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Sign of the overlap of Hartree-Fock-Bogoliubov wave functions

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The problem of how to compute accurately and efficiently the sign of the overlap between two general Hartree-Fock-Bogoliubov (HFB) wave functions is addressed. The results obtained can easily be extrapolated to the evaluation of the sign of the trace of a density operator exponential of one body operators.

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Introduction. Beyond mean field calculations are becoming very popular [1] as they allow a fairly good description of many nuclear state properties of both the ground state and several kinds of excited states all over the nuclide chart. In these calculations, overlaps of Hartree-Fock-Bogoliubov (HFB) wave functions have to be computed. Standard formulas [2] involve the square root of a determinant leaving the sign of the overlap undefined. However, when the HFB states preserve some kind of discrete symmetry like time reversal or simplex, the block structure of the matrices involved fixes the sign. This has been discussed, for instance, in some recent applications of angular momentum projection (AMP) using axially symmetric and time reversal preserving intrinsic wave functions [3,4]. To move forward, HFB wave functions that do not have any spatial symmetry (triaxial) and also breaking time reversal symmetry have to be considered in order to incorporate $K \neq 0$ configurations. This is the case to describe, for instance, the ground state of odd-A nuclei. For the usual time reversal breaking (TRB) mean field wave functions, the simplex symmetry endows the HFB amplitudes U and V with a common bipartite structure and the usual arguments used to extract out the sign of the overlap apply. However, when full triaxial angular momentum projection of HFB intrinsic states [5] is considered, the simplex symmetry is no longer preserved in the evaluation of rotated overlaps and the determination of the sign becomes more difficult. A general solution to the sign problem was given in Ref. [6], where it was shown that the overlap, including the sign, can be computed from the pairwise degenerate eigenvalues of a non-Hermitian matrix. Handling the eigenvalues of non-Hermitian matrices is a difficult task [7], that increases its complexity if the pairwise degenerate eigenvalues have to be obtained numerically without any symmetry enforcing degeneracy, as is the case with HFB wave functions breaking simplex. Neergard's method has been used along with small configuration spaces [8] but in the majority of the calculations continuity arguments are used (see Refs. [5,9,10] for recent examples) in spite of the difficulties with that procedure. The same sign problem is also present in the evaluation of the trace of statistical density operators [11,12]. In this case, however, Neergard's method has not been implemented up to date, leaving as the only choice the continuity method in such finite temperature calculations. The same difficulty also applies to the recently proposed method to compute multi-quasiparticle overlaps that relays on the statistical Wick's theorem [13]. Recently, [14] the group structure of the unitary Bogoliubov transformation has been discussed, as well as its implications in the relative phase between two HFB wave functions. However, its practical implications are still unclear.

In this paper, I will introduce a new way to compute the overlap of two HFB wave functions based on the concept of fermion coherent states [15–17]. The new formula involves a quantity similar to the determinant called pfaffian of a skew-symmetric matrix. The advantage of the proposed method is that the numerical evaluation of the pfaffian is simple and lacks the problems previously mentioned about pairwise degenerate eigenvalues. Another advantage of the present formulation is its applicability to the evaluation of the trace of density operators like the ones found in applications of the auxiliary-field shell model Monte Carlo [11] or symmetry restoration at finite temperature [12]. A reliable determination of the sign of the norm can also be useful in to order to pin down the location of the zeros of the HFB overlaps [10]. This determination would eventually be useful to get rid of the so called "pole problem" that plagues present beyond mean field calculations.

