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. Our method applies to an arbitrary number of fermionic operators, even in the case of a singular overlap matrix.

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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 calculation can be found in the seminal paper by the Swedish physicist Löwdin [1] who developed in 1955 a very smart strategy, based on a careful application of the properties of the determinant. 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 nonsingular [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 used to expand the wave functions of the fractional quantum Hall effect (FQHE) as discussed in Ref. [11]. In lattice QCD the study of physical systems involving several hadrons [12], as is the case in the description of collisions [13] or when the hadrons aggregate to form atomic nuclei [14–16], requires the evaluation of matrix elements involving the product of $(3N)^2$ (N is the number of hadrons) creation or annihilation operators coming from the quark fields. If the matrix elements are computed in terms of Wick contractions (see below), the required number of terms grows exponentially fast with N [12]. General overlaps of Slater determinants are also required in nuclear physics, in the framework of the Monte Carlo shell model (MCSM) [17,18], the in-medium similarity renormalization group [19], configuration interaction [20], or in the field of symmetry restored quasiparticle excitations [21,22].

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 hundred of thousands, if not millions, of operator overlaps calls for robust evaluation methods capable of handling 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,

$$|A\rangle = a^\dagger_{i_1} \cdots a^\dagger_{i_N} |-\rangle, \tag{1}$$

$$|B\rangle = b^\dagger_{j_1} \cdots b^\dagger_{j_N} |-\rangle, \tag{2}$$

of N particles. The $a_i^\dagger$ and $b_j^\dagger$ are arbitrary creation operators with quantum numbers denoted by i and j, respectively. Their Hermitian conjugate annihilates the true Fock vacuum $|-\rangle$:

$$a_i|-\rangle = b_j|-\rangle = 0, \tag{3}$$

such that

$$\{a_i^\dagger, b_j\} = S_{ij}^*, \tag{4}$$

$$\{a_i, b_j^\dagger\} = S_{ij}, \tag{5}$$

as well as

$$\{a_i^\dagger, b_j^\dagger\} = 0. \tag{6}$$

The overlap matrix is defined by $S_{ij} = \langle a_i|b_j\rangle = \langle -|a_i b_j^\dagger|-\rangle$. The overlap between both states, $\langle A|B\rangle$, is evaluated in a recursive way:

$$\begin{aligned}\langle A|B\rangle &= \langle -|a_N \cdots a_1 b_1^\dagger \cdots b_N^\dagger|-\rangle \\ &= -\langle -|a_N \cdots a_2 b_1^\dagger a_1 b_2^\dagger \cdots b_N^\dagger|-\rangle \\ &\quad + S_{11}\langle -|a_N \cdots a_2 b_2^\dagger \cdots b_N^\dagger|-\rangle \end{aligned} \tag{7}$$

by *jumping* with the $b_1^\dagger$ creation operator over the a_1 annihilation one. The notation has been also simplified by replacing indexes $i_1, \ldots$ by $1, \ldots$. Let us now introduce the quantity

$$\langle A|B\rangle_{[11]} = \langle -|a_N \cdots a_2 b_2^\dagger \cdots b_N^\dagger|-\rangle, \tag{8}$$

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,

$$\begin{aligned}\langle A|B\rangle &= S_{11}\langle A|B\rangle_{[11]} - S_{21}\langle A|B\rangle_{[21]} + \cdots \\ &\quad + (-1)^{N+1} S_{N1}\langle A|B\rangle_{[N1]}, \end{aligned} \tag{9}$$

and the expansion ends after N jumps because $\langle -|b_1^\dagger = 0$. 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. (9) becomes the minor expansion of the determinant of S by the first row, i.e.,

$$\langle A|B\rangle = \det(S). \tag{10}$$

Let us now expand $a_i^\dagger$ and $b_j^\dagger$ in terms of a common basis $\{c_k^\dagger, k = 1, \ldots, N_B\}$

