ENTANGLEMENT OF $1p0f$-SHELL NUCLEON PAIRS

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The entanglement of pure states of the $1p0f$-shell nucleon pairs has been studied. The Slater decomposition theorem has been used to verify if any pure state of a nucleon pair is an entangled state. The von Neumann entropy of the partial density matrix has been employed to quantify the entanglement of the $1p0f$-shell nucleon pairs. Results of calculations have evidenced that the spin J and isospin $T = 0$ states are strongly entangled. In the spin J and isospin $T = 1$ states, proton–neutron pairs are more entangled than proton–proton and neutron–neutron pairs.

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1. Introduction

The concept of quantum entanglement, first considered by Schrödinger [1, 2], has played a crucial role in the development of quantum physics. Entanglement, observed nowadays in composite quantum systems, is one of the most intriguing issues of modern quantum theory. Basic features of quantum entanglement manifest themselves in non-local correlations between measurements performed on interacting well-separated particles. In other words, quantum entanglement means that interacting multiple particles after their separation are linked together in such a way that the measurement of one particle's quantum state determines the possible quantum states of other particles independently of their spatial separation.

Formulated by Bell famous inequalities [3] have opened a possibility to experimental verification of the non-local features of quantum theory. Among many experiments performed to check Bell's inequalities, experiments involving entangled pairs of photons were performed by Aspect and co-workers [4, 5]. They confirmed an unambiguous violation of Bell's inequality and confirmed good agreement with quantum mechanics (see also [6–8]). All these results show us that entanglement is a fundamental, new resource, beyond the scope of classical physics.

The phenomenon of quantum entanglement of particles separated by macroscopic distances is rather well-known. On the contrary, the characterization of quantum entanglement of particles at short, microscopic distances is still an open problem. In this case, the indistinguishable character of identical, tightly bounded particles (fermions or bosons) is a challenging subject to study [9, 10].

In reference [11], we studied quantum entanglement between indistinguishable particles at short distances on the example of the $1s0d$-shell nucleon pairs. The choice of such particles was dictated by their relatively simple structure and by the fact that nucleon pairs in the truncated versions of the shell model are used as building blocks for wave functions of nuclei in the ground and excited states [12–14]. The main result of this study is that the isospin $T = 0$ pairs are more entangled than the isospin $T = 1$ pairs.

Fingerprints of entangled states of nucleon pairs obtained from nuclear decays and in reactions with exotic nuclei, *e.g.* ^{11}Li or ^{6}He, were reported in Ref. [15]. Simple quantum entanglements were also visible in peripheral reactions with rare isotopes [16]. Experimental results of Ref. [17] suggest that in the reaction ^{16}O–^{208}Pb, entangled proton pairs pass through the Coulomb barrier with high probability in collisions with energies well below those to breach this barrier. Therefore, fingerprints of entangled states of two-nucleon systems observed in experiments involving nuclei from different mass ranges justify the motivation to study the entanglement of nucleon pairs. The $1p0f$-shell nucleon pairs take part in two-nucleon transfer reactions involving nuclei from different shells and different mass ranges. In theoretical models of direct two-nucleon transfer reactions, it is generally assumed that nucleons are transferred in the shell-model two-nucleon configurations. So, transfer reactions can serve as a good tool to test an influence of the entanglement of nucleon pairs on the probability transfer.

The aim of this paper is to extend the formalism of Ref. [11] to analyse the entanglement of proton–proton, proton–neutron and neutron–neutron pairs in the $1p0f$ shell.

In spite of the fact that it is hard to perform experiments on the entanglement of nuclear systems, we hope that presented in this and previous paper [11] findings will stimulate interest in issues of entanglement of two-nucleon systems. We hope that in the near term, nuclear systems as well as atomic and optical systems can become an important tool to obtain outcomes for testing the non-local nature of quantum mechanics.

In order to quantify the amount of entanglement in quantum states of indistinguishable particles, an appropriate measure of entanglement is required. Such measure of the entanglement of pure states for two distinguishable particles is the von Neumann entropy of the partial density matrix, obtained by tracing over one subsystem [18]. The analog of the von

Neumann entropy remains a good measure of entanglement also for two identical fermions [10, 19]. Therefore, we will use the von Neumann entropy to quantify the entanglement of the $1p0f$-shell nucleon pairs.

The paper is organized as follows. In Section 2, the entanglement criteria for two distinguishable and two undistinguished particles are shortly presented. In Section 3, the von Neumann entropy is briefly described. Results of calculations of the von Neumann entropy of states of the $1p0f$-shell nucleon pairs are discussed in Section 4. Summary is in Section 5.

2. The entanglement criteria

2.1. System of two distinguishable particles

The impossibility of writing the pure state vector $|\Psi(1.2)\rangle$ of the system made from two distinguishable particles as a tensor product of two single-particle state vectors $|\Psi(1)\rangle$ and $|\Psi(2)\rangle$ indicates an appearance of entanglement in this systems. This implies that: *(i)* the state vector $|\Psi(1.2)\rangle$ turns out to be non-entangled if and only if the number of non-zero coefficients in the Schmidt decomposition of this state equals 1, *(ii)* the state is non-entangled if and only if the von Neumann entropy of the partial density matrix associated with both particles is equal to zero. (For more exhaustive discussion about entanglement of two particles see, for instance, [20].)

These statements have clear physical meaning: *(i)* the first refers to the possibility of attributing to each particle a complete set of eigenstates associated with the considered set of observables, *(ii)* the second ensures the complete and exhaustive information allowed by the quantum theory about situation of each constituent. For clarity, in factorized state $|\Psi(1.2)\rangle$, each particle is described by well-defined state vectors $|\Psi(1)\rangle$ and $|\Psi(2)\rangle$, and the reduced density operator for one of the two particles, for example, the one labelled 1, *i.e.* $\widehat{\rho}_1 = \mathrm{Tr}_2(|\Psi(1.2)\rangle\langle\Psi(1.2)|)$ is a projection operator onto a one dimension manifold. Correspondingly, its von Neumann entropy $S(\widehat{\rho}_1) = -\mathrm{Tr}(\widehat{\rho}_1 \log_2 \widehat{\rho}_1)$ equals zero since the von Neumann entropy measures the lack of information about the single-particle subsystem and there is no uncertainty concerning the state attributed to it.

