–particle system \cite{8,15,21,22}.
II. DENSITY MATRICES AND OVERLAP FUNCTIONS

The one–and the two–body density matrices are defined in coordinate space as:

\[ \rho^{(1)}(x, x') = \langle \Psi^{(A)}| a^+(x) a(x')|\Psi^{(A)} \rangle, \]

and

\[ \rho^{(2)}(x_1, x_2; x'_1, x'_2) = \langle \Psi^{(A)}| a^+(x_1) a^+(x_2) a(x'_1) a(x'_2)|\Psi^{(A)} \rangle \]

respectively, where \( |\Psi^{(A)} \rangle \) is the antisymmetric \( A \)-fermion ground state normalized to unity and \( a^+(x), a(x) \) are creation and annihilation operators at position \( x \). The coordinate \( x \) includes both the spatial coordinate \( r \) and the appropriate spin and isospin coordinates. The matrices \( \rho^{(1)} \) and \( \rho^{(2)} \) are trace–normalized to the number of particles and of pairs of particles:

\[ \text{Tr} \rho^{(1)} = \int \rho^{(1)}(x) \, dx = A, \]

\[ \text{Tr} \rho^{(2)} = \frac{1}{2} \int \rho^{(2)}(x_1, x_2) \, dx_1 \, dx_2 = \frac{A(A-1)}{2}. \]

Since \( \rho^{(1)} \) and \( \rho^{(2)} \) are hermitian matrices their eigenstates \( \psi^{(i)}_\alpha \) form a complete orthonormal set, in terms of which \( \rho^{(1)} \) and \( \rho^{(2)} \) can be decomposed as

\[ \rho^{(1)}(x, x') = \sum_{\alpha=1}^{\infty} \lambda^{(1)}_\alpha \psi^{(1)*}_\alpha(x) \psi^{(1)}_\alpha(x'), \]

\[ \rho^{(2)}(x_1, x_2; x'_1, x'_2) = \sum_{\alpha=1}^{\infty} \lambda^{(2)}_\alpha \psi^{(2)*}_\alpha(x_1, x_2) \psi^{(2)}_\alpha(x'_1, x'_2). \]

The eigenfunctions \( \psi^{(1)}_\alpha \) and eigenvalues \( \lambda^{(1)}_\alpha \) are usually referred to as natural orbitals and natural occupation numbers \( \lambda^{(1)}_\alpha \) are hermitian matrices their eigenstates \( \psi^{(i)}_\alpha \) form a complete orthonormal set, in terms of which \( \rho^{(1)} \) and \( \rho^{(2)} \) can be decomposed as

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The eigenfunctions \( \psi^{(1)}_\alpha \) and eigenvalues \( \lambda^{(1)}_\alpha \) are usually referred to as natural orbitals and natural occupation numbers \( \lambda^{(1)}_\alpha \). For fermionic systems the antisymmetry of the wave functions imposes the constraint \( 0 \leq \lambda^{(1)}_\alpha \leq 1 \). In analogy, the eigenfunctions \( \psi^{(2)}_\alpha(x_1, x_2) \) are called natural geminals and the associated real eigenvalues \( \lambda^{(2)}_\alpha \) – natural geminal occupation numbers \( \lambda^{(2)}_\alpha \). As a consequence of the antisymmetry of the nuclear ground state, the \( \lambda^{(2)}_\alpha \) obey the inequalities:

\[ 0 \leq \lambda^{(2)}_\alpha \leq (A-1)/2, \text{ for } A \text{ odd} \]

\[ 0 \leq \lambda^{(2)}_\alpha \leq A/2, \text{ for } A \text{ even} \]

In uncorrelated (non–interacting) systems only the values \( \lambda^{(i)}_\alpha = 0, 1 \) appear for both the one– and two–body natural occupation numbers. Whereas the presence of correlations always reduces the maximal one–body occupation number, this is not the case for the two–body occupation numbers. The upper bound in (7) is actually only reached for systems which are in a sense maximally correlated, as e.g. the occupation number of zero–coupled pairs in the seniority formalism in the limit of large shell degeneracy.