$$a_i^\dagger = \sum_{k=1}^{N_B} A_{ki} c_k^\dagger, \tag{11}$$

$$b_j^\dagger = \sum_{k=1}^{N_B} B_{kj} c_k^\dagger. \tag{12}$$

Then the $N\times N$ overlap matrix S becomes the product of the two expansion matrices, A and B, of dimension $N_B\times N$

$$S_{ij} = \sum_k A_{ki}^* B_{kj} = (A^\dagger B)_{ij}. \tag{13}$$

The previous result can be easily generalized to the calculation of a general overlap

$$\langle A|f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger|B\rangle, \tag{14}$$

where the f_l and $g_p^\dagger$ are arbitrary annihilation and creation operators expressed in the $c^\dagger$ basis as

$$f_l = \sum_{k=1}^{N_B} F_{kl} c_k, \tag{15}$$

$$g_p^\dagger = \sum_{k=1}^{N_B} G_{kp} c_k^\dagger, \tag{16}$$

in terms of the F and G matrices of dimension $N_B\times N$. These kind of overlaps appear when considering a system of $N + M = N'$ particles where M of them play a different role than the remaining N ones and therefore require a different set of orbitals. For instance, this is the case for unrestricted molecular orbitals [23]. We could also accommodate the situation where the N orbitals are considered as an inert core and only the M orbitals are active. As the f's anticonmute with the a's and the $g^\dagger$'s with the $b^\dagger$, we can repeat verbatim the previous considerations for $\langle A|B\rangle$. We only have to be careful and define four partial overlap matrices:

$$(S_{\rm fg})_{ij} = \langle -|f_i g_j^\dagger|-\rangle \quad (M\times M), \tag{17}$$

$$(S_{\rm ag})_{lj} = \langle -|a_l g_j^\dagger|-\rangle \quad (N\times M), \tag{18}$$

$$(S_{\rm fb})_{ip} = \langle -|f_i b_p^\dagger|-\rangle \quad (M\times N), \tag{19}$$

$$(S_{\rm ab})_{lp} = \langle -|a_l b_p^\dagger|-\rangle \quad (N\times N), \tag{20}$$

to arrive at the formula

$$\langle A|f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger|B\rangle = \det\begin{pmatrix} S_{\rm fg} & S_{\rm fb} \\ S_{\rm ag} & S_{\rm ab}\end{pmatrix}, \tag{21}$$

which is the general result for the overlap of Eq. (14). 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 based on the concept of the Schur complement [24]:

$$\begin{aligned}\det\begin{pmatrix} P & Q \\ R & S\end{pmatrix} &= \det P \, \det(S - RP^{-1}Q) \\ &= \det S \, \det(P - QS^{-1}R). \end{aligned} \tag{22}$$

Therefore,

$$\det\begin{pmatrix} S_{\rm fg} & S_{\rm fb} \\ S_{\rm ag} & S_{\rm ab}\end{pmatrix} = \det S_{\rm ab} \det\left(S_{\rm fg} - S_{\rm fb} S_{\rm ab}^{-1} S_{\rm ag}\right), \tag{23}$$

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 $N\times N$ matrices. This formula is also advantageous over Eq. (21) when $N \gg M \gg 1$ as only one costly matrix inversion is required. The expression above for the determinant is similar to the one used in the proof of Sylverster's theorem discussed in Ref. [25]. A similar expression has been obtained for the more general kind of product wave functions of the Hartree-Fock-Bogoliubov (HFB) type [26] using Pfaffians [27].

In the right-hand side of Eq. (23) a potential source of problems is identified in the inverse of $S_{\rm ab}$. If the inverse

exists, then $\det S_{\rm ab} \neq 0$ and it is possible to write

$$\frac{\langle A|f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger|B\rangle}{\langle A|B\rangle} = \det\left(S_{\rm fg} - S_{\rm fb} S_{\rm ab}^{-1} S_{\rm ag}\right), \quad (24)$$

which is the canonical form of the GLT where the sum of $(2M-1)!!$ contractions is replaced by the evaluation of the determinant of a $M\times M$ matrix which can be carried out efficiently in $O(M^3)$ operations. On the other hand, the result of Eq. (23) is required to resolve the implicit indeterminacy when $\det S_{\rm ab} = 0$ and $S_{\rm ab}$ is not invertible (see below).