2.2. Slater rank for system of two indistinguishable fermions

Considering systems composed of two identical particles, due to the symmetrization requirement of the vector state $|\Psi(1.2)\rangle$, one should pay particular attention to interpretation of criteria for determining whether a state is entangled. These criteria are both the Slater number and the von Neumann entropy of the reduced density operator [10, 19]. They are considered for systems of two fermions represented by two nucleons when each nucleon is described in a finite-dimensional single-particle Hilbert space.

The total Hilbert space H for system of two identical fermions sharing an n-dimensional single-particle space H_n is

$$H = \widehat{A}(H_n \otimes H_n)\,, \tag{1}$$

where $\widehat{A}$ denotes the antisymmetrization operator. A general state vector $|\Psi(1,2)\rangle \in H$ can be written as

$$|\Psi(1,2)\rangle = \sum_{i,j=1;i\neq j}^{n} c_{ij}\,|i(1)\rangle\,|j(2)\rangle\ , \tag{2}$$

where $|i(k)\rangle$, $|j(k)\rangle$ are orthonormal basis states to expand the space H_n and index $k = 1,2$ is used to enumerate the particles. Under a unitary transformation of the single-particle states

$$|i(k)\rangle \longmapsto \left|i'(k)\right\rangle = \sum_{j=1}^{n} U_{ji'}\,|j(k)\rangle\ , \tag{3}$$

a matrix $C = [c_{ij}]_{n\times n}$, defined by expansion coefficients c_{ij} of state (2), transforms in such a way that $C' = UCU^{\mathrm{T}}$ (where U^{T} is transpose of U) takes a block diagonal form [9, 10] containing blocks of the type

$$Z_i = \begin{bmatrix} 0 & z_i \\ -z_i & 0 \end{bmatrix}, \tag{4}$$

i.e.

$$C^{'} = \mathrm{diag}[Z_1, \ldots, Z_r, Z_0]\,, \tag{5}$$

where $z_i > 0$ for $i \in \{1,\ldots,r\}$, and Z_0 is the $(n-2r)\times(n-2r)$ null matrix. Each 2×2 block Z_i corresponds to an elementary Slater determinant. Thus, when expressed in such a basis, the state $|\Psi(1,2)\rangle$ of Eq. (2) is a sum of elementary Slater determinants where each single-particle basis state occurs at most in one term. These elementary Slater determinants are the analogues of product states of the Schmidt decomposition of systems consisting of two distinguishable parties. A minimum number r of elementary Slater determinants Z_i in Eq. (5) replaces the Schmidt rank for the distinguishable parties. It is called the fermionic Slater rank of $|\Psi 1,2)\rangle$ and expansion (5) is called a Slater decomposition of $|\Psi(1,2)\rangle$ [9]. Analogously to the Schmidt criterion, a pure state of two identical fermions at short distance is entangled if and only if Slater rank $r > 1$.

3. The von Neumann entropy

If a quantum system is described by the density operator

$$\widehat{\rho} = |\Psi(1.2)\rangle \langle\Psi(1.2)| \ , \tag{6}$$

its von Neumann entropy $S(\widehat{\rho})$ is defined as

$$S(\widehat{\rho}) = -\mathrm{Tr}\,(\widehat{\rho}\log_2\widehat{\rho}) \ . \tag{7}$$

(In what follows, the logarithm base will be omitted.) By employing the spectral decomposition of $S(\widehat{\rho})$, we obtain that

$$S(\widehat{\rho}) = -\sum_{i=1}^{k} \lambda_i \log \lambda_i \, , \tag{8}$$

where numbers $\lambda_i, i = 1, \ldots, k$ are the eigenvalues of the density operator $\widehat{\rho}$.

Given a density operator $\widehat{\rho}$ of a pure state of two distinguishable particles, we define the reduced density operators $\widehat{\rho}_1 = \mathrm{Tr}_2(\widehat{\rho})$ and $\widehat{\rho}_2 = \mathrm{Tr}_1(\widehat{\rho})$, where the partial trace has been taken over one subsystem, either 1 or 2. Eqations (6)–(8) indicate that the von Neumann entropy ensures complete information allowed by the quantum theory about constituents of bipartite pure states.

Considering a system of two indistinguishable fermions, it is no matter over which subsystem, 1 or 2, we perform tracing since the state $|\Psi(1,2)\rangle$ is antisymmetric under the exchange of the two particles. Its density operator (6) is a symmetric operator and the reduced density operators of the two particles are equal, *i.e.* $\widehat{\rho}_1 = \mathrm{Tr}_2(\widehat{\rho}) = \widehat{\rho}_2 = \mathrm{Tr}_1(\widehat{\rho})$. Then, the von Neumann entropy of the reduced density operator for two indistinguishable particles is

$$S(\widehat{\rho}_{1\,\mathrm{or}\,2}) = -\mathrm{Tr}(\widehat{\rho}_1 \log \widehat{\rho}_1) = -\mathrm{Tr}(\widehat{\rho}_2 \log \widehat{\rho}_2) \, . \tag{9}$$

As we already stated, the von Neumann entropy for disentangled, pure states of two distinguishable particles takes its minimum value $S_{\min}(\widehat{\rho}) = 0$ (Schmidt rank $r = 1$). On the contrary, for disentangled, pure states of two fermions $S_{\min}(\widehat{\rho}) = 1$ (Slater rank $r = 1$). Moreover, in the case of two identical bosons, the minimum of the analogous quantity is null. These problematic issues suggest at first glance that the von Neumann entropy is inappropriate measure of entanglement because it gives different values for non-entangled distinguished particle states, non-entangled fermion states and non-entangled boson states, respectively [10, 19, 21]. However, taking into account the real meaning of the von Neumann entropy as a measure of the uncertainty about the state of a quantum system allows us to explain this

puzzling situation. To illustrate it, let us consider similarly as in Ref. [20] a state $|\Psi(1,2)\rangle$ with Slater rank equal to 1, *i.e.* a non-entangled state

$$|\Psi(1,2)\rangle = \frac{1}{\sqrt{2}}\Big(|1\rangle_1 \otimes |2\rangle_2 - |2\rangle_1 \otimes |1\rangle_2 \Big) . \tag{10}$$

