

Robust Formulation of Wick's theorem for Computing Matrix Elements Between Hartree–Fock–Bogoliubov Wavefunctions

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Numerical difficulties associated with computing matrix elements of operators between Hartree–Fock–Bogoliubov (HFB) wavefunctions have plagued the development of HFB-based many-body theories for decades. The problem arises from divisions by zero in the standard formulation of the nonorthogonal Wick's theorem in the limit of vanishing HFB overlap. In this paper, we present a robust formulation of Wick's theorem that stays well-behaved regardless of whether the HFB states are orthogonal or not. This new formulation ensures cancellation between the zeros of the overlap and the poles of the Pfaffian, which appears naturally in fermionic systems. Our formula explicitly eliminates self-interaction, which otherwise causes additional numerical challenges. A computationally efficient version of our formalism enables robust symmetry-projected HFB calculations with the same computational cost as mean-field theories. Moreover, we avoid potentially diverging normalization factors by introducing a robust normalization procedure. The resulting formalism treats even and odd number of particles on equal footing, and reduces to Hartree–Fock as a natural limit. As proof of concept, we present a numerically stable and accurate solution to a Jordan–Wigner-transformed Hamiltonian, whose singularities motivated the present work. Our robust formulation of Wick's theorem is a most promising development for methods using quasiparticle vacuum states.

I. INTRODUCTION

The Hartree–Fock–Bogoliubov (HFB) wavefunction is a fermionic mean-field ansatz allowing particle number symmetry breaking.^{1, 2} It encompasses the Hartree–Fock (HF) wavefunction in the same sense that spin-unrestricted HF (UHF) reduces to spin-restricted HF (RHF) without spin S^2 symmetry breaking. HFB-based methods are not as conventional in quantum chemistry as in nuclear structure theory. This is a consequence of repulsive electronic interactions in the former, which results in number symmetry not breaking spontaneously in mean-field.³

Nevertheless, the emergence of variation-after-projection approaches to symmetry breaking and restoration^{4–7} has sparked growing interest in HFB and related ansätze in electronic structure theory.^{6, 8–26} Methods based on symmetry-projected HFB (PHFB) are particularly promising for describing strongly correlated systems, where traditional HF-based methods fail.^{6, 27–29}

Essential for the implementation of PHFB-based methods are matrix elements of many-body operators between nonorthogonal HFB states. Indeed, the PHFB formalism can be considered a general form of nonorthogonal configuration interaction (NOCI).^{30, 31} The computation of relevant matrix elements relies on the generalized Wick's theorem with respect to nonorthogonal HFB states, also known as the nonorthogonal Wick's theorem.^{32, 33}

However, when the overlap between right and left HFB states vanishes, the standard formula in the nonorthogonal Wick's theorem becomes numerically ill-conditioned,

and eventually ill-defined, causing large round-off errors. This problem occurs in PHFB calculations^{34, 35} and is exacerbated by self-interaction^{36, 37} if exchange- or pairing-type contractions are neglected, *e.g.*, within the context of nuclear density functional theory.^{37–40}

Our recent work mapping spin systems to fermions using the Jordan–Wigner transformation^{41, 42} is another example where orthogonal HFB wavefunctions arise and lead to large numerical errors. This happens when fermionic on-site occupations are equal to 1/2, which is frequently encountered in frustrated phases of transformed spin systems.

The main objective of this paper is demonstrating that with proper algorithmic design, the nonorthogonal Wick's theorem can be extended to the orthogonal limit, resulting in accurate and efficient computation of matrix elements between arbitrary HFB states. Related algorithms have been discussed for HF-based NOCI,^{43–46} and our formalism reduces to them in that limit. Remedies for the numerical problems encountered in the HFB case have been proposed for specific applications^{34, 35} or under certain restrictions.^{47, 48} However, a universal, low-scaling formula for robust computation of matrix elements between HFB states, as the one presented here, was lacking.

II. NONORTHOGONAL WICK'S THEOREM

We define unnormalized HFB wavefunctions or *quasi-particle vacuum states*, $|\Phi_0\rangle$ and $|\Phi_1\rangle$, as

$$|\Phi_j\rangle = \prod_{p=1}^M \beta_p^j |-\rangle \quad (1)$$

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for $j = 0, 1$, where $|- \rangle$ denotes the physical vacuum, and M is the dimension of the one-particle (spin-orbital) basis. The Bogoliubov quasiparticle annihilation operators β_p^j are related to the fermionic particle operators $c_q^\dagger$ and c_q through a unitary canonical transformation known as the *Bogoliubov transformation*:

$$\beta_p^j = \sum_{q=1}^M (U_{qp}^{j*} c_q + V_{qp}^{j*} c_q^\dagger). \quad (2)$$

To ensure nonvanishing $|\Phi_j\rangle$, we assume that V^j is non-singular, *i.e.*, all of the canonical orbitals of $|\Phi_j\rangle$ obtained from the Bloch–Messiah decomposition⁴⁹ of U^j and V^j (*vide infra*) are at least infinitesimally occupied. We will eliminate this assumption and address the normalization of $|\Phi_j\rangle$ in Sec. V.

