Efficient computation of matrix elements of generic Slater determinants

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We present an extension of the Löwdin strategy to find arbitrary matrix elements of generic Slater determinants. The new method applies to arbitrary number of fermionic operators, even in the case of a singular overlap matrix.

I. INTRODUCTION

Many developments in quantum many body physics require the efficient computation of matrix elements of fermionic operators between Slater determinant states. In many relevant cases, the matrix elements should be computed between Slater determinant states which are not based on the same set of single-body fermionic states. An early example of this kind of calculations can be found in the seminal paper by the Swedish physicist Per-Olov Löwdin [1] who developed in 1955 a very smart strategy, based on a careful application of the properties of the determinants. The strategy was developed in full for the case of two and four fermionic operators, and required the overlap matrix between the two Slater determinants to be non-singular [1]. Further developments, aimed to simplify the original complexity of the formulas and to facilitate their use in the framework of the valence bond theory, can be found in the literature [2, 3]. There are many applications in quantum chemistry requiring overlaps of operators between Slater determinant including Configuration Interaction (CI) and symmetry restoration methods (see Refs. [4–9] as an example). More recently Brouder [10] proposed a method to reduce the combinatorial complexity of Wick’s theorem to a more manageable algebraic complexity. As applications of the method, formulas for the overlap of a general product of creation and annihilation operators between arbitrary Slater determinants were proposed and used to compute, for instance, the generating function of the Green function or k-density correlation operators. The method uses general ideas coming from the world of quantum groups and Hopf algebras but leads to rather involved expressions. Slater determinants are also required in nuclear physics, in the framework of the Monte Carlo Shell Model (MCSM) [17, 18], or in the field of symmetry restored quasiparticle excitations [19, 20].

In all the above situations the matrix elements can be computed with the help of Wick’s theorem or its generalizations, but the number of contractions to consider grows with the factorial of the number of operators involved and therefore it becomes unmanageable very soon.

In this work we extend Löwdin’s results to the case of a generic number of fermionic operators in order to obtain compact and easily handled expressions prone to an efficient evaluation in a computer. In addition, the evaluation of hundreds of thousands, if not millions of operator overlaps, calls for robust evaluation methods capable to handle the cases of zero or nearly zero overlaps of the Slater determinants where Löwdin’s method becomes ill-defined. In our derivation we will use a second quantization formalism from the beginning, which makes calculations more transparent.

This article is organized as follows. Our generalized version of Löwdin’s theorem is described and proved in Sec. II. The case of zero overlap between both Slater determinants is discussed in Sec. III. A numerical application is provided in Sec. IV where our approach is used to estimate the entanglement of a block for a linear combination of Slater determinants. The article finishes with some conclusions and our proposals for further work.

II. GENERALIZED LöWDIN’S THEOREM

To start with, let us consider two generic Slater determinants

\[ |A\rangle = a^\dagger_i \cdots a^\dagger_{i_N} |\cdots\rangle, \]  
\[ |B\rangle = b^\dagger_{j_1} \cdots b^\dagger_{j_N} |\cdots\rangle. \]  

of \(N\) particles. The \(a^\dagger_i\) and \(b^\dagger_j\) are arbitrary creation operators with quantum numbers denoted by \(i\) and \(j\), respectively. Their hermitian conjugate annihilates the true Fock vacuum \(\{-\}\): 

\[ a_i |\cdots\rangle = b_j |\cdots\rangle = 0, \]  