In this situation, we can attribute definite states $|1\rangle$ or $|2\rangle$ to the particles. But, since they are indistinguishable, we cannot know which particle is associated to the state $|1\rangle$ or to the state $|2\rangle$. As a consequence, the von Neumann entropy $S(\widehat{\rho}_{1\,\mathrm{or}\,2}) = 1$ measures the uncertainty concerning the quantum state to attribute to each of the two identical subsystems. So, quantum correlations related only to the antisymmetrization of the state of identical fermions cannot be considered as a manifestation of entanglement.

If we consider an entangled state, *i.e.* a state with Slater rank $r > 1$, the von Neumann entropy of the associated reduced density operator turns out to be greater than 1. In this case, we cannot say that one particle is in state $|1\rangle$ and one in state $|2\rangle$ (contrary to the situation described by Eq. (10)). Besides, the greater value of the von Neumann entropy, the greater lack of information about considered system and, consequently, the greater entanglement of a given quantum state. Therefore, in this sense, the von Neumann entropy is considered as the measure of entanglement of composite quantum systems. If the density operator $\widehat{\rho}$ acts in an n-dimensional Hilbert space, then $1 \leq S(\widehat{\rho}) \leq S(\widehat{\rho})_{\max}$, where $S(\widehat{\rho})_{\max} = \log n$. To get a better insight how much the considered state is entangled, we proposed in Ref. [11] the factor

$$\eta(\widehat{\rho}_1) = \frac{S(\widehat{\rho}_1) - \log 2}{\log n - \log 2} . \tag{11}$$

This factor, $0 < \eta(\widehat{\rho}_1) \leq 1$, determines a fraction of the maximum value of entanglement ($S_{\max} = \log n, n > 2$) deposited in a given state.

In the next section, we will employ the von Neumann entropy of Eq. (9) to quantify the entanglement of the $1p0f$-shell nucleon pairs.

4. The entanglement of nucleon pairs — results of calculations

A nucleon pair can be compounded of two nucleons occupying the same single-particle orbit nlj (a single-particle orbit is specified by the n-main, l-orbital and j-spin quantum numbers) or occupying different orbits $n_1l_1j_1$ and $n_2l_2j_2$. In the $1p0f$ shell, there are four single-nucleon orbits: $1p\frac{1}{2}$, $1p\frac{3}{2}, 0f\frac{5}{2}$ and $0f\frac{7}{2}$ which can also be indicated clearly by the spin j only. In these orbits, we can construct 30 pairs for each total isospin $T = 0, 1$. The total angular momentum J of these pairs is ranging from 0 up to 7 (see Tables V and VI).

To study the entanglement of nucleon pairs in the $1p0f$ shell, we will employ the same formalism as in our previous paper [11] concerning the entanglement of nucleon pairs in the $1s0d$ shell. For the reader's convenience, this formalism is included in Appendixes A–D.

In the first step, we will consider the entanglement of nucleon pairs in states $|\Psi_{JmT\tau}(1,2)\rangle$ specified by spin–isospin angular momenta JT and their projections $m\tau$.

A set of $(2J+1)(2T+1)$ such states defines a basis to expand two-nucleon rotationally invariant states specified only by the spin–isospin JT quantum numbers. In the second step, we will discuss the entanglement of two-nucleon spin–isospin JT rotationally invariant states.

Rotationally invariant states with isospin $T=0$ describe proton–neutron pairs. Rotationally invariant states with total isospin $T=1$ describe a superposition of proton–proton (p–p), proton–neutron (p–n) and neutron–neutron (n–n) states. To consider the entanglement of the p–n, p–n and n–n pairs separately in the $T=1$ states, we will in the third step exploit states which are rotationally invariant only in the spin J space, *i.e.* $|\Psi_{JT=1\tau}(1,2)\rangle$ states (where $\tau=+1,0,-1$ in the case of p–p, p–n, and n–n pairs, respectively).

We will calculate the von Neumann entropy for all considered states of nucleon pairs according to the method stressed in Section 3. The matrices C for these states are made from elements c_{pq} calculated according to formulas given in Appendix A for states $|\Psi_{JmT\tau}(n_1l_1j_1,n_2l_2j_2)\rangle$, in Appendix B, for spin–isospin JT rotationally invariant states $|\Psi_{JT}(n_1l_1j_1,n_2l_2j_2)\rangle$ and in Appendix C, for spin J rotationally invariant states $|\Psi_{JT\tau}(n_1l_1j_1,n_2l_2j_2)\rangle$, respectively. We will use these matrices to calculate the reduced density matrices ρ_1 (see Appendix D). The order of density matrix $\rho_1 = CC^\dagger$ is equal to the number of its eigenvalues $\lambda_i > 0$ (note that eigenvalues appear pairwise). We assume that the order of a given density matrix ρ_1 determines only the number of eigenvalues $\lambda_i \geq 0.00001$. Values of $\lambda_i < 0.00001$ are random ones which arise due to the accuracy of numerical operations and, practically, do not affect the values of the von Neumann entropy (9). To verify a correctness of our calculations, we have also performed the Slater decomposition of the matrices C into block matrices C' (Eq. (5)).

Results of calculations for selected spin–isospin $m\tau$-dependent states, for spin–isospin JT rotationally invariant and spin J rotationally invariant states, respectively, are presented in the next subsections.