Overlaps and traces: Preliminaries. Let $|\phi_0\rangle$ and $|\phi_1\rangle$ be two HFB wave functions defined in terms of a set of single particle creation and annihilation operators a_k^+ and a_k that are assumed to be related by hermitian conjugation and also to satisfy fermion commutation relations. The HFB wave functions, in the Thouless representation [2,16], are given by

$$|\phi_i\rangle = \exp\left(\frac{1}{2}\sum_{kk'} M_{kk'}^{(i)} a_k^+ a_{k'}^+\right)|0\rangle, \quad (1)$$

where the skew-symmetric matrices

$$M^{(i)} = \left(V_i U_i^{-1}\right)^*$$

are defined in terms of the U_i and V_i coefficients of the Bogoliubov transformations defining the HFB wave functions and $|0\rangle$ is the true vacuum. The arbitrary phase that can always be associated with a vector state in quantum mechanics has been implicitly fixed in the definition of Eq. (1) by requiring $\langle 0|\phi_i\rangle = 1$. Ways to enforce this normalization for general HFB wave functions are discussed, for instance in Refs. [2,16]. In the event of having $\langle 0|\phi_i\rangle = 0$ (as a consequence of divergent $M^{(i)}$ and/or zero occupancies) the best practical strategy is to use another reference wave function instead of

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the true vacuum $|0\rangle$. The new reference HFB wave function $|\bar{\phi}\rangle$ has to be conveniently chosen as to stay close to both $|\phi_i\rangle$ (for instance by taking a wave function with similar deformation parameters as those of $|\phi_i\rangle$). The matrices $\bar{M}^{(i)}$ referred to $|\bar{\phi}\rangle$ can be straightforwardly computed in terms of the previous quantities and the Bogoliubov transformation amplitudes of the reference state. In the rare event of not finding a convenient reference wave function $|\bar{\phi}\rangle$ a regularization procedure to handle the divergent $\bar{M}^{(i)}$ matrix elements (or the zero occupancies) is in order. In this case, the expressions get more involved and a detailed account is deferred to a forthcoming publication. Another way to deal with that problem is presented in Ref. [6] but the resulting expressions are rather involved.

Let me now introduce fermion coherent states $|\mathbf{z}\rangle$, which are parametrized in terms of the anticommuting elements z_k and z_k^* of a Grassmann algebra [15–18] and fulfilling the equations

$$a_k|\mathbf{z}\rangle = z_k|\mathbf{z}\rangle \tag{2}$$

and

$$\langle\mathbf{z}|a_k^+ = z_k^*\langle\mathbf{z}|. \tag{3}$$

From the above definition is clear that $|\mathbf{z}\rangle$ is a right eigenstate of the annihilation operator a_k with eigenvalue z_k whereas $\langle\mathbf{z}|$ is a left eigenvector of a_k^+ with eigenvalue z_k^* (the notation used for the members of the Grassmann algebra is the usual one but can be a little misleading as z_k^* is not connected to z_k by complex conjugation). The coherent states satisfy a closure relation

$$\mathbb{1} = \int d\mu(\mathbf{z})|\mathbf{z}\rangle\langle\mathbf{z}|, \tag{4}$$

where the metric of the integral is given by $d\mu(\mathbf{z}) = e^{-\mathbf{z}^*\mathbf{z}}\prod_k dz_k^* dz_k$. These and other relevant definitions and properties of fermion coherent states can be found in many textbook or in the original literature [15–18].

Evaluation of the overlap. To compute the overlap $\langle\phi_0|\phi_1\rangle$, the closure relation of Eq. (4) is inserted to obtain

$$\langle\phi_0|\phi_1\rangle = \int d\mu(\mathbf{z})\langle 0|e^{\frac{1}{2}\sum_{kk'} M^{(0)*}_{kk'} a_{k'} a_k}|\mathbf{z}\rangle \times \langle\mathbf{z}|e^{\frac{1}{2}\sum_{kk'} M^{(1)}_{kk'} a_k^+ a_{k'}^+}|0\rangle.$$