of Wick contractions (see below), the required number of terms grows exponen-
and such that
\[ \{a_i^\dagger, b_j\} = S_{ij}, \]
(4)\[
\{a_i, b_j^\dagger\} = S_{ij}, \]
(5)
as well as
\[ \{a_i^\dagger, b_j^\dagger\} = 0. \]
(6)
The overlap matrix is defined by \( S_{ij} = \langle a_i | b_j \rangle = \langle a_i | b_j \rangle \). The overlap between both states, \( \langle A | B \rangle \) is evaluated in a recursive way:
\[ \langle A | B \rangle = \langle \cdots a_N a_1 b_1^\dagger \cdots b_N^\dagger | \rangle \]
(7)
\[ = -\langle \cdots a_N a_2 b_2^\dagger a_1 b_1^\dagger \cdots b_N^\dagger | \rangle \]
(8)
\[ + S_{11} \langle \cdots a_N a_2 b_2^\dagger \cdots b_N^\dagger | \rangle \]
(9)
by jumping with the \( b_1^\dagger \) creation operator over the \( a_1 \) annihilation one. The notation has been also simplified by replacing indexes \( i_1, \ldots, k \) by \( 1, \ldots, \). Let us now introduce the quantity
\[ \langle A | B \rangle_{[11]} = \langle \cdots a_N a_2 b_2^\dagger \cdots b_N^\dagger | \rangle, \]
(10)
that corresponds to the overlap of the two Slater determinants, but “removing the \( a_1 b_1^\dagger \) pair from \( \langle A | B \rangle \). Then,
\[ \langle A | B \rangle = S_{11} \langle A | B \rangle_{[11]} - S_{21} \langle A | B \rangle_{[21]} + \cdots \]
(11)
and the expansion ends after \( N \) jumps because \( \langle \cdots | b_1^\dagger \rangle = 0 \).
We easily recognize in \( \langle A | B \rangle_{[11]} \) the minor of \( S \) with respect to the matrix element \( (1, 1) \), i.e. \( S_{11} \). Viewed from this perspective, the expression of \( \langle A | B \rangle \) given in Eq. (11) becomes the minor expansion of the determinant of \( S \) by the first row, i.e.
\[ \langle A | B \rangle = \text{det}(S), \]
(12)
Let us now expand \( a_i^\dagger \) and \( b_j^\dagger \) in terms of a common basis \( \{c_k, k = 1, \ldots, N_B\} \)
\[ a_i^\dagger = \sum_{k=1}^{N_B} A_{ki} c_k^\dagger, \]
(13)
\[ b_j^\dagger = \sum_{k=1}^{N_B} B_{kj} c_k, \]
(14)
then the \( N \times N \) overlap matrix \( S \) becomes the product of the two expansion matrices, \( A \) and \( B \), of dimension \( N_B \times N \)
\[ S_{ij} = \sum_k A_{ki}^* B_{kj} = (A^\dagger B)_{ij}. \]
(15)
The previous result can be easily generalized to the calculation of a general overlap
\[ \langle A | f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger | B \rangle, \]
(16)
where the \( f_i \) and \( g_i^\dagger \) are arbitrary annihilation and creation operators expressed in the \( c_i^\dagger \) basis as
\[ f_i = \sum_{k=1}^{N_B} F_{ik} c_k, \]
(17)
\[ g_i^\dagger = \sum_{k=1}^{N_B} G_{ik} c_k^\dagger, \]
(18)
in terms of the \( F \) and \( G \) matrices of dimension \( N_B \times N \). This kind of overlaps appear when considering a system of \( N + M \) particles where \( M \) of them play a different role than the remaining \( N \) ones and therefore require of a different set of orbitals. As the \( f \)’s anti-commute with the \( a \)’s and the \( g \)’s with the \( b \)’s, we can repeat verbatim the previous considerations for \( \langle A | B \rangle \). We only have to be careful and define four partial overlap matrices:
\[ (S_{fg})_{ij} = \langle \cdots f_i g_j^\dagger | \rangle \quad (M \times M), \]
(19)
\[ (S_{ag})_{ip} = \langle \cdots a_j g_j^\dagger | \rangle \quad (N \times M), \]
(20)
\[ (S_{fb})_{ij} = \langle \cdots f_i b_j^\dagger | \rangle \quad (M \times N), \]
(21)
\[ (S_{ab})_{ip} = \langle \cdots a_j b_j^\dagger | \rangle \quad (N \times N), \]
(22)
to arrive to the formula
\[ \langle A | f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger | B \rangle = \text{det} \left( \begin{array}{cc} S_{fg} & S_{fb} \\ S_{ag} & S_{ab} \end{array} \right) \]
(23)
which is the general result for the overlap of Eq. (16). In order to disentangle the contributions from each set of orbitals it is convenient to use the well known formula for the determinant of a partitioned matrix
\[ \text{det} \left( \begin{array}{cc} P & Q \\ R & S \end{array} \right) = \text{det}(S - Q P^{-1} Q) \]
(24)
in order to obtain
\[ \text{det} \left( \begin{array}{cc} S_{fg} & S_{fb} \\ S_{ag} & S_{ab} \end{array} \right) = \text{det}(S_{fb} - S_{fb} S_{ab}^{-1} S_{ag}) \]
(25)
which we can call generalized Löwdin’s theorem (GLT). It requires the evaluation of the determinant of one \( M \times M \) matrix and the determinant and inverse of a \( N \times N \) matrix. This formula is also advantageous over Eq. (23) when \( N \gg M \gg 1 \) and many matrix elements for different \( g \) or \( f \) orbitals are required as only one costly matrix inversion is required. A similar expression has been obtained for the more general kind of product wave functions of the Hartree-Fock-Bogoliubov (HFB) type [21] using pfaffians [22].