The above derivation assumes that the f and $g^\dagger$ 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 $\hat{Q}$

$$\langle A|f_M \cdots f_1 \hat{Q} g_1^\dagger \cdots g_M^\dagger|B\rangle, \quad (25)$$

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

$$\hat{Q} = \sum_{m,n} Q_{mn} r_m^\dagger t_n. \quad (26)$$

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

$$\begin{aligned}&\langle A|f_M \cdots f_1 r_m^\dagger t_n g_1^\dagger \cdots g_M^\dagger|B\rangle \\ &= (S_{\rm tr})_{mn} \det\begin{pmatrix} S_{\rm fg} & S_{\rm fb} \\ S_{\rm ag} & S_{\rm ab}\end{pmatrix} - \det\begin{pmatrix} S_{\rm tr} & S_{\rm tg} & S_{\rm tb} \\ S_{\rm fr} & S_{\rm fg} & S_{\rm fb} \\ S_{\rm ar} & S_{\rm ag} & S_{\rm ab}\end{pmatrix}. \quad (27)\end{aligned}$$

Please note that in this case the n and m are specific indices and therefore $S_{\rm tr}$ is a 1×1 matrix with a single element corresponding to the overlap $\langle -|t_n r_m^\dagger|-\rangle$. With obvious notation, we introduce the row $S_{\rm t,gb}$ and column $S_{\rm fa,r}$ vectors as well as the matrix $S_{\rm fa,gb}$ to be able to use property (22). Straightforward manipulations lead to the final expression

$$\langle A|f_M \cdots f_1 r_m^\dagger t_n g_1^\dagger \cdots g_M^\dagger|B\rangle = S_{\rm t,gb} S_{\rm fa,gb}^{-1} S_{\rm fa,r} \det(S_{\rm fa,gb}). \quad (28)$$

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

$$\langle A|f_M \cdots f_1 r_{m_1}^\dagger r_{m_2}^\dagger t_{n_1} t_{n_2} g_1^\dagger \cdots g_M^\dagger|B\rangle \quad (29)$$

is required. As in the previous case the commutation relations are used to move the $r^\dagger$ operators to the right of the t operators to use (21). Further application of Eq. (22) and after a few manipulations that require the expression of $\det(A-B)$ we obtain

$$\begin{aligned}&\langle A|f_M \cdots f_1 r_{m_1}^\dagger r_{m_2}^\dagger t_{n_1} t_{n_2} g_1^\dagger \cdots g_M^\dagger|B\rangle \\ &\quad = \det\left(S_{\rm t,gb} S_{\rm fa,gb}^{-1} S_{\rm fa,r}\right) \det(S_{\rm fa,gb}), \quad (30)\end{aligned}$$

where $S_{\rm t,gb}$ and $S_{\rm fa,r}$ are now matrices with dimensions $2\times(M+N)$ and $(M+N)\times 2$, respectively. The matrix element is given by the product of $\det(S_{\rm fa,gb})$ times the determinant of a 2×2 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 involving matrices $S_{\rm t,gb}$ and $S_{\rm fa,r}$ of dimensions $k\times(M+N)$ and $(M+N)\times k$, respectively. The combinatorial increase in the number of terms as k increases is thus hidden in the form of a determinant of low dimensionality that can be evaluated efficiently using standard numerical analysis techniques. This result is the generalization of Eq. (51) of [28].

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

$$\hat{\mathcal{T}} b_m^\dagger \hat{\mathcal{T}}^\dagger = \tilde{b}_m^\dagger = \sum_n (T_b)_{nm} b_n^\dagger. \quad (31)$$

The overlap becomes

$$\langle A|f_M \cdots f_1 g_1^\dagger \cdots g_M^\dagger \hat{\mathcal{T}}|B\rangle = \det\begin{pmatrix} S_{\rm fg} & S_{\rm f\tilde{b}} \\ S_{\rm ag} & S_{\rm a\tilde{b}}\end{pmatrix}, \quad (32)$$

where the only modification with respect to Eq. (21) is in the overlaps $S_{\rm f\tilde{b}}$ and $S_{\rm a\tilde{b}}$, which have to be computed with the $\tilde{\rm b}_m^\dagger$ of Eq. (31).