Of more direct physical interest is the decomposition of the density matrices in terms of the overlap functions between the \( A \) particle ground state and the eigenstates of the \( (A-1) \) and \( (A-2) \) particle systems, since overlap functions can be probed in exclusive knock–out reactions.

Inserting a complete set of \( (A-1) \) eigenstates \( |\alpha(A-1)\rangle \) into eq. (8) one gets

\[ \rho^{(1)}(x, x') = \sum_{\alpha} \varphi^{(1)*}_\alpha(x) \varphi^{(1)}_\alpha(x'), \]

where \( \varphi^{(1)}_\alpha(x) = \langle \alpha(A-1)|a(x)|\Psi(A) \rangle \) is the one–body overlap function associated with the state \( |\alpha(A-1)\rangle \). The spectroscopic factors are then defined by the norm
\[ S^{(1)}_\alpha = \langle \varphi_\alpha | \varphi_\alpha \rangle. \]  

The two–nucleon overlap functions are defined as the overlap between the ground state of the target nucleus \( \Psi^{(A)} \) and a specific state \( \Psi^{(C)}_\alpha \) of the residual nucleus \( (C = A - 2) \) [24]:

\[ \Phi_\alpha(x_1, x_2) = \langle \Psi^{(C)}_\alpha | a(x_1) a(x_2) | \Psi^{(A)} \rangle. \]  

(10)

The two–particle spectroscopic factor is analogously defined by the norm

\[ S^{(2)}_\alpha = \langle \Phi_\alpha | \Phi_\alpha \rangle \]  

(11)

and the two–body density matrix reads

\[ \rho^{(2)}(x_1, x_2; x'_1, x'_2) = \sum_\alpha \Phi^*_\alpha(x_1, x_2) \Phi_\alpha(x'_1, x'_2). \]  

(12)

As in the case of the single–particle spectroscopic factors where \( S^{(1)}_\alpha \leq \lambda^{(1)}_{\text{max}} \) [1], one can find that \( S^{(2)}_\alpha \leq \lambda^{(2)}_{\text{max}} \). Therefore, both one- and two-particle spectroscopic factors cannot exceed the corresponding maximal natural occupation numbers.

**III. RELATIONSHIPS BETWEEN OVERLAP FUNCTIONS AND DENSITY MATRICES**

It has been shown in [1] that the one-body overlap functions associated with the bound states of the \( (A - 1) \) system can be expressed in terms of the ground state one-body density matrix of the \( A \) nucleon system. For example, in the case of a target nucleus with \( J^2 = 0^+ \), the lowest \( (n_0l_0j) \) bound state overlap function is determined by the asymptotic behavior \( (a \to \infty) \) of the corresponding partial radial contribution \( \rho_{lj}(r, r') \) of the one-body density matrix:

\[ \varphi_{n_0l_0j}(r) = \frac{\rho_{lj}(r, a)}{C_{n_0l_0j} \exp(-k_{n_0l_0j} a) / a}, \]  

(13)

where the constants \( C_{n_0l_0j} \) and \( k_{n_0l_0j} \) are completely determined by \( \rho_{lj}(r, r') \). In this way, both \( \varphi_{n_0l_0j}(r) \) and \( k_{n_0l_0j} \) define the separation energy

\[ \epsilon_{n_0l_0j} \equiv E^{(A-1)}_{n_0l_0j} - E^{(A)}_0 = \frac{\hbar^2 k^2_{n_0l_0j}}{2m} \]  

(14)

and the spectroscopic factor \( S_{n_0l_0j} = \langle \varphi_{n_0l_0j} | \varphi_{n_0l_0j} \rangle \). The procedure gives also the next bound state overlap functions with the same multipolarity if they exist and its applicability has been demonstrated in Refs. [1,22].