In the right hand side of Eq. (25) a potential source of problems is identified in the inverse of \( S_{ab} \). If the inverse exists, then det \( S_{ab} \neq 0 \) and it is possible to write
\[ \langle A | f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger | B \rangle = \text{det} \left( S_{fg} - S_{fb} S_{ab}^{-1} S_{ag} \right) \]
(26)
which is the canonical form of the GLT where the sum of $N!$ contractions is replaced by the evaluation of the determinant of a $M \times M$ matrix. On the other hand, the result of Eq. (25) is required to resolve the implicit indeterminacy when $\det S_{ab} = 0$ and $S_{ab}$ is not invertible (see below).

The above derivation assumes that the $f$ and $g^t$ are in normal order. If this is not the case, operators can always be brought to normal order using commutation relations of fermion operators. To illustrate the procedure and to obtain a compact expression we evaluate now the overlap of a one-body operator $\hat{Q}$

$$\langle A | f_M \cdots f_1 \hat{Q} g_1^\dagger \cdots g_M^\dagger | B \rangle$$

where $\hat{Q}$ is written in terms of fermion operators $r_i^\dagger$ and $t_n$ as

$$\hat{Q} = \sum_{m,n} Q_{mn} r_i^\dagger t_n.$$  \hspace{1cm} (28)

The matrix element $\langle A | f_M \cdots f_1 r_i^\dagger t_n g_1^\dagger \cdots g_M^\dagger | B \rangle$ is evaluated by using the commutation relation $r_i^\dagger t_n = -t_n r_i^\dagger + (S_{t})_{mn}$ as

$$\langle A | f_M \cdots f_1 r_i^\dagger t_n g_1^\dagger \cdots g_M^\dagger | B \rangle = (S_{t})_{mn} \det \begin{pmatrix} S_{fg} & S_{fh} \\ S_{ag} & S_{ab} \end{pmatrix} - \det \begin{pmatrix} S_{tr} & S_{tg} \\ S_{br} & S_{bg} \end{pmatrix}$$ \hspace{1cm} (29)

With obvious notation, we introduce the row $S_{t,gb}$ and column $S_{fa,r}$ vectors as well as the matrix $S_{ba,gb}$ to be able to use property (24). Straightforward manipulations lead to the final expression

$$\langle A | f_M \cdots f_1 r_i^\dagger t_n g_1^\dagger \cdots g_M^\dagger | B \rangle = S_{t,gb} S_{fa,r}^{-1} S_{fa,gb} \det (S_{fa,gb})$$ \hspace{1cm} (30)

For the evaluation of the overlap of a two body operator the matrix element

$$\langle A | f_M \cdots f_1 r_i^\dagger t_n r_2^\dagger t_n g_1^\dagger \cdots g_M^\dagger | B \rangle$$ \hspace{1cm} (31)

is required. Using the same procedure as before and after a few manipulations we obtain

$$\langle A | f_M \cdots f_1 r_i^\dagger t_n g_1^\dagger \cdots g_M^\dagger | B \rangle = \det \begin{pmatrix} S_{t,gb} S_{fa,gb}^{-1} S_{fa,r} \end{pmatrix} \det (S_{fa,gb})$$ \hspace{1cm} (32)

where $S_{t,gb}$ and $S_{fa,gb}$ have dimensions $2 \times (M + N)$ and $(M + N) \times 2$, respectively. The matrix element is given by the product of $\det(S_{fa,gb})$ times the determinant of a $2 \times 2$ matrix with entries corresponding to the “elementary contractions”. The generalization to more general $k$-particle, $k$-hole matrix elements is straightforward and leads to the determinant of a $k \times k$ matrix of contractions. The combinatorial increase in the number of terms as $k$ increases is thus hidden in the form of a determinant of low dimensionality. This result is the generalization of Eq. (51) of [23].