An important issue in the application of the above formulas is the scaling of the computational cost with the number of particles N', the dimension of the Hilbert space, N_B, and the order of the involved operators, k. The naive evaluation of a generic k-body operator in the basis of the particle orbitals requires computing $O(N_B^{2k})$ determinant of a $(N'+k)\times(N'+k)$ matrix, which amounts to a computer time of order $O(N_B^{2k}(N'+k)^3)$. Using the generalized Löwdin expression, Eq. (30), we can precalculate the inverse of $S_{\rm fa,gb}$, which takes $O(N^3)$ operations, we can also precalculate the two matrix multiplications for all possible values of the m and n indices, which takes $O(N_B N'^2)$ operations, and finally evaluate only N_B^{2k} determinants of $k\times k$, matrices, with a cost $O(N_B^{2k}k^3)$. In terms of *amortized cost*, this route is much more convenient when $N' \gg k$ and $N_B \gg k$.

III. CASE OF ZERO OVERLAP

Let us study how to apply the GLT of Eq. (23) 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. (30). When $\langle A|B\rangle = 0$, S_{ab} is a singular matrix and Eq. (23) becomes indeterminate. To avoid the problem one can always use the full determinant in Eq. (21), of order $(N+M)\times(N+M)$, but this comes at a higher cost than just using (23). 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

$$S_{\rm ab} = U \Sigma V^\dagger, \quad (33)$$

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

$$\Sigma = \begin{pmatrix} \sigma_1 & & & & & & \\ & \ddots & & & & & \\ & & \sigma_{N-k} & & & & \\ & & & \varepsilon_1 & & & \\ & & & & \ddots & & \\ & & & & & \varepsilon_k \end{pmatrix} \equiv \begin{pmatrix} \Sigma^{\rm R} & \\ & E \end{pmatrix}, \tag{34}$$

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

$$\det S_{\rm ab} = f\ \det \Sigma, \tag{35}$$

where $f = e^{i\varphi_{UV}} \equiv \det U\ \det V^\dagger$. One also has

$$S_{\rm ab}^{-1} = V\Sigma^{-1}U^\dagger. \tag{36}$$

Let us define now $S^V_{\rm fb} \equiv S_{\rm fb}V$ and $S^U_{\rm ag} \equiv U^\dagger S_{\rm ag}$, and decompose them in a *regular* (R) and a *singular* (S) part, according to the decomposition in Eq. (34):

$$S^V_{\rm fb} = \underbrace{\left(\bar S^{V,{\rm R}}_{\rm fb}\right.}_{N-k} \underbrace{\left.\bar S^{V,{\rm S}}_{\rm fb}\right)}_{k} \Big\}\, M \tag{37}$$

and

$$S^U_{\rm ag} = \underbrace{\begin{pmatrix} \bar S^{U,{\rm R}}_{\rm ag} \\ \bar S^{U,{\rm S}}_{\rm ag} \end{pmatrix}}_{M} \begin{matrix} \} \ N\text{-}k \\ \} \ k \end{matrix}. \tag{38}$$

Using this decomposition we can write

$$\det \begin{pmatrix} S_{\rm fg} & S_{\rm fb} \\ S_{\rm ag} & S_{\rm ab} \end{pmatrix} = f\ \det\Sigma\ \det\left(S_{\rm fg} - S^V_{\rm fb}\Sigma^{-1}S^U_{\rm ag}\right), \tag{39}$$

with

$$S^V_{\rm fb}\Sigma^{-1}S^U_{\rm ag} = \bar S^{V,{\rm R}}_{\rm fb}(\Sigma^{\rm R})^{-1}\bar S^{U,{\rm R}}_{\rm ag} + \bar S^{V,{\rm S}}_{\rm fb}E^{-1}\bar S^{U,{\rm S}}_{\rm ag}. \tag{40}$$