Using now Eqs. (2) and (3) one arrives to

$$\langle\phi_0|\phi_1\rangle = \int d\mu(\mathbf{z}) e^{\frac{1}{2}\sum_{kk'} M^{(0)*}_{kk'} z_{k'} z_k} e^{\frac{1}{2}\sum_{kk'} M^{(1)}_{kk'} z_k^* z_{k'}^*}, \tag{5}$$

where the property $|\langle 0|\mathbf{z}\rangle|^2 = 1$ is used. The integral is of the Gaussian type but for Grassmann variables. The techniques to evaluate this kind of integrals can be found in many textbooks [15–17] but its evaluation will be carried out explicitly here. The reason is that in order to determine the sign of the norm we have to be careful with some intermediate steps. The above integral can be written in a more compact way by introducing the bipartite skew-symmetric matrix

$$\mathbb{M}_{\mu'\mu} = \begin{pmatrix} M^{(1)}_{k'k} & -\mathbb{1}_{k'k} \\ \mathbb{1}_{k'k} & -M^{(0)*}_{k'k} \end{pmatrix}$$

and the vector of Grassmann variables $z_\mu = (z_{k'}^*, z_{k'})$ as

$$\langle\phi_0|\phi_1\rangle = \int \prod_k (dz_k^* dz_k) e^{\frac{1}{2}\sum_{\mu\mu'} z_{\mu'}\mathbb{M}_{\mu'\mu} z_\mu}. \tag{6}$$

The skew-symmetric matrix $\mathbb{M}$ can always be transformed [19] to canonical form by means of a unitary transformation U

$$\mathbb{M} = U \begin{pmatrix} 0 & \cdots & 0 & \beta_1 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & \ddots & 0 \\ 0 & \cdots & 0 & 0 & 0 & \beta_N \\ -\beta_1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \vdots & \ddots & \vdots \\ 0 & 0 & -\beta_N & 0 & \cdots & 0 \end{pmatrix} U^T = U\mathbb{M}_c U^T$$

and the $\beta_1, \ldots, \beta_N$ coefficients of the "canonical form" of the matrix $\mathbb{M}$ are real and positive. Introducing now the new Grassmann variables $\eta_\mu = \sum_{\mu'}(U^T)_{\mu\mu'} z_{\mu'}$ the exponent in the integrand of Eq. (5) becomes

$$\frac{1}{2}\sum_{\mu\mu'} \eta_\mu \mathbb{M}_{c\,\mu\mu'}\eta_{\mu'} = \sum_{k=1}^{N} \beta_k \eta_k^* \eta_k,$$

which is straightforward to integrate. The Jacobian of the transformation can be shown to be simply $\det(U^T) = \det(U)$. The remaining integrals can be performed easily being the result

$$\int d\eta^* d\eta e^{\beta\eta^*\eta} = -\beta.$$

The final expression for the overlap is then

$$\langle\phi_0|\phi_1\rangle = (-1)^N \det(U)\prod_{k=1}^{N}\beta_k.$$

This expression can be cast in terms of the pfaffian of a skew-symmetric matrix. The pfaffian of a skew-symmetric matrix (see, for instance, [20]) is a number obtained out of the matrix elements of the skew-symmetric matrix in a way quite similar to the one used to define the determinant (see Appendix A for details and properties used below). The connection between the product of β_i's and the pfaffian is a consequence of Eq. (A2) and reads $\prod_{k=1}^N \beta_k = (-1)^{N(N-1)/2}\mathrm{pf}(\mathbb{M}_c)$ where $\mathrm{pf}(\mathbb{M}_c)$ obviously denotes the pfaffian of $\mathbb{M}_c$. Using the property (A1) $\mathrm{pf}(\mathbb{M}) = \mathrm{pf}(U\mathbb{M}_c U^T) = \det(U)\mathrm{pf}(\mathbb{M}_c)$ the final result is obtained,

$$\langle\phi_0|\phi_1\rangle = s_N \mathrm{pf}(\mathbb{M}) = s_N \mathrm{pf}\begin{pmatrix} M^{(1)} & -\mathbb{1} \\ \mathbb{1} & -M^{(0)*}\end{pmatrix}, \tag{7}$$

where $s_N = (-1)^{N(N+1)/2}$. To make the connection with the standard formula for the overlap [2] the relation $\mathrm{pf}(A)^2 = \det A$ is used (and this is here where the sign is lost) to write

$$\langle\phi_0|\phi_1\rangle = \left(\det\begin{pmatrix} M^{(1)} & -\mathbb{1} \\ \mathbb{1} & -M^{(0)*}\end{pmatrix}\right)^{1/2}. \tag{8}$$