To finish this section let us consider a common situation concerning to symmetry restoration where the overlap includes a multi-particle unitary operator $\hat{T}$ in the form of an exponentiated one body-operator. Typical examples are the rotation and translation operator. Then the operator $\hat{b}_m^\dagger$ generating the $|B\rangle$ configuration are transformed to $\hat{b}_m^\dagger$ given by

$$\hat{T} \hat{b}_m^\dagger \hat{T}^\dagger = \hat{b}_m^\dagger = \sum_n (T_b)_{nm} \hat{b}_n^\dagger$$ \hspace{1cm} (33)

The overlap becomes

$$\langle A | f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger \hat{T} | B \rangle = \det \begin{pmatrix} S_{fg} & S_{fh} \\ S_{ag} & S_{ab} \end{pmatrix}$$ \hspace{1cm} (34)

where the only modification with respect to Eq. (25) is in the overlaps $S_{fg}$ and $S_{ab}$ which have to be computed with the $\hat{b}_m^\dagger$ of Eq. (33).

III. CASE OF ZERO OVERLAP

Let us study how to apply the GLT of Eq. (25) when the overlap between the states $|A\rangle$ and $|B\rangle$ is zero. The methodology used can be used straightforwardly for the other form of Löwdin’s theorem, Eq. (32). When $\langle A | B \rangle = 0$, $S_{ab}$ is a singular matrix and Eq. (25) becomes indeterminate. To avoid the problem one can always use the full determinant in Eq. (25), of order $(N + M) \times (N + M)$, but this comes at a higher cost than just using (25). In addition, resolving the indeterminacy explicitly is always beneficial in order to avoid numerical artifacts that could eventually appear. To this end, we introduce the singular value decomposition (SVD) of $S$

$$S_{ab} = U \Sigma \Sigma^\dagger,$$ \hspace{1cm} (35)

where $U$ and $V$ are orthogonal matrices ($U^\dagger U = I$) and $\Sigma$ is diagonal. If $S_{ab}$ is near singular, it can be expressed as

$$\Sigma = \begin{pmatrix} \sigma_1 & \cdots & \cdots & \cdots \\ & \sigma_{N-k} \\ & & \varepsilon_1 \\ & & & \ddots \\ & & & & \varepsilon_k \end{pmatrix} \equiv \begin{pmatrix} \Sigma^R \\ E \end{pmatrix}$$ \hspace{1cm} (36)

with $\varepsilon_i$ a set of $k$ small numbers, while $E$ is the $k \times k$ diagonal matrix with $\varepsilon_i$ in the diagonal. Using this decomposition we arrive at

$$\det S_{ab} = f \det \Sigma,$$ \hspace{1cm} (37)

where $f = e^{\text{det}U V} \equiv \det U \det V$. One also has

$$S_{ab}^{-1} = V \Sigma^{-1} U^\dagger.$$ \hspace{1cm} (38)
Let us define now $S^V_{\alpha \beta} = S_{\alpha \beta} V$ and $S^U_{\alpha \beta} = U^\dagger S_{\alpha \beta}$, and decompose them in a regular (R) and a singular (S) part, according to the decomposition in Eq. (36)

$$S^V_{\beta} = \left( \begin{array}{c} S^{V,R}_{\beta} \\ S^{V,S}_{\beta} \end{array} \right) \} M$$

and

$$S^U_{\alpha \beta} = \left( \begin{array}{c} S^{U,R}_{\alpha \beta} \\ S^{U,S}_{\alpha \beta} \end{array} \right) \} k$$

Using this decomposition we can write

$$\det \left( \begin{array}{c} S_{\alpha \beta} \\ S_{\alpha \beta} \end{array} \right) = f \det \Sigma \det \left( S_{\alpha \beta} - S^V_{\alpha \beta} \Sigma^{-1} S^U_{\alpha \beta} \right),$$

with

$$S^V_{\alpha \beta} \Sigma^{-1} S^U_{\alpha \beta} = S^{V,R} \Sigma^{-1} S^{R,U} + S^{V,S} \Sigma^{-1} S^{S,U},$$