The nonorthogonal Wick’s theorem can be concisely stated using the *Pfaffian* as follows:⁵⁰ For $\langle \Phi_0 | \Phi_1 \rangle \neq 0$, a matrix element of a d -body operator is expressed as

$$\langle \Phi_0 | \gamma^1 \gamma^2 \cdots \gamma^{2d} | \Phi_1 \rangle = \langle \Phi_0 | \Phi_1 \rangle \text{pf}(\Gamma), \quad (3)$$

where $\{\gamma^k\}_{1 \leq k \leq 2d}$ is a set of arbitrary fermionic operators, and Γ is a $2d \times 2d$ antisymmetric matrix whose strict upper triangular part is defined by *contractions* of the form

$$\Gamma_{kl} = \overline{\gamma^k \gamma^l} = \frac{\langle \Phi_0 | \gamma^k \gamma^l | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \quad (4)$$

for $k < l$. The Pfaffian $\text{pf}(\Gamma)$ automatically generates all possible full contractions of the fermionic operators

with the correct signs, reflecting the fermionic anticommutation relations. For example, Eq. (3) reduces to the conventional statement of the nonorthogonal Wick’s theorem^{1,2,32,33} for the two-particle reduced transition matrix (2-RTM),^{51–53} or second-order transition density matrix:

$$\begin{aligned} \mathcal{D}_{pq,p'q'}^{(2)} &= \langle \Phi_0 | c_p^\dagger c_q^\dagger c_{q'} c_{p'} | \Phi_1 \rangle \\ &= \langle \Phi_0 | \Phi_1 \rangle (\overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} + \overline{c_p^\dagger c_q^\dagger c_{p'} c_{q'}} + \overline{c_p^\dagger c_{q'} c_q c_{p'}}) \\ &= \langle \Phi_0 | \Phi_1 \rangle (\rho_{p'p}^{01} \rho_{q'q}^{01} - \rho_{p'q}^{01} \rho_{q'p}^{01} + \kappa_{pq}^{10*} \kappa_{p'q'}^{01}), \end{aligned} \quad (5)$$

where

$$\rho_{pq}^{01} = \overline{c_q^\dagger c_p}, \quad \kappa_{pq}^{01} = \overline{c_q c_p}, \quad \kappa_{pq}^{10*} = \overline{c_p^\dagger c_q^\dagger}, \quad (6)$$

and we follow the convention that each crossing between contraction lines introduces a minus sign, which is implied by the properties of the Pfaffian. In general, we can write γ^k as a quasiparticle

$$\gamma^k = \sum_{q=1}^M (A_{qk}^* c_q + B_{qk}^* c_q^\dagger), \quad (7)$$

where A and B are $M \times 2d$ matrices. Note that for $k \neq l$, γ^k and γ^l may come from different Bogoliubov transformations, hence the superscript in our notation.

We see from Eq. (4) that the nonorthogonal Wick’s theorem becomes ill-defined when $\langle \Phi_0 | \Phi_1 \rangle = 0$. In this case, we may fall back to the original Wick’s theorem with respect to the physical vacuum.^{54–56} We have⁵⁷

$$\langle \Phi_0 | \gamma^1 \gamma^2 \cdots \gamma^{2d} | \Phi_1 \rangle = (-1)^{M(M-1)/2} \langle - | \beta_1^{0\dagger} \beta_2^{0\dagger} \cdots \beta_M^{0\dagger} \gamma^1 \gamma^2 \cdots \gamma^{2d} \beta_1^1 \beta_2^1 \cdots \beta_M^1 | - \rangle \quad (8a)$$

$$= (-1)^{M(M-1)/2} \text{pf} \begin{pmatrix} V^0 \text{T} U^0 & V^0 \text{T} B^* & V^0 \text{T} V^{1*} \\ -B^\dagger V^0 & \Gamma^{(-)} & A^\dagger V^{1*} \\ -V^{1\dagger} V^0 & -V^{1\dagger} A^* & U^{1\dagger} V^{1*} \end{pmatrix}, \quad (8b)$$

where $\Gamma^{(-)}$ is a $2d \times 2d$ antisymmetric matrix defined by

$$\Gamma_{kl}^{(-)} = \langle - | \gamma^k \gamma^l | - \rangle \quad (9)$$

for $k < l$. Compared with Eq. (3), Eq. (8) is always well-defined, but the Pfaffian of a much larger matrix needs to be evaluated, greatly increasing the computational cost.