This expression reduces, by using standard formulas for the determinant of a bipartite matrix (see below), to

$$\langle\phi_0|\phi_1\rangle = (\det(\mathbb{1} - M^{(0)*}M^{(1)}))^{1/2} \tag{9}$$

which is the usual expression for the norm (Onishi formula). Please notice that in going from Eq. (7) to Eq. (8) the sign present in the first equation is lost as a consequence of the writing of the square of the pfaffian as a determinant. Also signs appearing in the manipulations needed to obtain Eq. (9) have been neglected. We clearly see that the sign problem appears in the standard formulas because of the wrong implicit use of the above relation between the pfaffian and the determinant.

If both HFB wave functions $|\phi_0\rangle$ and $|\phi_1\rangle$ share a common discrete symmetry like simplex or time reversal, then the matrices $M^{(i)}$ defining them can acquire a common block structure

$$M^{(i)} = \begin{pmatrix} 0 & \overline{M}^{(i)} \\ -\overline{M}^{(i)T} & 0 \end{pmatrix}$$

that can be used to simplify the result of Eq. (7). In this case

$$\mathbb{M} = \begin{pmatrix} 0 & \overline{M}^{(1)} & -\mathbb{1} & 0 \\ -\overline{M}^{(1)T} & 0 & 0 & -\mathbb{1} \\ \mathbb{1} & 0 & 0 & -\overline{M}^{(0)*} \\ 0 & \mathbb{1} & \overline{M}^{(0)+} & 0 \end{pmatrix}.$$

By exchanging blocks 2 and 4 we obtain

$$\mathrm{pf}(\mathbb{M}) = (-1)^N \mathrm{pf}\begin{pmatrix} 0 & 0 & -\mathbb{1} & \overline{M}^{(1)} \\ 0 & 0 & \overline{M}^{(0)+} & \mathbb{1} \\ \mathbb{1} & -\overline{M}^{(0)*} & 0 & 0 \\ -\overline{M}^{(1)T} & -\mathbb{1} & 0 & 0 \end{pmatrix}$$

that can be evaluated using Eq. (A2) to give

$$\langle\phi_0|\phi_1\rangle = \det\begin{pmatrix} -\mathbb{1} & \overline{M}^{(1)} \\ \overline{M}^{(0)+} & \mathbb{1} \end{pmatrix} = \det(\mathbb{1} + \overline{M}^{(0)+}\overline{M}^{(1)}). \tag{10}$$

Evaluation of statistical traces. Now I turn to the evaluation of the trace of density operators. In the statistical HFB theory the statistical density operator $\hat{\mathcal{D}}$ is given by the exponential of a one-body operator $\hat{\mathcal{D}} = \exp[\frac{1}{2}\sum_{\mu\nu}\gamma_\mu \mathcal{R}_{\mu\nu}\gamma_\nu]$ where γ_μ is a shorthand notation for $(\beta_1,\ldots,\beta_N,\beta_1^+,\ldots,\beta_N^+)$ and $\mathcal{R}$ is a skew-symmetric matrix of dimension $2N$ characterizing the density operator (see Ref. [12] for details). Another way to characterize the density operator is to define how it transforms quasiparticle creation and annihilation operators $\hat{\mathcal{D}}^{-1}\gamma_\mu\hat{\mathcal{D}} = \sum_\nu T_{\mu\nu}\gamma_\nu$ where the matrix $T = \exp(\sigma\mathcal{R})$ and $\sigma_{\mu\nu} = \{\gamma_\mu,\gamma_\nu\}$. Introducing the bipartite structure of T

$$T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$

the Balian and Brezin's decomposition [21] of $\hat{\mathcal{D}}$ is given by

$$\hat{\mathcal{D}} = e^{\frac{1}{2}\sum_{ij}\beta_i^+X_{ij}\beta_j^+}e^{-\frac{1}{2}\mathrm{Tr[Y]}}e^{\sum_{ij}\beta_i^+Y_{ij}\beta_j}e^{\frac{1}{2}\sum_{ij}\beta_iZ_{ij}\beta_j} \tag{11}$$