Let us now introduce the $M \times M$ matrix

$$C \equiv S_{\alpha \beta} - S^{V,R} \Sigma^{-1} S^{S,U},$$

and consider the determinant

$$\det \left( C - S^{V,S} \Sigma^{-1} S^{S,U} \right),$$

It can be computed using the Woodbury formula for the determinant (see, for instance, Ref [24])

$$\det (A + U W V) = \det (W^{-1} + V^\dagger A^{-1} U) \det W \det A$$

to obtain

$$\det \left( \begin{array}{c} S_{\alpha \beta} \\ S_{\alpha \beta} \end{array} \right) = f \det \Sigma \det E \times$$

$$\times \det \left( E - S^{V,S} \Sigma^{-1} S^{S,V} \right) \frac{1}{\det E} \det C,$$

which is well defined in the limit $\varepsilon_i \to 0$

$$\det \left( \begin{array}{c} S_{\alpha \beta} \\ S_{\alpha \beta} \end{array} \right) = f \det \Sigma \det \left( -S^{U,S} \Sigma^{-1} S^{S,U} \right) \det C,$$

which is a finite quantity when $\varepsilon_i \to 0$. This quantity requires the SVD of $S_{ab}$ to get $\Sigma^R$ and the $U$ and $V$ matrices. For large values of $N$ this can be a costly operation of order $N^3$. The inverse of the diagonal $\Sigma^R$ is also required as well as the construction of the $S^U_{\alpha \beta}$ and $S^V_{\alpha \beta}$ matrices. Once we have all the ingredients, the evaluation of the determinants in Eq. (47) require little extra work due to the low dimensionality of the matrices involved $(k \times k$ and $M \times M)$. Please note that the dimensionality of the different matrices appearing in Eq. (47) is not the same ($\Sigma^R$ is $(N-k) \times (N-k)$, $S^U_{\alpha \beta} \Sigma^{-1} S^V_{\alpha \beta}$ is $k \times k$ and $C$ is $M \times M$) and therefore the formula for the product of a determinant does not apply here.

Note that the derivation above can also be extended to the case where the matrix $S_{ab}$ is ill-conditioned and has a very small (but non-zero) determinant. A blind use of the traditional formulas may contaminate the final results due to numerical artifacts consequence of the finite representation of floating point numbers in computer’s arithmetic.

IV. NUMERICAL EXPERIMENTS

In this section we put the extended Löwdin approach to the test, characterizing the entanglement behavior of a linear combination of two Slater determinants.

A. The rainbow system

As our physical system, we have chosen the rainbow system [23–27], a 1D inhomogeneous fermionic hopping system which presents volumetric entanglement between its left and right halves. It can be described on an open chain through the following Hamiltonian,

$$H = - \sum_{m=-L+1}^{L-1} J_m c_m^\dagger c_{m+1} + \text{h.c.},$$

with hopping amplitudes given by

$$J_m = \begin{cases} \alpha^{m+1} & \text{if } m \neq 0, \\ 1 & \text{otherwise} \end{cases},$$

in terms of an inhomogeneity parameter $\alpha \in (0,1]$. For $\alpha = 1$, the system reduces to the homogeneous case. For small $\alpha$, the ground state (GS) of Hamiltonian (48) becomes approximately a valence bond solid with concentric bonds around the center, see Fig. [1]. This GS violates maximally the area-law [29], giving rise to a volumetric growth of entanglement.

B. Entanglement and number fluctuations

The eigenstates of Hamiltonian (48) are Slater determinants. Therefore, the exact entanglement entropy for any block can be efficiently evaluated [29]. Yet, this technique of evaluating the entanglement entropy cannot be extended to a linear combination of Slater determinants. Let us consider an arbitrary linear combination of the ground state and first excited states of Hamiltonian (48), both within the half-filling sector, i.e. with $N/2$ particles.

$$|\Psi\rangle = \alpha \, |0\rangle + \beta \, |1\rangle.$$
The quadratic term is more involved:

\[
\langle n_A^2 \rangle = \sum_{i,j \in A} [|\alpha|^2 \langle 0 | n_i n_j | 0 \rangle + |\beta|^2 \langle 1 | n_i n_j | 1 \rangle + 2\text{Re} \bar{\alpha} \beta \langle 0 | n_i n_j | 1 \rangle].
\]  