4.1. Selected states $|\Psi_{JmT\tau}(1,2)\rangle$

4.1.1. The $j_1 = j_2$ case

As an example, let us consider the entanglement of states $|\Psi_{J=3mT=0}(0f_{5/2}, 0f_{5/2})\rangle$. From results stored in Table I, we see that states corresponding to all m projections are almost maximally entangled ($\eta(\widehat{\rho}_1)$ factor of Eq. (11) is ≥ 0.814). However, due to the interference of m-projected states, the amount of entanglement in the rotationally invariant state $|\Psi_{J=3T=0}(0f_{5/2}, 0f_{5/2})\rangle$ is reduced to the value of $\eta(\widehat{\rho}_1) = 0.624$.

TABLE I

Description of the entanglement of the $|\Psi_{J=3mT=0\tau}(0f_{5/2}0f_{5/2})\rangle$ states. The columns list the spin–isospin projections $m\tau$, Slater rank r, von Neumann entropy of the reduced density matrix $S(\rho_1)$, maximum value of the von Neumann entropy $S_{\max}$ and factor $\eta(\rho_1)$ (Eq. (11)), respectively.

m	τ	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
$3, -3$	0	3	2.547	2.585	0.976
$2, -2$	0	4	2.650	3	0.825
$1, -1$	0	5	2.892	3.322	0.814
0	0	6	3.434	3.585	0.942

Let us now consider the entanglement for selected example of $T = 1$ states, namely for $|\Psi_{J=2mT=1\tau}(1p_{3/2}, 1p_{3/2})\rangle$ states. From data collected in Table II, it is seen that for $(m, \tau) = (2,1), (2,-1), (-2,1), (-2,-1), (1,1), (1,-1).(-1,1)$ and $(-1,-1)$, projected states (see Eq. (19) of Appendix A) Slater rank $r = 1$ and von Neumann entropy $S(\widehat{\rho}_1) = 1$. So, each such state is represented by only one elementary Slater determinant and is disentangled. Other $m\tau$ projected states are maximally entangled, $\eta(\widehat{\rho}_1) = 1$. However, the rotationally invariant state $|\Psi_{J=2T=1}(1p_{3/2}, 1p_{3/2})\rangle$ superposed from states $|\Psi_{J=2mT=1\tau}(1p_{3/2}, 1p_{3/2})\rangle$ is weakly entangled, $\eta(\widehat{\rho}_1) = 0.134$.

TABLE II

The same as in Table I but for the $|\Psi_{J=2mT=1\tau}(1p_{3/2}1p_{3/2})\rangle$ state.

m	τ	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
$2, -2$	$1, -1$	1	1	1	0
$2, -2$	0	2	2	2	1
$1, -1$	$1, -1$	1	1	1	0
$1, -1$	0	2	2	2	1
0	$1, -1$	2	2	2	1
0	0	4	3	3	1

4.1.2. The $j_1 \neq j_2$ case

In Table III, there are stored results for the $|\Psi_{J=3mT=0}(1p_{3/2}0f_{5/2})\rangle$ states. For all m projections, they are strongly entangled ($\eta(\widehat{\rho}_1) \geq 840$). The corresponding, rotationally invariant $JT = 30$ state composed from m projected states is, due to their interference, less entangled ($\eta(\widehat{\rho}_1) = 0.712$). Similar situation is observed in the case of the $|\Psi_{J=1mT=1\tau}(0f_{5/2}, 0f_{7/2})\rangle$ states (Table IV). Namely, all $m\tau$ states are strongly entangled ($\eta(\widehat{\rho}_1) \geq 0.835$) and entanglement of corresponding rotationally invariant state is characterized by the factor $\eta(\widehat{\rho}_1) = 0.668$.

TABLE III

The same as in Table I but for the $|\Psi_{J=3mT=0\tau}(1p_{3/2}0f_{5/2})\rangle$ state.

m	τ	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
$3, -3$	0	4	2.954	3	0.977
$2, -2$	0	6	3.325	3.585	0.899
$1, -1$	0	8	3.519	4	0.840
0	0	8	3.971	4	0.990

TABLE IV

The same as in Table I but for the $|\Psi_{J=1mT=1\tau}(0f_{5/2}0f_{7/2})\rangle$ state.

m	τ	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
$1, -1$	$1, -1$	6	3.159	3.585	0.835
$1, -1$	0	12	4.159	4.585	0.881
0	$1, -1$	6	3.531	3.585	0.979
0	0	12	4.531	4.585	0.984

4.2. Spin–isospin JT rotationally invariant states $|\Psi_{JT}(1,2)\rangle$

In the full $1p0f$ shell, nucleons occupy $1p\frac{1}{2}, 1p\frac{3}{2}$ $0f\frac{5}{2}$ and $0f\frac{7}{2}$ levels. This gives in the $1p0f$ shell 30 two-nucleon pairs for each total isospin $T = 0, 1$. Similarly as in the $1s0d$ shells, a majority of the isospin $T = 0$ rotationally invariant states are strongly entangled. For twenty four states from thirty such states in the $1p0f$ shell, the factor $\eta(\rho_1)$ of Eq. (11) is larger than 0.6. But, in the case of thirty $T = 1$ rotationally invariant states, only for eight states $\eta(\rho_1) > 0.6$. The rotationally invariant $JT = 0$ states (*i.e.* spin J and isospin $T = 0$ states) describe p–n pairs. Rotationally invariant $JT = 1$ states (*i.e.* spin J and isospin $T = 1$ states) are a superposition of p–p ($\tau = 1$), p–n ($\tau = 0$) and n–n ($\tau = -1$) pairs. The fact that dominating part of the $JT = 1$ rotationally invariant states is less entangled than $JT = 0$

states is a consequence of a destructive interference of the p–p pairs and n–n pairs with the p–n pairs. Results stored in Tables V and VI describe the entanglement of rotationally invariant isospin $T = 0$ and isospin $T = 1$ states.

TABLE V

Description of the entanglement of the isospin $T = 0$ rotationally invariant states $|\Psi_{JT}(n_1 l_1 j_1, n_2 l_2 j_2)\rangle$. The columns list the spin J of pairs, orbits of nucleons $n_i l_i j_i$ ($i = 1, 2$, Slater rank r, von Neumann entropy of the reduced density matrix $S(\rho_1)$, maximum value of the von Neumann entropy $S_{\max}(\rho_1)$ and factor $\eta(\rho_1)$ (Eq. (11)), respectively.