with $X = T_{12}T_{22}^{-1}$ and $Z = T_{22}^{-1}T_{21}$ skew-symmetric (as a consequence of the relation $T^T\sigma T = \sigma$ that T satisfies) and $\exp(-Y) = T_{22}^T$. To evaluate the trace of $\hat{\mathcal{D}}$ using fermion coherent states we have to use the formula [17]

$$\mathrm{Tr}(\hat{\mathcal{D}}) = \int d\mu(\mathbf{z})\langle -\mathbf{z}|\hat{\mathcal{D}}|\mathbf{z}\rangle, \tag{12}$$

where $|\mathbf{z}\rangle$ are again a set of fermion coherent states but chosen this time as eigenstates of the quasiparticle annihilation operators β_i, i.e., $\beta_i|\mathbf{z}\rangle = z_i|\mathbf{z}\rangle$. Using Eq. (11) the evaluation of the overlap between the fermion coherent states gives

$$\langle -\mathbf{z}|\hat{\mathcal{D}}|\mathbf{z}\rangle = e^{-\frac{1}{2}\mathrm{Tr[Y]}}e^{\frac{1}{2}\sum_{ij}z_i^*X_{ij}z_j^*}e^{\frac{1}{2}\sum_{ij}z_iZ_{ij}z_j} \times \langle -\mathbf{z}|e^{\sum_{ij}\beta_i^+Y_{ij}\beta_j}|\mathbf{z}\rangle.$$

To evaluate the remaining overlap the standard result $\exp(\sum_{ij}\beta_i^+Y_{ij}\beta_j)|\mathbf{z}\rangle = |e^Y\mathbf{z}\rangle$ used together with $\langle -\mathbf{z}|\mathbf{z}'\rangle = \exp(-\mathbf{z}^*\mathbf{z}')$ (see Refs. [15–17]) gives

$$\langle -\mathbf{z}|\hat{\mathcal{D}}|\mathbf{z}\rangle = e^{-\frac{1}{2}\mathrm{Tr[Y]}}e^{\frac{1}{2}\sum_{ij}z_i^*X_{ij}z_j^*}e^{-\sum_{ij}z_i^*(e^Y)_{ij}z_j} \times e^{\frac{1}{2}\sum_{ij}z_iZ_{ij}z_j}.$$

Combining this result with Eq. (12), the following integral is obtained:

$$\mathrm{Tr}(\hat{\mathcal{D}}) = e^{-\frac{1}{2}\mathrm{Tr[Y]}}\int\prod_k(dz_k^*dz_k)e^{\frac{1}{2}\sum_{\mu\mu'}z_{\mu'}\mathbb{M}_{\mu'\mu}z_\mu},$$

where the same notation as in Eq. (6) is used. In this case

$$\mathbb{M} = \begin{pmatrix} X & -(e^Y+\mathbb{1}) \\ (e^Y+\mathbb{1})^T & Z \end{pmatrix}.$$

Applying the same considerations as in the evaluation of the overlap we finally arrive to

$$\mathrm{Tr}(\hat{\mathcal{D}}) = s_N \exp\left(-\tfrac{1}{2}\mathrm{Tr[Y]}\right)\mathrm{pf}(\mathbb{M}),$$

where $s_N = (-1)^{N(N+1)/2}$. Taking into account the relationship between X, Z, and Y and the blocks of the matrix T the above result can be expressed as

$$\mathrm{Tr}(\hat{\mathcal{D}}) = s_N(\det T_{22})^{1/2}\,\mathrm{pf}\begin{pmatrix} T_{12}T_{22}^{-1} & -\left((T_{22}^T)^{-1}+\mathbb{1}\right) \\ \left((T_{22})^{-1}+\mathbb{1}\right) & T_{22}^{-1}T_{21} \end{pmatrix}.$$