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

$$C \equiv S_{\rm fg} - \bar S^{V,{\rm R}}_{\rm fb}(\Sigma^{\rm R})^{-1}\bar S^{U,{\rm R}}_{\rm ag}, \tag{41}$$

and consider the determinant

$$\det\left(C - \bar S^{V,{\rm S}}_{\rm fb}E^{-1}\bar S^{U,{\rm S}}_{\rm ag}\right). \tag{42}$$

It can be computed using the Woodbury formula for the determinant (see, for instance, Ref. [29])

$$\det(A + UWV^\dagger) = \det(W^{-1} + V^\dagger A^{-1}U)\det W\ \det A \tag{43}$$

to obtain

$$\det \begin{pmatrix} S_{\rm fg} & S_{\rm fb} \\ S_{\rm ag} & S_{\rm ab} \end{pmatrix} = f\ \det\Sigma^{\rm R}\det E\det\left(E - \bar S^{U,{\rm S}}_{\rm ag}C^{-1}\bar S^{V,{\rm S}}_{\rm fb}\right) \times \frac{1}{\det E}\det C. \tag{44}$$

Simplifying this expression we get

$$\det \begin{pmatrix} S_{\rm fg} & S_{\rm fb} \\ S_{\rm ag} & S_{\rm ab} \end{pmatrix} = f\ \det\Sigma^{\rm R}\det\left(-\bar S^{U,{\rm S}}_{\rm ag}C^{-1}\bar S^{V,{\rm S}}_{\rm fb}\right)\det C, \tag{45}$$

which is a finite quantity when $\varepsilon_i \to 0$. This quantity requires the SVD of $S_{\rm ab}$ to get $\Sigma^{\rm R}$ 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 $\Sigma^{\rm R}$ is also required, as well as the construction of the $S^U_{\rm ag}$ and $S^V_{\rm fb}$ matrices. Once we have all the ingredients, the evaluation of the determinants in Eq. (45) 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. (45) is not the same [$\Sigma^{\rm R}$ is $(N-k)\times(N-k)$, $\bar S^{U,{\rm S}}_{\rm ag}C^{-1}\bar S^{V,{\rm S}}_{\rm fb}$ 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 $S_{\rm ab}$ is ill conditioned and has a very small (but nonzero) 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.

The zero overlap case has also been considered for one and two body operators in [2–4] using the LDU decomposition of the overlap matrix $S_{\rm ab}$. We prefer our approach as it is independent of the type of operator at stake and uses the SVD which is an always defined decomposition.

In terms of computational cost, the analysis of the previous section still holds. Indeed, we can precompute the SVD of the $N\times N$ matrix $S_{\rm a,b}$, with a cost $O(N^3)$, and then evaluate N_B^{2k} small determinants of order $k\times k$.

IV. NUMERICAL EXPERIMENTS

In this section we put the extended Löwdin approach to the test, characterizing the fluctuations in the number of particles in a block of a fermionic state described by a linear combination of two Slater determinants. Our motivation to consider these fluctuations is that they are known to constitute a *witness of entanglement* [30], as we will briefly discuss.

Given any pure state for a quantum system $|\Psi\rangle$ and a subsystem A, we can define the associated reduced density matrix, $\rho_A = {\rm Tr}_A|\Psi\rangle\langle\Psi|$, where ${\rm Tr}_A$ denotes the partial trace over A. Also, we can define the *entanglement entropy* associated with A,

$$S_A = -{\rm Tr}(\rho_A \ln \rho_A). \tag{46}$$

Entanglement entropy often follows the *area law*, i.e., the entanglement entropy of A is proportional to the measure of its boundary, $S_A \propto |\partial A|$ [31]. For a Slater determinant, the entanglement entropy of any block can be efficiently computed in polynomial time with the number of sites [32]. Unfortunately, those techniques cannot be extended even to linear combinations of Slater determinants.