$T = 0$												
J	$n_1 l_1 j_1$	$n_1 l_1 j_1$	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$	J	$n_1 l_1 j_1$	$n_1 l_1 j_1$	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
1	$1p\frac{1}{2}$	$1p\frac{1}{2}$	2	1.872	2	0.187	3	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	3.135	4	0712
1	$1p\frac{1}{2}$	$1p\frac{3}{2}$	4	2.833	3	0.917	3	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	3.425	4	0.808
1	$1p\frac{3}{2}$	$1p\frac{3}{2}$	4	2.554	3	0.777	3	$0f\frac{5}{2}$	$0f\frac{5}{2}$	6	2.612	3.585	0.624
1	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	3.689	4	0.896	3	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.904	4.585	0.810
1	$0f\frac{5}{2}$	$0f\frac{5}{2}$	6	3.249	3.585	0.870	3	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	3.225	4	0.742
1	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	4.209	4.585	0.895	4	$1p\frac{1}{2}$	$0f\frac{7}{2}$	4	2.386	3	0.693
1	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	3.708	4	0.903	4	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	2.634	4	0.545
2	$1p\frac{1}{2}$	$1p\frac{3}{2}$	4	2.308	3	0.654	4	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	3.157	4	0.719
2	$1p\frac{1}{2}$	$0f\frac{5}{2}$	4	2.729	3	0.864	4	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.646	4.585	0.738
2	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	3.486	4	0.829	5	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	2.694	4	0.565
2	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	3.484	4	0.828	5	$0f\frac{5}{2}$	$0f\frac{5}{2}$	6	1.767	3.585	0.297
2	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	4.132	4.585	0.847	5	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.330	4.585	0.650
3	$1p\frac{1}{2}$	$0f\frac{5}{2}$	4	2.358	3	0.679	5	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	2.733	4	0.578
3	$1p\frac{1}{2}$	$0f\frac{7}{2}$	4	2.671	3	0.835	6	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	2.848	4.585	0.516
3	$1p\frac{3}{2}$	$1p\frac{3}{2}$	4	1.531	3	0.265	7	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	1.945	4	0.315

4.3. Spin J rotationally invariant states $|\Psi_{JT\tau}(1,2)\rangle$

The rotationally invariant $JT = 0$ states describe p–n pairs whilst rotationally invariant $JT = 1$ states describe a superposition of p–p ($\tau = 1$), p–n ($\tau = 0$) and n–n ($\tau = -1$) pairs. The rotationally invariant $JT = 0$ states and $JT = 1\tau = 0$ states describe p–n pairs. These states for fixed spin J and fixed orbits $n_1 l_1 j_1, n_2 l_2 j_2$ are the same since the Clebsch–Gordan coefficient $\langle \frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2} \mid 00\rangle = \langle \frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2} \mid 10\rangle$. Consequently, in this case, the entanglement of rotationally invariant $JT = 0$ states and $JT = 1\tau = 0$ states takes the same value. Noticeable is also that regardless of whether nucleons occupy the same ($n_1 l_1 j_1 = n_2 l_2 j_2$) or different ($n_1 l_1 j_1 \neq n_2 l_2 j_2$) orbits, the n–n and p–p pairs in the $JT = 1\tau = \pm 1$ states are less entangled than the p–n pairs in the corresponding $JT = 1\tau = 0$ states. In Table VII, there are collected selected data which illustrate described above properties.

TABLE VI

The same as in Table V but for the isospin $T = 1$ states.

$T = 1$													
J	$n_1l_1j_1$	$n_1l_1j_1$	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$	J	$n_1l_1j_1$	$n_1l_1j_1$	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
0	$1p\frac{1}{2}$	$1p\frac{1}{2}$	2	1.187	2	0.187	3	$1p\frac{1}{2}$	$0f\frac{5}{2}$	4	1.545	3	0.273
0	$1p\frac{3}{2}$	$1p\frac{3}{2}$	4	2.187	3	0.594	3	$1p\frac{1}{2}$	$0f\frac{7}{2}$	4	1.858	3	0.429
0	$0f\frac{5}{2}$	$0f\frac{5}{2}$	6	2.772	3.585	0.686	3	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	2.323	4	0.441
0	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	3.187	4	o.729	3	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	2.613	4	0.538
1	$1p\frac{1}{2}$	$1p\frac{3}{2}$	4	2.021	3	0.510	3	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.092	4.585	0.583
1	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	2.876	4	0.626	4	$1p\frac{1}{2}$	$0f\frac{7}{2}$	4	1.573	3	0.287
1	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.396	4.585	0.668	4	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	1.821	4	0.274
2	$1p\frac{1}{2}$	$1p\frac{3}{2}$	4	1.495	3	0.247	4	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	2.344	4	0.448
2	$1p\frac{1}{2}$	$0f\frac{5}{2}$	4	1.916	3	0.458	4	$0f\frac{5}{2}$	$0f\frac{5}{2}$	6	1.453	3.585	0.175
2	$1p\frac{3}{2}$	$1p\frac{3}{2}$	4	1.269	3	0.134	4	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	2.833	4.585	0.511
2	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	2.673	4	0.558	4	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	2.178	4	0.393
2	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	2.672	4	0.557	5	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	1.882	4	0.294
2	$0f\frac{5}{2}$	$0f\frac{5}{2}$	6	2.114	3.585	0.431	5	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	2.517	4.585	0.423
2	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.320	4.585	0.647	6	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	2.036	4.585	0.289
2	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	2.654	4	0.551	6	$0f\frac{7}{2}$	$0f\frac{7}{2}$	8	1.608	4	0.203

5. Summary

Results presented in Tables I–IV indicate that, in general, isospin $T = 0$ and $T = 1$ states $|\Psi_{JmT\tau}(n_1l_1j_1, n_2l_2j_2)\rangle$ are strongly entangled. However, for some $m\tau$ projections, there are disentangled states. For instance, states $|\Psi_{J=2mT=1\tau}(1p_{3/2}1p_{3/2})\rangle$ with projections $(m\tau) = (2,1), (2,-1), (-2,1), (-2,-1), (1,1), (1,-1), (-1,1), (-1,-1)$ are disentangled and they are represented by one Slater determinant (see Table II). On the contrary, similarly as in the case of $1s0d$ shell [11], all rotationally invariant states $|\Psi_{JT}(n_1l_1j_1, n_2l_2j_2)\rangle$ are entangled (Tables V–VI). This is so, since rotationally invariant states are a superposition of the $m\tau$-dependent, entangled and disentangled states.