In the following, we sketch a proof of the nonorthogonal Wick’s theorem stated in Eq. (3), introducing our notation along the way. Unlike the proof by induction presented in Ref. 50, our proof follows a more direct approach inspired by Ref. 58. We start by rewriting Eq. (8) using the properties of the Pfaffian:

$$\langle \Phi_0 | \gamma^1 \gamma^2 \cdots \gamma^{2d} | \Phi_1 \rangle = (-1)^{M(M-1)/2} \text{pf}(\mathcal{M}), \quad (10)$$

where

$$\mathcal{M} = \begin{pmatrix} \mathcal{S} & \mathcal{G} \\ -\mathcal{G}^\text{T} & \Gamma^{(-)} \end{pmatrix}, \quad (11)$$

$$\mathcal{S} = \begin{pmatrix} V^0 \text{T} U^0 & V^0 \text{T} V^{1*} \\ -V^{1\dagger} V^0 & U^{1\dagger} V^{1*} \end{pmatrix}, \quad \mathcal{G} = \mathcal{V}^\text{T} \mathcal{C}^* \quad (12)$$

and

$$\mathcal{V} = \begin{pmatrix} 0 & -V^{1*} \\ V^0 & 0 \end{pmatrix}, \quad \mathcal{C} = \begin{pmatrix} A \\ B \end{pmatrix}. \quad (13)$$

When $\langle \Phi_0 | \Phi_1 \rangle \neq 0$, the $2M \times 2M$ antisymmetric matrix $\mathcal{S}$ is non-singular since⁵⁷

$$\langle \Phi_0 | \Phi_1 \rangle = (-1)^{M(M-1)/2} \text{pf}(\mathcal{S}). \quad (14)$$

We therefore have the Pfaffian identity

$$\text{pf}(\mathcal{M}) = \text{pf}(\mathcal{S})\text{pf}(\mathcal{M}/\mathcal{S}), \quad (15)$$

where $\mathcal{M}/\mathcal{S}$ denotes the Schur complement of the block $\mathcal{S}$ of the supermatrix $\mathcal{M}$, *i.e.*,

$$\mathcal{M}/\mathcal{S} = \Gamma^{(-)} + \mathcal{G}^T \mathcal{S}^{-1} \mathcal{G}. \quad (16)$$

On the other hand, as shown in detail in the supplementary material, we find

$$\mathcal{K} = \mathcal{V} \mathcal{S}^{-1} \mathcal{V}^T = \begin{pmatrix} -\kappa^{01} & -\rho^{01} \\ \rho^{01T} & \kappa^{10*} \end{pmatrix}, \quad (17)$$

and it follows that

$$\mathcal{M}/\mathcal{S} = \Gamma^{(-)} + \mathcal{C}^\dagger \mathcal{K} \mathcal{C}^* = \Gamma. \quad (18)$$

Inserting Eqs. (14) and (18) into Eqs. (10) and (15) completes the proof.

Without loss of generality, we hereafter assume that $\gamma^1 \gamma^2 \dots \gamma^{2d}$ are particle operators in normal order with respect to the physical vacuum. Thus, we have $\Gamma^{(-)} = 0_{2d \times 2d}$ and

$$\langle \Phi_0 | \gamma^1 \gamma^2 \dots \gamma^{2d} | \Phi_1 \rangle = (-1)^{M(M-1)/2} \text{pf}(\mathcal{S}) \text{pf}(\mathcal{G}^T \mathcal{S}^{-1} \mathcal{G}). \quad (19)$$

These particular matrix elements contain those that arise in the d -particle or d th-order reduced transition matrix (d -RTM),^{51–53}

$$\mathcal{D}_{p_1 p_2 \dots p_d, q_1 q_2 \dots q_d}^{(d)} = \langle \Phi_0 | c_{p_1}^\dagger c_{p_2}^\dagger \dots c_{p_d}^\dagger c_{q_d} \dots c_{q_2} c_{q_1} | \Phi_1 \rangle. \quad (20)$$

Eq. (19) is reminiscent of Löwdin's formula for d -RTM between HF wavefunctions,⁵⁹ for which singular value decomposition (SVD) can be used to extract the zeros and poles in order to evaluate the zero-overlap limit.^{43–46} We show in the next section that this idea can be generalized to the HFB case.