The introduction of $(\det T_{22})^{1/2}$ in place of $\exp(-\frac{1}{2}\mathrm{Tr[Y]})$ can lead to the (right) conclusion that a sign indeterminacy has been introduced in the expression of the trace. The definition of $\hat{\mathcal{D}}$ in terms of the transformation matrix T leaves a phase open in the definition of the density operator which is also present in the expression of Eq. (11). A way to fix the phase is to require some condition like, for instance, the realness and positiveness of $\langle\phi_0|\hat{\mathcal{D}}|\phi_0\rangle = (\det T_{22})^{1/2}$ where $|\phi_0\rangle$ is the vacuum of the quasiparticle operators β_i entering in the definition of $\hat{\mathcal{D}}$. This condition implies the replacement of $(\det T_{22})^{1/2}$ by its modulus. Using property (A1) of the pfaffian the final result is obtained

$$\mathrm{Tr}(\hat{\mathcal{D}}) = s_N\frac{|\det T_{22}|^{1/2}}{\det T_{22}} \times \mathrm{pf}\begin{pmatrix} T_{12}T_{22}^{-1} & -(T_{22}^T+\mathbb{1}) \\ (T_{22}+\mathbb{1}) & T_{21}T_{22}^T \end{pmatrix}. \tag{13}$$

This result is apparently quite different from the standard one of [11,12], but after some tedious manipulations (see Appendix B) one can obtain the usual result.

Conclusions. I have used the technique of fermion coherent states to compute unambiguously the sign of the overlap of two HFB wave functions. The result given in terms of pfaffians is simpler to implement than previous considerations [6] based on pairwise degenerate eigenvalues of a general matrix and it is free from the uncertainties of other methods based on continuity arguments. Indications on how to evaluate efficiently the pfaffian are also given. Hopefully, this new method will help to simplify the implementation of ambitious projects like triaxial angular momentum projection. On the other hand, the method used is straightforwardly extended to the evaluation of the sign of the trace of statistical density operators which is a new result not considered previously in the literature.

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APPENDIX A

Definition, basic properties, and numerical evaluation of the pfaffian. The pfaffian of a skew-symmetric matrix R of dimension $2N$ and with matrix elements r_{ij} is defined as [20]

$$\mathrm{pf}(R)=\frac{1}{2^n}\frac{1}{n!}\sum_{\mathrm{Perm}}\epsilon(P)r_{i_1i_2}r_{i_3i_4}r_{i_5i_6}\ldots r_{2n-1,2n},$$

where the sum extends to all possible permutations of $i_1,\ldots,i_{2n}$ and $\epsilon(P)$ is the parity of the permutation. For matrices of odd dimension the pfaffian is by definition equal to zero. As an example, the pfaffian of a 2×2 matrix R is $\mathrm{pf}(R)=r_{12}$ and for a 4×4 one $\mathrm{pf}(R)=r_{12}r_{34}-r_{13}r_{24}+r_{14}r_{23}$. Similarly to the case of determinants, exchanging rows i and j and the same time columns i and j, multiplies the pfaffian by minus one. Other useful properties of the pfaffian are

$$\mathrm{pf}(P^TRP)=\det(P)\mathrm{pf}(R), \tag{A1}$$

$$\mathrm{pf}\begin{pmatrix}0 & R\\ -R^T & 0\end{pmatrix}=(-1)^{N(N-1)/2}\det(R), \tag{A2}$$

$$\mathrm{pf}(R)=(\det R)^{1/2}. \tag{A3}$$

A useful formula to compute pfaffians of small or simple matrices is

$$\mathrm{pf}(R)=\sum_j(-1)^{i+j-1}r_{ij}\mathrm{pf}(R_{ij}), \tag{A4}$$

where R_{ij} is the pfaffian-minor obtained by eliminating from R the two rows and two columns i and j.