Majority of the isospin $T = 0$ rotationally invariant states are strongly entangled. For twenty two out of thirty such states in the $1p0f$ shell, the factor $\eta(\rho_1) > 0.6$. But, in the case of thirty $T = 1$ rotationally invariant states, only for five states $\eta(\rho_1) > 0.6$. The rotationally invariant $JT = 1$ states are a superposition of p–p, p–n and n–n states, therefore, one can infer that in these states, a destructive interference of n–n and p–p states with n–p states reduces the entanglement of p–n pairs observed in the $JT = 0$ states.

Spin J rotationally invariant states with well-defined isospin $T = 1$ and projection $\tau = 1, 0, -1$ describe p–p, p–n, n–n pairs, respectively. For all such states, p–p and n–n pairs are less entangled than p–n pairs (see

TABLE VII

Description of the entanglement of selected spin J rotationally invariant $|\Psi_{JT=1\tau}(n_1l_1j_1, n_2l_2j_2)\rangle$ states in the $1p0f$ shell. The columns list the spin J, isospin projections τ, specification of nucleon orbits $n_il_ij_i$ $(i = 1, 2)$, Slater rank r, von Neumann entropy of the reduced density matrix $S(\rho_1)$, maximum value of the von Neumann entropy $S_{\max}$ and factor $\eta(\rho_1)$ (Eq. (11)), respectively.

$T = 1$							
J	τ	$n_1l_1j_1$	$n_2l_2j_2$	r	$S(\rho_1)$	$S_{\max}$	$\eta(\rho_1)$
1	$1, -1$	$1p\frac{1}{2}$	$1p\frac{3}{2}$	2	1.833	2	0.833
1	0	$1p\frac{1}{2}$	$1p\frac{3}{2}$	4	2.833	3	0.917
1	$1, -1$	$1p\frac{3}{2}$	$0f\frac{5}{2}$	4	2.689	3	0.845
1	0	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	3.689	4	0.896
1	$1, -1$	$0f\frac{5}{2}$	$0f\frac{7}{2}$	6	3.209	3.585	0.854
1	0	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	4.209	4.585	0.895
2	$1, -1$	$1p\frac{1}{2}$	$1p\frac{3}{2}$	2	1.307	2	0.307
2	0	$1p\frac{1}{2}$	$1p\frac{3}{2}$	4	2.307	3	0.654
2	$1, -1$	$1p\frac{1}{2}$	$0f\frac{5}{2}$	2	1.729	2	0.729
2	0	$1p\frac{1}{2}$	$0f\frac{5}{2}$	4	2.729	3	0.864
2	$1, -1$	$1p\frac{3}{2}$	$0f\frac{5}{2}$	4	2.486	3	0.743
2	0	$1p\frac{3}{2}$	$0f\frac{5}{2}$	8	3.486	4	0.829
2	$1, -1$	$1p\frac{3}{2}$	$0f\frac{7}{2}$	4	2.484	3	0.742
2	0	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	3.484	4	0.828
3	$1, -1$	$1p\frac{1}{2}$	$0f\frac{5}{2}$	2	1.358	2	0.358
3	0	$1p\frac{1}{2}$	$0f\frac{5}{2}$	4	2.358	3	0.679
3	$1, -1$	$1p\frac{1}{2}$	$0f\frac{7}{2}$	2	1.671	2	0.671
3	0	$1p\frac{1}{2}$	$0f\frac{7}{2}$	4	2.671	3	0.835
4	$1, -1$	$1p\frac{1}{2}$	$0f\frac{7}{2}$	2	1.386	2	0.386
4	0	$1p\frac{1}{2}$	$0f\frac{7}{2}$	4	2.386	3	0.693
4	$1, -1$	$1p\frac{3}{2}$	$0f\frac{7}{2}$	4	2.157	3	0.578
4	0	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	3.157	4	0.719
5	$1, -1$	$1p\frac{3}{2}$	$0f\frac{7}{2}$	4	1.694	3	0.347
5	0	$1p\frac{3}{2}$	$0f\frac{7}{2}$	8	2.694	4	0.565
5	$1, -1$	$0f\frac{5}{2}$	$0f\frac{7}{2}$	6	2.330	3.585	0.514
5	0	$0f\frac{5}{2}$	$0f\frac{7}{2}$	12	3.330	4.585	0.650

Table VII). This is due to the fact that wave functions of p–n pairs are made from more interfering terms than wave functions of n–n and p–p pairs (see Eqs. (12), (13), (25)). Besides, the entanglement of $JT = 1\tau = 0$ states is larger than entanglement of rotationally invariant $JT = 1$ states (see Tables VI and VII).

The entanglement of the $JT = 0$ rotationally invariant states and entanglement of p–n pairs in corresponding $JT = 1\tau = 0$ states is the same (see Tables V and VII) since in both cases wave functions are the same (see Eqs. (12), (13), (22), (25) and notice that the Clebsch–Gordan coefficient $\langle \frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2} \mid 00\rangle = \langle \frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2} \mid 10\rangle$).

Nucleon pairs are building blocks to expand wave functions for many-nucleon systems governed by many-body Hamiltonian. Taking into account that nucleon pairs, particularly the $T = 0$ pairs, are strongly entangled, one can expect that many-nucleon pure, stationary states of the $1p0f$-shell nuclei are strongly entangled.