III. ROBUST WICK'S THEOREM

The antisymmetric matrix $\mathcal{S}$ can be written in canonical form,^{60,61}

$$\mathcal{S} = \mathcal{Q} \bar{\mathcal{S}} \mathcal{Q}^T, \quad (21)$$

where $\mathcal{Q}$ is unitary and

$$\bar{\mathcal{S}} = \begin{pmatrix} 0 & \text{diag}(s) \\ -\text{diag}(s) & 0 \end{pmatrix}. \quad (22)$$

The elements of the vector s are nonnegative and they reduce to the singular values of the overlap matrix in the HF case, as shown in the supplementary material. Moreover, it follows from Eq. (14) that

$$\langle \Phi_0 | \Phi_1 \rangle = \zeta \prod_r s_r, \quad (23)$$

where $\zeta = \det(\mathcal{Q})$ is a complex phase factor. We observe that the poles of $\mathcal{S}^{-1}$ in Eq. (19) get cancelled out by the zeros of the overlap, hinting at a more general and robust formula for computing matrix elements.

Define

$$\tilde{\mathcal{K}}^r = \begin{pmatrix} -\tilde{\kappa}^{01,r} & -\tilde{\rho}^{01,r} \\ (\tilde{\rho}^{01,r})^T & (\tilde{\kappa}^{10,r})^* \end{pmatrix} \quad (24)$$

where

$$\tilde{\rho}_{pq}^{01,r} = [L_{11}]_{pr} [L_{22}]_{qr} - [L_{12}]_{pr} [L_{21}]_{qr}, \quad (25a)$$

$$\tilde{\kappa}_{pq}^{01,r} = [L_{11}]_{pr} [L_{12}]_{qr} - [L_{12}]_{pr} [L_{11}]_{qr}, \quad (25b)$$

$$(\tilde{\kappa}_{pq}^{10,r})^* = [L_{22}]_{pr} [L_{21}]_{qr} - [L_{21}]_{pr} [L_{22}]_{qr}, \quad (25c)$$

and

$$\mathcal{L} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} = \mathcal{V} \mathcal{Q}^* \quad (26)$$

It is straightforward to show

$$\Gamma = \sum_r s_r^{-1} \tilde{\Gamma}^r, \quad \tilde{\Gamma}^r = \mathcal{C}^\dagger \tilde{\mathcal{K}}^r \mathcal{C}^*. \quad (27)$$

We now propose a robust formulation of Wick's theorem for computing matrix elements between HFB wavefunctions:

$$\begin{aligned} \langle \Phi_0 | \gamma^1 \gamma^2 \dots \gamma^{2d} | \Phi_1 \rangle &= (2d-1)!! \zeta \\ &\times \sum_{r_1 r_2 \dots r_d} \lambda_{r_1 r_2 \dots r_d} \text{hpf}(\tilde{\Gamma}^{r_1} \otimes \tilde{\Gamma}^{r_2} \otimes \dots \otimes \tilde{\Gamma}^{r_d}) \end{aligned} \quad (28)$$

with

$$\lambda_{r_1 \dots r_d} = \begin{cases} \prod_{r \neq r_1, \dots, r_d} s_r & (r_1, \dots, r_d \text{ are distinct}) \\ 0 & (\text{otherwise}) \end{cases} \quad (29)$$

$$\begin{aligned} \text{hpf}(\tilde{\Gamma}^{r_1} \otimes \tilde{\Gamma}^{r_2} \otimes \dots \otimes \tilde{\Gamma}^{r_d}) &= \\ \frac{1}{(2d)!} \sum_{\sigma \in S_{2d}} \text{sgn}(\sigma) \tilde{\Gamma}_{\sigma(1)\sigma(2)}^{r_1} \tilde{\Gamma}_{\sigma(3)\sigma(4)}^{r_2} \dots \tilde{\Gamma}_{\sigma(2d-1)\sigma(2d)}^{r_d} \end{aligned} \quad (30)$$

where $\otimes$ denotes tensor product, σ enumerates permutations in the symmetric group S_{2d} , and $\text{sgn}(\sigma)$ is the signature of σ . Eq. (30) defines a special case of the *hyper-Pfaffian*,^{62,63} denoted by $\text{hpf}(\cdot)$, which generalizes the Pfaffian to tensors. For the general definition of the hyper-Pfaffian, we refer the reader to the supplementary material.