Moreover, let us also define the variance of the number of particles in A,

$$\sigma_N^2 \equiv \left\langle n_A^2\right\rangle - \langle n_A\rangle^2, \tag{47}$$

where the operator n_A is defined through

$$n_A \equiv \sum_{i\in A} n_i = \sum_{i\in A} c_i^\dagger c_i. \tag{48}$$

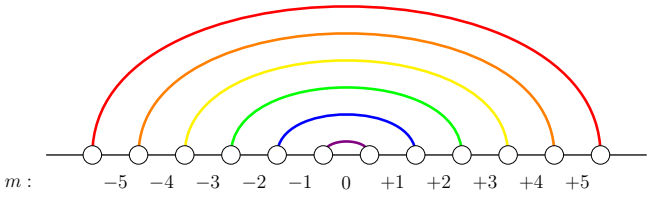

FIG. 1. Illustration of the rainbow ground state in the small α limit: a valence bond solid with concentric bonds around the center of the chain. Notice that the entanglement entropy of a left block is proportional to the block size, i.e., a volumetric growth of the entropy.

There is a very interesting connection between the fluctuations in the number of particles and the entanglement entropy for a block within a Slater determinant [30],

$$S_A \geqslant 4\ \ln 2\sigma_N^2, \tag{49}$$

which sets a lower bound on the entanglement entropy of a block provided by the variance of the number of particles. Hence our claim that σ_N^2 is an *entanglement witness*.

A. Rainbow system

As our physical system, we have chosen the *rainbow system* [33–35], a 1D inhomogeneous fermionic hopping system which violates strongly the area law, presenting *volumetric entanglement*, $S_A \propto |A|$. It can be described on an open chain through the following Hamiltonian:

$$H = -\sum_{m=-L+1}^{L-1} J_m c_m^\dagger c_{m+1} + \text{H.c.}, \tag{50}$$

with hopping amplitudes given by

$$J_m = \begin{cases} \alpha^{2m+1} & \text{if } m \neq 0, \\ 1 & \text{otherwise,} \end{cases} \tag{51}$$

in terms of an inhomogeneity parameter $\alpha \in (0, 1]$. For $\alpha = 1$, the system reduces to the homogeneous case. For small α, the ground state (GS) of Hamiltonian (50) becomes approximately a *valence bond solid* with concentric bonds around the center; see Fig. 1. The entanglement entropy of a block A in a valence bond solid can be shown to be proportional to the number of bonds connecting it to its environment [34,35]. Thus the entanglement between the left and right halves is proportional to the number of sites in the chain, and hence volumetric.

B. Fluctuations in the number of particles

Let us consider an arbitrary linear combination of the ground state and first excited states of Hamiltonian (50), both within the half-filling sector, i.e., with $N/2$ particles:

$$|\Psi\rangle = \eta_0|0\rangle + \eta_1|1\rangle. \tag{52}$$

Let us use Eq. (47) to compute the fluctuations in the number of particles in a block A. The expected value of the number of particles is given by

$$\langle n_A\rangle = \sum_{i\in A}\langle\Psi|n_i|\Psi\rangle = \sum_{i\in A}[|\eta_0|^2\langle 0|n_i|0\rangle + |\eta_1|^2\langle 1|n_i|1\rangle + 2\,\text{Re}\,\bar\eta_0\eta_1\langle 0|n_i|1\rangle]. \tag{53}$$

The first two terms are easily obtained, because they refer to a single Slater determinant. The third, notwithstanding, must be found using the (generalized) Löwdin tricks described:

$$\langle 0|n_i|1\rangle = \langle 0|c_i^\dagger c_i|1\rangle = \langle 0|1\rangle - \langle 0|c_i c_i^\dagger|1\rangle. \tag{54}$$

The quadratic term is more involved:

$$\langle n_A^2\rangle = \sum_{i,j\in A}[|\eta_0|^2\langle 0|n_i n_j|0\rangle + |\eta_1|^2\langle 1|n_i n_j|1\rangle + 2\,\text{Re}\,\bar\eta_0\eta_1\langle 0|n_i n_j|1\rangle]. \tag{55}$$