Appendix A

The $|\Psi_{JmT\tau}(1,2)\rangle$ states

If nucleons occupy the same single-particle orbit nlj, the wave function of a nucleon pair in a state specified by the spin–isospin angular momenta quantum numbers JT and their projections $m\tau$ is written as

$$\begin{aligned} |\Psi_{JmT\tau}(1,2)\rangle \;=\; & \sum_{m_1 m_2 \tau_1 \tau_2} \langle jm_1 jm_2 |\, Jm\rangle \\ & \times \left\langle \tfrac{1}{2}\tau_1 \tfrac{1}{2}\tau_2 \right| T\tau\rangle \\ & \times |\Psi_{nljm_1\tau_1}(1)\rangle\, |\Psi_{nljm_2\tau_2}(2)\rangle \;, \end{aligned} \tag{12}$$

where $\ldots \mid \ldots\rangle$ are spin and isospin Clebsch–Gordan coefficients, $|\Psi_{nljm_i\tau_i}(i)\rangle$ is a wave function of a nucleon $i = 1, 2$ and m_i, τ_i are projection quantum numbers of the spin j and isospin $(= \frac{1}{2})$, respectively. Since the wave function of two fermions has to be antisymmetric, the spin J and isospin T angular momenta of a nucleon pair fulfil the condition $(-1)^{2j+1-J-T} = -1$. Because $2j + 1$ is even, this condition implies that $J + T$ is odd.

If nucleons occupy different orbits $n_1 l_1 j_1$ and $n_2 l_2 j_2$, the wave function of a nucleon pair reads

$$\begin{aligned} |\Psi_{JmT\tau}(1,2)\rangle \;=\; & \frac{1}{\sqrt{2}} \sum_{m_1 m_2 \tau_1 \tau_2} \langle j_1 m_1 jm_2 |\, Jm\rangle \\ & \times \left\langle \tfrac{1}{2}\tau_1 \tfrac{1}{2}\tau_2 \right| T\tau\rangle \\ & \times [|\Psi_{n_1 l_1 j_1 m_1 \tau_1}(1)\rangle\, |\Psi_{n_2 l_2 j_2 m_2 \tau}(2)\rangle + \\ & - |\Psi_{n_1 l_1 j_1 m_1 \tau_1}(2)\rangle\, |\Psi_{n_2 l_2 j_2 m_2 \tau_2}(1)\rangle] \,. \end{aligned} \tag{13}$$

States of equations (12) and (13) can be expressed as

$$|\Psi_{JmT\tau}(1,2)\rangle = \sum_{p \neq q} c_{pq}\, |\Psi_p(1)\rangle\, |\Psi_q(2)\rangle \;, \tag{14}$$

where states $|\Psi_p(1)\rangle = |\Psi_{n_p l_p j_p m_p \tau_p}(1)\rangle$ and $|\Psi_q(2)\rangle = |\Psi_{n_q l_q j_q m_q \tau_q}(2)\rangle$ define the n-dimensional single-nucleon basis in considered shell. Besides, for states of Eq. (12) (*i.e.* if $j_p = j_q$),

$$\begin{aligned} c_{pq} &= \langle j_p m_p j_q m_q | \, Jm \rangle \left\langle \tfrac{1}{2}\tau_p \tfrac{1}{2}\tau_q \right| T\tau \rangle \,, \\ c_{qp} &= (-1)^{j_p + j_q + 1 - J - T} c_{pq} = -c_{pq} \,, \end{aligned} \tag{15}$$

and for states of Eq. (13) (*i.e.* if $j_p \neq j_q$),

$$c_{pq} = -c_{qp} = \frac{1}{\sqrt{2}} \langle j_p m_p j_q m_q | \, Jm \rangle \left\langle \tfrac{1}{2}\tau_p \tfrac{1}{2}\tau_q \right| T\tau \rangle \,. \tag{16}$$

Coefficients c_{pq} of Eq. (14) define an antisymmetric matrix $C = [c_{pq}]_{n\times n}$. Given a density operator for nucleon pairs

$$\widehat{\rho} = |\Psi_{JmT\tau}(1,2)\rangle \langle \Psi_{JmT\tau}(1,2)| \,, \tag{17}$$

we can calculate the reduced density operator $\widehat{\rho}_1 = \mathrm{Tr}_2(\widehat{\rho}) = \mathrm{Tr}_1(\widehat{\rho})$ for the subsystem represented by a nucleon, either 1 or 2. Its matrix representation can also be obtained with the aid of matrix C as follows (see Appendix D)

$$\rho_1 = CC^\dagger \,, \tag{18}$$

where $C^\dagger$ is the Hermitian conjugate of C. Then, solving the eigenvalue problem of ρ_1, we can calculate the von Neumann entropy according to Eq. (8). From the property $\langle j_1 m_1 j_2 m_2 | jm \rangle = (-1)^{j_1 + j_2 - j} \langle j_1 - m_1 j_2 - m_2 | j - m \rangle$ of the Clebsch–Gordan coefficients applied to coefficients c_{pq} of Eqs. (15) and (16), one can deduce that the reduced density matrix ρ_1 (Eq. (18)) has the following property:

$$\begin{aligned} \rho_1 &= \rho_1(M_J, M_T) = \rho_1(-M_J, M_T) = \rho_1(M_J, -M_T) \\ &= \rho_1(-M_J, -M_T) \,. \end{aligned} \tag{19}$$

Since states (12) and (13) have well-defined projections $m\tau$ of the spin–isospin angular momenta JT, therefore, their entanglement measured by the von Neumann entropy is $m\tau$-dependent. Due to the property $S(\widehat{\rho}) = S(U\widehat{\rho}U^\dagger)$ with U being a unitary transformation (note that $S(\widehat{\rho})$ depends only on the eigenvalues of $\widehat{\rho}$ which are basis-independent), the von Neumann entropy remains unchanged for given $m\tau$ projections, even if we express the density operator $\widehat{\rho}$ in a new basis obtained by the unitary transformation.