The proof of the theorem is presented in the supplementary material. We emphasize that the formula in Eq. (28) remains well-behaved with vanishing $\langle \Phi_0 | \Phi_1 \rangle$ because all potential divisions by zero have been prevented by construction. Specifically, all s_r^{-1} factors are cancelled out by the factors of $\langle \Phi_0 | \Phi_1 \rangle$ in Eq. (23), while all terms involving s_r^{-2} , s_r^{-3} , *etc.*, drop out due to the

cancellation of self-interaction. The latter is guaranteed by the properties of the Pfaffian and is further enforced numerically by setting $\lambda_{r_1 \dots r_d}$ to zero when its indices are not distinct. From the definition of $\lambda_{r_1 \dots r_d}$, we can also see that the matrix element vanishes if the number of zero elements in s exceeds d , consistent with the Slater–Condon rules between HF wavefunctions;^{51,64,65} see the next section for generalization to the HFB case.

In practical calculations, we do not need to explicitly evaluate the hyper-Pfaffian for each individual matrix element. Instead, Eq. (28) generates expressions of high-order RTMs in terms of the modified contractions defined in Eq. (25). As an example, the robust Wick’s theorem implies the following expression of the 2-RTM:

$$\begin{aligned} \mathcal{D}_{pq,p'q'}^{(2)} &= \langle \Phi_0 | \overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} + \overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} + \overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} | \Phi_1 \rangle \\ &= \zeta \sum_{r_1 r_2} \lambda_{r_1 r_2} \left(\tilde{\rho}_{p'p}^{01,r_1} \tilde{\rho}_{q'q}^{01,r_2} - \tilde{\rho}_{p'q}^{01,r_1} \tilde{\rho}_{q'p}^{01,r_2} \right. \\ &\quad \left. + (\tilde{\kappa}_{pq}^{10,r_1})^* \tilde{\kappa}_{p'q'}^{01,r_2} \right), \end{aligned} \quad (31)$$

where we have used $\lambda_{r_1 r_2} = \lambda_{r_2 r_1}$. Computing the full 2-RTM using Eq. (31) scales as $\mathcal{O}(M^5)$. In practice, however, we never construct the full 2-RTM. To compute the

matrix element of a two-body operator, we can directly contract its parameters (*e.g.*, two-electron integrals) with the factorized form of the 2-RTM in Eq. (31). For example, the tensor contraction between the two-electron integrals and the 2-RTM should scale as $\mathcal{O}(M^3)$ to $\mathcal{O}(M^4)$ after exploiting locality using standard techniques.^{66–68}

IV. LOW-SCALING VERSION

We may further reduce the scaling by enforcing the cancellation only of the smallest elements in s . We partition Γ into singular (S) and regular (R) parts according to

$$\Gamma = \Gamma^S + \Gamma^R = \sum_{r \in S} s_r^{-1} \tilde{\Gamma}^r + \Gamma^R, \quad (32)$$

where $S = \{s_r < \epsilon \mid 1 \leq r \leq M, \epsilon > 0\}$. The value of ϵ should be so chosen that Γ^R is well-conditioned while the size of S is small. Similarly, we define $\rho^{01,R}$, $\kappa^{01,R}$, and $\kappa^{10,R}$ as the regular parts of ρ^{01} , κ^{01} , and κ^{10} , respectively. By the properties of the hyper-Pfaffian, we can now establish a low-scaling robust Wick’s theorem, which states that

$$\begin{aligned} \langle \Phi_0 | \gamma^1 \gamma^2 \dots \gamma^{2d} | \Phi_1 \rangle &= \zeta \lambda^R \left(\lambda^S \text{pf}(\Gamma^R) + (2d-1)!! \binom{d}{1} \sum_{r_1 \in S} \lambda_{r_1}^S \text{hpf}(\tilde{\Gamma}^{r_1} \otimes (\Gamma^R)^{\otimes(d-1)}) \right. \\ &\quad + (2d-1)!! \binom{d}{2} \sum_{r_1, r_2 \in S} \lambda_{r_1 r_2}^S \text{hpf}(\tilde{\Gamma}^{r_1} \otimes \tilde{\Gamma}^{r_2} \otimes (\Gamma^R)^{\otimes(d-2)}) \\ &\quad \left. + \dots + (2d-1)!! \sum_{r_1, r_2, \dots, r_d \in S} \lambda_{r_1 r_2 \dots r_d}^S \text{hpf}(\tilde{\Gamma}^{r_1} \otimes \tilde{\Gamma}^{r_2} \otimes \dots \otimes \tilde{\Gamma}^{r_d}) \right), \end{aligned} \quad (33)$$