Again, the first two terms are straightforward to obtain. Let $C_{A,0}$ be the submatrix of the correlation matrix corresponding to block A on state $|0\rangle$; then

$$\langle 0|n_i n_j|0\rangle = \text{Tr}(C_{A,0})^2 + \text{Tr}[C_{A,0}(I - C_{A,0})]. \tag{56}$$

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

$$\begin{aligned}\langle 0|n_i n_j|1\rangle &= \langle 0|(1 - c_i c_i^\dagger)(1 - c_j c_j^\dagger)|1\rangle \\ &= \langle 0|1\rangle - \langle 0|c_j c_j^\dagger|1\rangle - \langle 0|c_i c_i^\dagger|1\rangle \\ &\quad + \delta_{ij}\langle 0|c_i c_j^\dagger|1\rangle - \langle 0|c_i c_j c_i^\dagger c_j^\dagger|1\rangle.\end{aligned} \tag{57}$$

C. Numerical experiments

For concreteness, let $\eta_0 = \sqrt{x}$ and $\eta_1 = \sqrt{1-x}$ for $x \in [0, 1]$ in Eq. (52). Thus our state will be given by

$$|\Psi\rangle = \sqrt{x}|0\rangle + \sqrt{1-x}|1\rangle. \tag{58}$$

Let us notice that the first excitation is obtained from the ground state by performing a parity transformation on the Fermi level [35]. 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 σ_N^2 of the number of particles in the left half of the rainbow system with $N = 8$, for different values of α. Notice that only in the $\alpha \to 0^+$ limit the variance is the same for $x = 0$ and $x = 1$, i.e., 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.

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, $\sigma_N = \sqrt{N/8}$, that we can readily check in Fig. 2. Also, the entanglement entropy will grow up to its maximal possible value, $(N\ \ln 2)/2$. The lower panel of Fig. 2 shows the von Neumann entropy for the same blocks as the top panel, which could only be evaluated through expression (46), taking an exponential time.

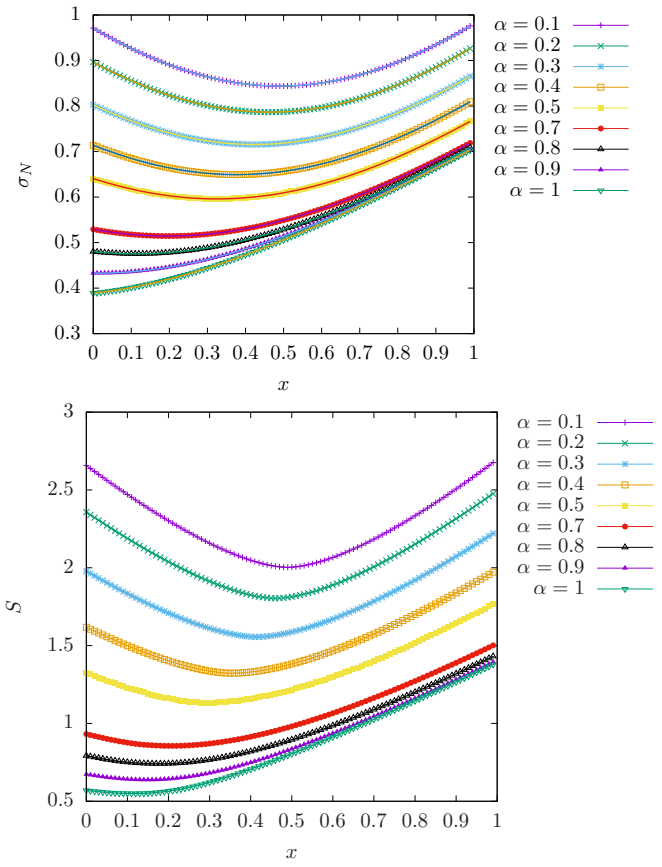

FIG. 2. Top: deviation of the number of particles in the left half of state (58) with $N = 8$ sites and various values of α, computed with the full Slater determinants and with our generalized Löwdin scheme. The theoretical value in the $\alpha \to 0^+$ limit is $\sigma_N = 1$. Bottom: entanglement of the left half of state (58), computed with the full Slater determinants. The theoretical value in the $\alpha \to 0^+$ limit is $4 \ln 2 \approx 2.77$.