The pfaffian of a complex skew-symmetric matrix R of dimension $2N$ is evaluated numerically by first reducing the matrix to tridiagonal form R_T. This reduction is accomplish by means of a set of $2(N-1)$ successive Householder transformations P_i exactly in the same way as in the standard reduction of a symmetric matrix to tridiagonal form [7]. We have $P_{2(N-1)}\ldots P_2P_1RP_1^TP_2^T\ldots P_{2(N-1)}^T=R_T$ with

$$R_T=\begin{pmatrix}0 & r_1 & 0 & 0 & \ldots & 0\\ -r_1 & 0 & r_2 & 0 & \ldots & 0\\ 0 & -r_2 & 0 & \ddots & \ldots & \vdots\\ 0 & 0 & \ddots & 0 & \ddots & 0\\ \vdots & \vdots & \ldots & \ddots & 0 & r_{2N-1}\\ 0 & 0 & \cdots & 0 & -r_{2N-1} & 0\end{pmatrix},$$

where the special structure of a skew-symmetric and tridiagonal matrix is evident. Using now Eq. (A1) we obtain $\det(P_1)\ldots\det(P_{2(N-1)})\mathrm{pf}(R)=\mathrm{pf}(R_T)$. As Householder matrices are Hermitian, unitary, and have determinant $\det(P_i)=-1$ we finally arrive to $\mathrm{pf}(R)=\mathrm{pf}(R_T)$. To evaluate the pfaffian of the tridiagonal matrix we use the minor expansion of Eq. (A4) that gives $\mathrm{pf}(R_T)=r_1r_3\ldots r_{2N-1}=\prod_{i=1}^N r_{2i-1}$.

APPENDIX B

Derivation of the standard formula for the trace. In this appendix the standard result of [12] for the trace of a density operator is deduced from Eq. (13). I start considering

$$\tilde{\mathbb{M}}=\begin{pmatrix}T_{12}T_{22}^{-1} & -\left(T_{22}^T+\mathbb{1}\right)\\ (T_{22}+\mathbb{1}) & T_{21}T_{22}^T\end{pmatrix}.$$

Using Eq. (A3) the pfaffian of $\tilde{\mathbb{M}}$ is written as the square root of its determinant, $\mathrm{pf}\tilde{\mathbb{M}}=\left(\det\tilde{\mathbb{M}}\right)^{1/2}$. By exchanging rows and columns conveniently

$$\det\tilde{\mathbb{M}}=(-)^N\begin{pmatrix}(T_{22}+\mathbb{1}) & T_{21}T_{22}^T\\ T_{12}T_{22}^{-1} & -\left(T_{22}^T+\mathbb{1}\right)\end{pmatrix}$$

and applying the formula of a bipartite determinant $\det\begin{pmatrix}A & B\\ C & D\end{pmatrix}=\det A\det(D-CA^{-1}B)$ the following result is obtained:

$$\det\tilde{\mathbb{M}}=\det T_{22}\det(\mathbb{1}+T_{22})\det\left(\mathbb{1}+\left(T_{22}^T\right)^{-1}+T_{12}T_{22}^{-1}(\mathbb{1}+T_{22})^{-1}T_{21}\right).$$

But $T_{11}=(T_{22}^T)^{-1}+T_{12}T_{22}^{-1}T_{21}$ and $T_{22}^{-1}[(\mathbb{1}+T_{22})^{-1}-\mathbb{1}]=-(\mathbb{1}+T_{22})^{-1}$ so that

$$\begin{aligned}\det\tilde{\mathbb{M}}&=\det T_{22}\det(\mathbb{1}+T_{22})\\&\quad\times\det(\mathbb{1}+T_{11}-T_{12}(\mathbb{1}+T_{22})^{-1}T_{21})\\&=\det T_{22}\det\begin{pmatrix}(T_{11}+\mathbb{1}) & T_{12}\\ T_{21} & (T_{22}+\mathbb{1})\end{pmatrix}.\end{aligned}$$

When the pfaffian is written as the square of the determinant the sign is lost and therefore phases are irrelevant in the derivation. Taking all this into account the result

$$\mathrm{Tr}(\hat{\mathcal{D}})=\left[\det\begin{pmatrix}(T_{11}+\mathbb{1}) & T_{12}\\ T_{21} & (T_{22}+\mathbb{1})\end{pmatrix}\right]^{1/2}$$

is obtained up to a sign, which is the sought formula of Ref. [12].

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