where

$$\lambda^S = \prod_{r \in S} s_r, \quad \lambda^R = \prod_{r \notin S} s_r, \quad (34a)$$

$$\lambda_{r_1 \dots r_d}^S = \begin{cases} \prod_{S \ni r \neq r_1, \dots, r_d} s_r & (r_1, \dots, r_d \text{ are distinct}) \\ 0 & (\text{otherwise}) \end{cases} \quad (34b)$$

and we have used

$$\underbrace{\text{hpf}(\Gamma^R \otimes \dots \otimes \Gamma^R)}_d = \text{hpf}((\Gamma^R)^{\otimes d}) = \frac{\text{pf}(\Gamma^R)}{(2d-1)!!} \quad (35)$$

If S is empty, Eq. (33) reduces to the nonorthogonal Wick’s theorem in Eq. (3).

Applying the low-scaling robust Wick’s theorem to 2-RTM, we have

$$\begin{aligned} \langle \Phi_0 | \overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} | \Phi_1 \rangle &= \\ \zeta \lambda^R &\left(\lambda_{pq}^S \rho_{p'q'}^{01,R} + \sum_{r_1 \in S} \lambda_{r_1}^S \tilde{\rho}_{pq}^{01,r_1} \rho_{p'q'}^{01,R} \right. \\ &\quad \left. + \sum_{r_1 \in S} \lambda_{r_1}^S \rho_{pq}^{01,R} \tilde{\rho}_{p'q'}^{01,r_1} + \sum_{r_1, r_2 \in S} \lambda_{r_1 r_2}^S \tilde{\rho}_{pq}^{01,r_1} \tilde{\rho}_{p'q'}^{01,r_2} \right) \end{aligned} \quad (36)$$

and similarly for $\langle \Phi_0 | \overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} | \Phi_1 \rangle$ and $\langle \Phi_0 | \overline{c_p^\dagger c_q^\dagger c_{q'} c_{p'}} | \Phi_1 \rangle$. Each term in the above expression stays factorized, facilitating low-scaling tensor contractions with the electron integrals. Besides, the indices r_1, r_2 now only run over a small subset of s

elements. As a result, the computational cost of the matrix element of a two-body operator scales the same as that of HF, *i.e.*, $\mathcal{O}(M^2)$ to $\mathcal{O}(M^3)$, albeit with a larger prefactor. For d -RTM with $2 < d \ll M$, the reduction of computational scaling from Eq. (28) to Eq. (33) is even more significant.

We can now generalize the Slater–Condon rules to the HFB case using the low-scaling robust Wick’s theorem. Let μ be the number of s elements that are strictly zero. Loosely speaking, μ equals the smallest number of levels we need to block in both $|\Phi_0\rangle$ and $|\Phi_1\rangle$ in order to make them nonorthogonal. The blocking should be done in a biorthogonal basis that simultaneously brings both $|\Phi_0\rangle$ and $|\Phi_1\rangle$ to the canonical form of the Bardeen–Cooper–Schrieffer (BCS) ansatz.^{47,48,69} This biorthogonal basis is generally nonunitary and does not always exist as noted in Ref. 48. It is readily seen from Eq. (33) that the λ^S term vanishes for $\mu = 1$, the λ^S and $\lambda_{r_1}^S$ terms vanish for $\mu = 2$, and so forth. These results resemble the generalized Slater–Condon rules for HF transition matrix elements,^{44,46,70} in which case μ corresponds to the smallest number of biorthogonal occupied orbital pairs that need to be emptied in order to make the HF wavefunctions nonorthogonal. Here the biorthogonalization is guaranteed by Löwdin pairing and realized by SVD.^{71–73} We should point out that, as opposed to the generalized Slater–Condon rules, our Eq. (33) also ensures numerical stability when some elements of s are small but not strictly zero.