Figure 3 shows σ_N in the same system, using $N = 40$ sites. The entanglement entropy calculations are now out of our computational reach, but the variance of the number of particles, σ_N, can be efficiently computed in polynomial time.

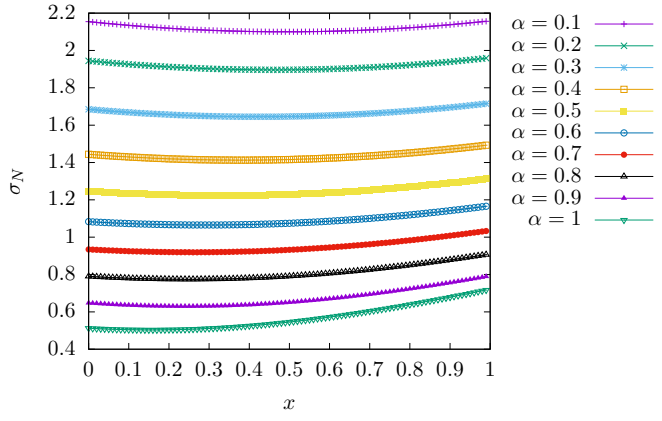

FIG. 3. Same observable as in the top panel of Fig. 2 for a rainbow system with $N = 40$. The theoretical value for the deviation of the particle number of the left half in the $\alpha \to 0^+$ limit is $\sqrt{N/8} = \sqrt{5} \approx 2.23$.

D. Computational cost

As it was discussed at the end of Sec. II, the total cost of evaluating the variance is the sum of the evaluation of the SVD, $O(N^3)$, and $O(N^2)$ determinants [less than the expected value for two-body operators, which is $O(N^4)$], whose cost is bounded. Thus we obtain that the final cost is bounded by $O(N^3)$. Avoiding the use of the generalized Löwdin theorem would lead to an order $O(N^5)$ cost [$O(N^2)$ determinants of $N \times N$ matrices, each $O(N^3)$].

E. Generalized Löwdin C++ code

We have uploaded our C++ libraries to compute matrix elements of Slater determinants using the generalized Löwdin approach to the repository `github` as *free software* [36]. The same material can also be downloaded from the Supplemental Material section of the electronic version of the journal [37], briefly described in the Appendix.

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 nonorthogonal 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 for future work, we would like to mention the extension of the previous calculations to the full reduced density matrix, combining our results with those of [32] for the reduced density matrix of a block of a single Slater determinant.

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APPENDIX: GENERALIZED LÖWDIN CODE

The reader can find a C++ library at [36] which implements the computational framework for the evaluation of matrix elements of k-body operators between different Slater determinants. This Appendix is devoted to a brief description of this library. The library is based on HVB, a multipurpose scientific library built on BLAS and LAPACK (more information in [36]).

The class structure is simple. A class `Lowdin` is defined, whose constructor takes two arguments: the (complex) matrices whose columns contain the occupied in the left and right

Slater determinants. Thus their dimension must be $N_B \times N$. It precomputes the inverse of the $S_{a,b}$ matrix if it is possible, or the SVD when it is not, using an internal flag (transparent to the user) to determine which route was needed in this case. Then, it implements two basic methods: `Lowdin::Elem` takes two integers i and j as arguments and returning $\langle U|c_i^\dagger c_j|V\rangle$. `Lowdin::NiNj` returns the expected value of $\langle U|n_i n_j|V\rangle$. The reader can extend easily these methods to other higher-order operators.

The repository contains the example code used to obtain Figs. 2 and 3, called `xfluctrb.cc`. A suitable `Makefile` is provided, assuming that BLAS and LAPACK are correctly installed in the system. Other HVB functions are used, and the reader can find documentation in [38].

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[37] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevA.101.012105 for the computer code.
[38] http://github.com/jvrlag/hvb.