Again, the first two terms are straightforward to obtain. If \( C_{A,0} \) is the submatrix of the correlation matrix corresponding to block \( A \) on state \( |0\rangle \), then

\[
\langle 0 | n_i n_j | 0 \rangle = \text{Tr}(C_{A,0})^2 + \text{Tr}(C_{A,0}(I - C_{A,0})).
\]  

The last term of Eq. (55) is the most involved one, because we cannot assume Wick’s theorem. We find

\[
\langle 0 | n_i n_j | 1 \rangle = \langle 0 | (1 - c_i c_j^\dagger)(1 - c_j c_i^\dagger) | 1 \rangle = \\
\qquad = \langle 0 | 1 \rangle - \langle 0 | c_j c_i^\dagger | 1 \rangle - \langle 0 | c_i c_j^\dagger | 1 \rangle \\
\qquad + \delta_{ij} \langle 0 | c_i c_i^\dagger c_j c_j^\dagger | 1 \rangle - \langle 0 | c_i c_j c_j^\dagger c_i^\dagger | 1 \rangle.
\]  

It has been proved that, for a single Slater determinant \[30\],

\[
S_A \geq 4 \log 2 \sigma_N^2.
\]  

Thus, even though Eq. (58) is not proved for a generic linear combination of Slater determinants, we will employ \( \sigma_N \) as our estimate for an entanglement witness.

### C. Numerical experiments

For concreteness, let us set \( \alpha = \sqrt{x} \) and \( \beta = \sqrt{1 - x} \) for \( x \in [0, 1] \) in Eq. (50). Thus, our state will be given by

\[
|\Psi\rangle = \sqrt{x} |0\rangle + \sqrt{1 - x} |1\rangle,
\]  

Let us notice that the first excitation is obtained from the ground state by performing a parity transformation on the Fermi level \[27\]. Notice that, by construction \( \langle 0 | 1 \rangle = 0 \), thus forcing us to make all our computations in the zero overlap case.

In the top panel of Fig. 2 we show the variance \( \sigma_N \) of the number of particles in the left half of the rainbow system with \( N = 8 \), for different values of \( \alpha \). Notice that only in the \( \alpha \to 0^+ \) limit the variance is the same for \( x = 0 \) and \( x = 1 \), i.e.: in the GS and the first excited. This variance has been computed in two different ways: the dots correspond to the exact calculation, with the full Slater determinant, and the continuous line corresponds to the computation performed with the generalized Löwdin formulas derived in this article. The agreement is complete, and the computational time is enormously reduced with our tools.
will grow up to the maximal possible value, \( (N/8)^{\alpha} \). Also, the entanglement entropy for the same blocks as the top panel. Notice that, in this case, our calculations cannot be easily extended. Our generalized Löwdin calculation scheme is much more efficient, and can be extended to larger system sizes.

The lower panel of Fig. 2 shows the Von Neumann entropy for the same blocks as the top panel. Notice that, in this case, our calculations cannot be easily extended. Our generalized Löwdin calculation scheme is much more efficient, and can be extended to larger system sizes. Fig. 3 shows the deviation in the number of particles of state (59), computed with the full Slater determinants. The theoretical value in the \( \alpha \to 0^+ \) limit is 4 log 2 \( \approx 2.77 \).

In the \( \alpha \to 0^+ \) limit, the left-half of the rainbow system becomes an infinite temperature mixed state. Thus, the fluctuations in the particle number are easy to obtain, following a binomial distribution, \( \sigma_A = \sqrt{N/8} \), that we can readily check in Fig. 2. Also, the entanglement entropy will grow up to the maximal possible value, \( (N \log 2)/2 \).

The theoretical value in the \( \alpha \to 0^+ \) limit is 4 log 2 \( \approx 2.77 \).

**V. CONCLUSIONS AND FURTHER WORK**

We have extended the seminal results of Löwdin to obtain efficiently the matrix elements of an arbitrarily large product of fermionic operators between arbitrary Slater determinants. Our results are still applicable when the overlap matrix between the orbitals of the Slater determinants is singular, i.e. when the corresponding states are orthogonal.

Efficient computation of matrix elements in non-orthogonal Slater determinants will open a very interesting possibility: the creation of Ansätze including Slater determinants obtained from different procedures and, therefore, using different orbitals.

As proposals of future work, we would like to remark the extension of the previous calculations to the obtention of the full reduced density matrix, combining our results with those of [29] for the reduced density matrix of a block of a single Slater determinant.

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