V. ROBUST NORMALIZATION

So far we have considered unnormalized HFB wavefunctions $|\Phi_j\rangle$ for $j = 0, 1$ as defined in Eq. (1). The corresponding normalized HFB wavefunction is⁵⁷

$$|\Phi'_j\rangle = \frac{\det(C^j)}{\prod_{p=1}^{m_P^j} v_p^j} |\Phi_j\rangle, \quad (37)$$

where C^j and v^j come from the Bloch–Messiah decomposition,⁴⁹

$$U^j = D^j \bar{U}^j C^j, \quad V^j = (D^j)^* \bar{V}^j C^j \quad (38)$$

with D^j and C^j being unitary and

$$\bar{U}^j = \begin{pmatrix} 0_{M_C^j \times M_C^j} & \\ & -\bigoplus_{p=1}^{m_P^j} i\sigma_y u_p^j \\ & & I_{M_V^j} \end{pmatrix}, \quad (39a)$$

$$\bar{V}^j = \begin{pmatrix} I_{M_C^j} & \\ & \bigoplus_{p=1}^{m_P^j} I_2 v_p^j \\ & & 0_{M_V^j \times M_V^j} \end{pmatrix}. \quad (39b)$$

Here I_k denotes the $k \times k$ identity matrix, and σ_y denotes the y -component of the 2×2 Pauli matrices; u_p^j, v_p^j are positive real numbers and satisfy $(u_p^j)^2 + (v_p^j)^2 = 1$. Note that we use an unconventional definition of $(\bar{U}^j, \bar{V}^j)$ in Eq. (39), which is physically inconsequential but will ease the notation in what follows. The Bloch–Messiah decomposition implies that, in the canonical basis of $|\Phi_j\rangle$ with orbital coefficients D^j , we have M_C^j fully occupied core orbitals, $2m_P^j$ paired fractionally occupied orbitals, and M_V^j unoccupied or virtual orbitals, with $M_C^j + 2m_P^j + M_V^j = M$.

The normalization factor in Eq. (37) is generally unbounded, which may introduce additional numerical challenges. To overcome this problem, we define a set of unnormalized quasiparticles by an unnormalized Bogoliubov transformation:

$$\beta_p^{j'} = \sum_{q=1}^M \left((U_{qp}^{j'})^* c_q + (V_{qp}^{j'})^* c_q^\dagger \right) \quad (40)$$

for $1 \leq p \leq M_C^j + 2m_P^j$, with

$$U^{j'} = D^{j'} \bar{U}^{j'} (\bar{V}^{j'})^{-\frac{1}{2}}, \quad V^{j'} = (D^{j'})^* (\bar{V}^{j'})^{\frac{1}{2}}, \quad (41)$$

where $D^{j'}$ is built from the first $M_C^j + 2m_P^j$ columns of D^j as suggested in Ref. 74, and

$$\bar{U}^{j'} = \begin{pmatrix} 0_{M_C^j \times M_C^j} & \\ & -\bigoplus_{p=1}^{m_P^j} i\sigma_y u_p^j \end{pmatrix}, \quad (42a)$$

$$\bar{V}^{j'} = \begin{pmatrix} I_{M_C^j} & \\ & \bigoplus_{p=1}^{m_P^j} I_2 v_p^j \end{pmatrix}. \quad (42b)$$

It is readily shown that the normalized HFB wavefunction $|\Phi'_j\rangle$ is the vacuum state of a set of unnormalized quasiparticles, *i.e.*,

$$|\Phi'_j\rangle = \prod_{p=1}^{M_C^j + 2m_P^j} \beta_p^{j'} |-\rangle. \quad (43)$$

Furthermore,

$$\mathcal{S}' = \begin{pmatrix} (V^{0'})^T U^{0'} & (V^{0'})^T (V^{1'})^* \\ - (V^{1'})^\dagger V^{0'} & (U^{1'})^\dagger (V^{1'})^* \end{pmatrix} \quad (44a)$$

$$= \begin{pmatrix} \bar{U}^{0'} & (V^{0'})^T (V^{1'})^* \\ - (V^{1'})^\dagger V^{0'} & -\bar{U}^{1'} \end{pmatrix}, \quad (44b)$$

whose elements are bounded by 1 in absolute value even though $U^{j'}$ is generally unbounded. Therefore, we no longer have to deal with the problematic normalization

factor in Eq. (37) as long as we compute the overlap between normalized HFB wavefunctions using

$$\langle \Phi'_0 | \Phi'_1 \rangle = (-1)^{(M_C^0 + 2m_P^0)(M_C^0 + 2m_P^0 - 1)/2} \text{pf}(\mathcal{S}'). \quad (45)$$

This procedure for computing the overlap is similar to the one proposed in Ref. 75; however, we emphasize that our formalism, as opposed to those in Refs. 57 and 75, treats even- and odd-particle systems on the same footing, since the number of core orbitals M_C^j from the Bloch–Messiah decomposition is not restricted to be even. Other formalisms for equally accounting for even and odd number parities have been suggested, without addressing the numerical pitfalls of the unbounded normalization factors.^{76–78}