Similar procedure but applied to the two-body density matrix is of significant physical interest for analyzing properties of transfer reactions when two nucleons are removed from the target’s ground state \( \Psi^{(A)} \) leaving the residual \( C = A - 2 \) system in a state \( \Psi^{(A-2)}_\alpha \). The procedure is possible again due to the particular asymptotic properties of the two-body overlap functions [20]. They satisfy the general equation [20]:

\[ \left( -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 + v_{12} + \epsilon_{\alpha}^{(2)} \right) \Phi_\alpha(r_1, r_2) = \sigma(r_1, r_2), \]  

(15)

where \( \epsilon_{\alpha}^{(2)} = E^{(A-2)}_\alpha - E^{(A)}_0, \) \( v_{12} \) is the internal di–nucleon interaction and \( \sigma(r_1, r_2) \) is the nonlocal residual source term which contains the interaction between the two extra nucleons and the \( C \)–nucleus.

The condition to obtain the asymptotic solution of eq. (13) for the two–body overlap function are considered in [20,25,26]. In [25] the restrictions on the two–body interactions in the case of the system of three nonrelativistic spinless neutral particles have been formulated and the coordinate asymptotics of the discrete spectrum wave functions have been studied. In [20,26] the asymptotic behavior of wave functions and overlap functions have been investigated generalizing the amplitudes of Merkuriev [25] and different types of overlap functions necessary in calculations of direct transfer amplitudes have been shown. In case when a cluster of two like nucleons (neutrons or protons) unbound to the rest of the system is transferred with a simultaneous transfer of both nucleons, as e.g., in reactions \( ^{18}O - 2n \to ^{16}O \), or \( ^{16}O - 2p \to ^{14}C \), the following hyperspherical type of asymptotics is valid for the two-body overlap functions [20,25,26].
\[ \Phi(r, R) \to N \exp \left\{ -\sqrt{\frac{4m|E|}{R^2}} \left( \frac{R^2 + \frac{1}{4}r^2}{\frac{1}{2}r^2} \right)^{5/2} \right\}, \] 

(16)

where \( r = r_1 - r_2 \) and \( R = (r_1 + r_2)/2 \) are the magnitudes of the relative and center of mass coordinates, respectively, \( m \) is the nucleon mass and \( E \) is the two-nucleon separation energy

\[ E = E^{(A)} - E^{(C)} = -E_C. \] 

(17)

In the case of a target nucleus with \( J^\pi = 0^+ \) the two-body overlap function can be written in the form:

\[ \Phi_{AJM}^C(x_1, x_2) = \sum_{LS} \{ \Phi_{a,LS}(r_1, r_2) \otimes \chi_S(\sigma_1, \sigma_2) \}_{JM}, \] 

(18)

where

\[ \chi_{S \lambda \sigma}(\sigma_1, \sigma_2) = \left\{ \chi_\lambda^\lambda(\sigma_1) \otimes \chi_\lambda^\lambda(\sigma_2) \right\}_{S \lambda \sigma} \]

\[ = \sum_{m_1, m_2} \left( \frac{1}{2} m_1 \frac{1}{2} m_2 \right) \chi_{m_1, m_2}^S(\sigma_1) \chi_{m_2, \sigma_2}^S \] 

(19)

and \( \Phi_{a,LS\lambda \sigma}(r_1, r_2) \) is the spatially dependent part of the overlap function. As suggested in [20] it is possible to perform a decomposition into angular momenta \( l = l_r \) and \( L_{\lambda \sigma} (L = l + L_r) \), corresponding to the relative and center of mass coordinates:

\[ \Phi_{a,LS\lambda \sigma}(r, R) = \sum_{lL_R} \Phi_{a,LS\lambda \sigma}(r, R) \left\{ Y_{LM}(\hat{R}) \otimes Y_l(\bar{r}) \right\}_{LM}. \] 

(20)