Appendix B

Spin–isospin JT rotationally invariant states $|\Psi_{JT}(1,2)\rangle$

Set of $(2J+1)(2T+1)$ states of Eqs. (12) and (13) defines the basis to expand any two-nucleon state $|\Psi_{JT}(1,2)\rangle$ which has well-defined spin–isospin angular momenta JT, namely

$$|\Psi_{JT}(1,2)\rangle = \sum_{m=-J}^{J} \sum_{\tau=-T}^{T} a_{m\tau} \, |\Psi_{JmT\tau}(1,2)\rangle \ , \tag{20}$$

where $a_{m\tau}$ are expansion coefficients satisfying the normalization condition $\sum_{m\tau} |a_{m\tau}|^2 = 1$. In this expansion, quantum numbers n, l, j are fixed for both particles, so coefficients $a_{m\tau}$ do not depend on these quantum numbers. Substituting for the coefficients

$$a_{m\tau} = \frac{1}{\sqrt{(2J+1)(2T+1)}} \, , \tag{21}$$

state (20) takes the averaged form of all substates $|\Psi_{JmT\tau}(1,2)\rangle$, *i.e.*

$$|\Psi_{JT}(1,2)\rangle = \frac{1}{\sqrt{(2J+1)(2T+1)}} \sum_{m=-J}^{J} \sum_{\tau=-T}^{T} |\Psi_{JmT\tau}(1,2)\rangle \ . \tag{22}$$

State (22) like state (20) is rotationally invariant and thus $m\tau$-independent. Due to this property, the entanglement of nucleon pairs calculated with the aid of wave functions (22) is $m\tau$-independent. Now, the coefficients c_{pq} of Eqs. (15) and (16) are slightly modified and take the form:

(i) if $j_1 = j_2$

$$\begin{aligned} c_{pq} &= \frac{1}{\sqrt{(2J+1)(2T+1)}} \sum_{m,\tau} \langle j_p m_p j_q m_q | \, Jm \rangle \left\langle \tfrac{1}{2}\tau_p \tfrac{1}{2}\tau_q \right| T\tau \rangle \, , \\ c_{qp} &= (-1)^{j_p + j_q + 1 - J - T} c_{pq} = -c_{pq} \, , \end{aligned} \tag{23}$$

(ii) if $j_1 \neq j_2$

$$\begin{aligned} c_{pq} &= -c_{qp} = \frac{1}{\sqrt{2(2J+1)(2T+1)}} \sum_{m,\tau} \langle j_p m_p j_q m_q | \, Jm \rangle \\ &\quad \times \left\langle \tfrac{1}{2}\tau_p \tfrac{1}{2}\tau_q \right| T\tau \rangle \, . \end{aligned} \tag{24}$$

Appendix C

Spin J rotationally invariant states $|\Psi_{JT\tau}(1,2)\rangle$

Similarly as in Appendix B, the set of $(2J+1)$ states of Eqs. (12) and (13) defines the basis to expand a two-nucleon state in the $1p0f$ shell which is rotationally invariant in the spin J space. By a simple modification of the Eq. (22), we obtain

$$|\Psi_{JT\tau}(1,2)\rangle = \frac{1}{\sqrt{(2J+1)}} \sum_{m=-J}^{J} |\Psi_{JmT\tau}(1,2)\rangle \ . \tag{25}$$

States (25) are rotationally invariant in the J space and thus m-independent. Depending on the projection τ of the isospin T, they describe p–p ($\tau = 1$), p–n ($\tau = 0$) and n–n ($\tau = -1$) pairs, respectively.

To calculate the reduced density matrix ρ for states (25), we need to modify matrix elements c_{pq} of Eqs. (23) and (24).

We have:

(i) if $j_1 = j_2$

$$\begin{aligned} c_{pq} &= \frac{1}{\sqrt{(2J+1)}} \sum_{m} \langle j_p m_p j_q m_q | \, Jm \rangle \left\langle \tfrac{1}{2}\tau_p \tfrac{1}{2}\tau_q \middle| \, T\tau \right\rangle , \\ c_{qp} &= (-1)^{j_p + j_q + 1 - J - T} c_{pq} = -c_{pq} \, , \end{aligned} \tag{26}$$

(ii) if $j_1 \neq j_2$

$$\begin{aligned} c_{pq} &= -c_{qp} = \frac{1}{\sqrt{2(2J+1)}} \sum_{m} \langle j_p m_p j_q m_q | \, Jm \rangle \\ &\quad \times \left\langle \tfrac{1}{2}\tau_p \tfrac{1}{2}\tau_q \middle| \, T\tau \right\rangle . \end{aligned} \tag{27}$$

Appendix D

Reduced density matrix

For a general state of Eq. (2), a density operator is of the form of

$$\widehat{\rho} = |\Psi\rangle \langle \Psi| = \sum_{i,j=1;i\neq j}^{n} \sum_{k,l=1;k\neq l}^{n} c_{ij} c^{*}_{kl} \, |i(1)\rangle \, |j(2)\rangle \, \langle k(1)| \, \langle l(2)| \ . \tag{28}$$

Taking the partial trace over one subsystem, say subsystem 2 (since system under consideration is composed of two identical fermions, it is no matter which subsystem we select for tracing), the reduced density operator reads

$$\widehat{\rho}_1 = \sum_{m=1}^{n} \langle m(2)| \widehat{\rho} |m(2)\rangle = \sum_{i,k,m=1}^{n} c_{im} c^*_{km} |i(1)\rangle \langle k(1)| \tag{29}$$

and its matrix representation is

$$[\rho_1]_{ik} = \langle i(1)| \widehat{\rho}_1 |k(1)\rangle = \sum_{m=1}^{n} c_{im} c^*_{km} . \tag{30}$$

We can define the matrix $C = [c_{im}]_{n\times n}$ and $C^\dagger = [c^*_{mk}]^T_{n\times n}$. Then, we have

$$\rho_1 = CC^\dagger . \tag{31}$$

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