Then the two-body density matrix has the form:

\[ \rho^{(2)}(x_1, x_2; x_1', x_2') = \sum_{JM} \sum_{LS} \sum_{lL_R} \rho^{(2)}_{S' L' L'' R} (r, R; r', R') \times \]

\[ A_{S' L' L'' R}^{JM} (\sigma_1, \sigma_2; \bar{r}, \hat{R}) \chi_{S \lambda \sigma} (\sigma_1, \sigma_2) \] 

\[ \times A_{S' L' L'' R}^{JM} (\sigma_1', \sigma_2'; \bar{r}', \hat{R}') \] 

(21)

where the radial part of the density matrix is

\[ \rho^{(2)}_{S' L' L'' R} (r, R; r', R') = \sum_{\alpha} \Phi_{a,LS\lambda \sigma}(r, R) \Phi_{a,LS' L' \lambda \sigma}(r', R') \] 

(22)

and the spin-angular function is:

\[ A_{S' L' L'' R}^{JM} (\sigma_1, \sigma_2; \bar{r}, \hat{R}) = \left\{ \left\{ Y_{LM}(\hat{R}) \otimes Y_l(\bar{r}) \right\}_{LM} \otimes \chi_S(\sigma_1, \sigma_2) \right\}_{JM}. \] 

(23)

In eqs. (18)–(22) \( \alpha \) is the number of the state of the residual nucleus with a given total momentum \( J \).

Let us further consider the diagonal part of eq. (24):

\[ \rho^{(2)}_{S' L' L'' R} (r, R; r', R') = \sum_{\alpha} \Phi_{a,LS\lambda \sigma}(r, R) \Phi_{a,LS\lambda \sigma}(r', R'). \] 

(24)

Eq. (16) implies that for large \( r' = a \) and \( R' = b \) a single term \( \alpha_0 \) (corresponding to the smallest two-nucleon separation energy) will dominate in the sum of the right hand side of eq. (24). As a consequence the two-body overlap function \( \Phi_{a,LS\lambda \sigma}(r, R) \) can be expressed in terms of the two-body density matrix:

\[ \Phi_{a,LS\lambda \sigma}(r, R) = \frac{\rho^{(2)}_{LS\lambda \sigma}(r, R; a, b)}{\Phi_{a,LS\lambda \sigma}(a, b)} \] 

\[ = \frac{\rho^{(2)}_{LS\lambda \sigma}(r, R; a, b)}{N \exp \left\{ -k \sqrt{(b^2 + \frac{1}{4}a^2)} \right\} \left( b^2 + \frac{1}{4}a^2 \right)^{5/2}. \] 

(25)
Here the asymptotic form of the two-body overlap function is used with a constant $k$ which defines the two-nucleon separation energy.

Therefore, if the two-body density matrix $\rho(2)$ is known, the constant $k$ entering eq. (26) can be determined by the slope of the partial radial contribution $\rho_{JSLLR}^{(2)}(r; a, b)$ at large $a$ and $b$, while the unknown coefficients $N$ can be obtained from the asymptotic behavior of the spatially diagonal part $\rho_{JSLLR}^{(2)}(a; a, b)$. In this way, the constant $k$ will give information about the two-nucleon separation (17), and the norm of the overlap function (26) about the associated two–particle spectroscopic factor. The relationships obtained can be useful in analyzing the processes such as $(e, e'NN)$ and $(\gamma, NN)$ which are studied widely nowadays. Of course, the method will be reliable when realistic density matrices are considered.

In conclusion, the derivation of eq.(26) makes it possible to find a solution of the complicated problem about the relationship between the two-body overlap functions and the two-body density matrix. The use of the asymptotics of the overlap function in the particular case of two like nucleons unbound to the rest of the system can help in analyzing the overlap functions for two–nucleon knock–out processes on the basis of correlated two-body density matrix for the target nucleus. In our future work, which is now in progress, the density matrices obtained in the Jastrow–type model are used for actual calculations of the two–particle overlap functions.

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