More importantly, our robust normalization procedure for computing the overlap is compatible with the robust Wick’s theorem and its low-scaling version. Namely, Eqs. (28) and (33) remain valid for the d -RTM between the normalized $|\Phi'_0\rangle$ and $|\Phi'_1\rangle$ after formally replacing (U^j, V^j) with $(U^{j'}, V^{j'})$, or equivalently replacing $\mathcal{S}$ with $\mathcal{S}'$ and $\mathcal{V}$ with

$$\mathcal{V}' = \begin{pmatrix} 0 & -(V^{1'})^* \\ V^{0'} & 0 \end{pmatrix}. \quad (46)$$

This correspondence is apparent from Eq. (19), whose derivation does not rely on the normalization of the Bogoliubov transformations.

Finally, we note in passing that, when $m_P^j = 0$, $|\Phi'_j\rangle$ reduces to a HF wavefunction, so the robust Wick’s theorem and its low-scaling variant can also be used to compute HF reduced transition matrices (see the supplementary material). All pairing-type contractions are removed in this case due to vanishing κ^{01} and κ^{10} .

VI. NUMERICAL EXAMPLE

We here present a prototypical example to demonstrate the power of our proposed robust Wick’s theorem. The Heisenberg XXZ Hamiltonian can be treated as a fermionic system after Jordan–Wigner (JW) transformation. The claim to fame of this mapping is that in 1D at $\Delta = 0$, a maximally degenerate point, the transformed Hamiltonian becomes a free fermion system readily solvable by mean-field HF theory. Here, Δ is the anisotropy parameter. We refer the reader to Ref. 42 for details of the transformed Hamiltonian. For $\Delta < 0$, number symmetry breaks spontaneously, necessitating HFB solutions. Matrix elements of the form

$$\langle \Phi | c_p^\dagger c_q | \Phi^{pq} \rangle = \langle \Phi | c_p^\dagger c_q \phi_p \phi_q | \Phi \rangle \quad (47)$$

need to be computed for $1 \leq p < q \leq M$, where the JW string

$$\phi_p = \prod_{q < p} (1 - 2n_q) = \exp(i\pi \sum_{q < p} n_q) \quad (48)$$

is a Thouless rotation acting on $|\Phi\rangle$ with $n_q = c_q^\dagger c_q$. The overlap

$$\langle \Phi | \Phi^{pq} \rangle = \langle \Phi | \phi_p \phi_q | \Phi \rangle = \langle \Phi | \prod_{r=p}^{q-1} (1 - 2n_r) | \Phi \rangle \quad (49)$$

vanishes when $\langle \Phi | n_r | \Phi \rangle = 1/2$ for $p \leq r < q$, a situation we observe across the critical $-1 \lesssim \Delta \lesssim 1$ region of the 1D phase diagram. On the other hand, because XXZ possess only nearest neighbor interactions, one can avoid dealing with JW strings all together, and analytically show that

$$\langle \Phi | c_p^\dagger c_{p+1} | \Phi^{p,p+1} \rangle = -\langle \Phi | c_p^\dagger c_{p+1} | \Phi \rangle. \quad (50)$$

The right hand side of Eq. (50) is numerically well-posed because $\langle \Phi | \Phi \rangle = 1$, after applying the normalization procedure in Sec. V. Therefore, we have two analytically equivalent forms of evaluating the same matrix elements. Comparing numerical results from Eq. (47), which generates orthogonal HFB states, and Equation (50), we can measure the round-off errors due to vanishing $\langle \Phi | \Phi^{pq} \rangle$ and verify that our robust Wick’s theorem eliminates them.

Consider a JW-transformed 8-site XXZ chain with open boundary conditions. We constrain $\langle \Phi | \sum_p n_p | \Phi \rangle = M/2$, which corresponds to $\langle S^z \rangle = 0$. We find that $\langle \Phi | \Phi^{p,p+1} \rangle = 0$ for all $1 \leq p < M$ with $-1.12 \leq \Delta \leq 0.98$. We observe equal site occupations ($\langle S_p^z \rangle = 0$ in the original spin representation) within this range of Δ values, consistent with our previous calculations using a spin antisymmetrized geminal power ansatz.⁷⁹ As shown in Fig. 1, the HFB energies obtained from Eq. (47) using the nonorthogonal Wick’s theorem indeed suffer from severe numerical error in this regime. In contrast, the robust Wick’s theorem, yields energies on top of the exact results computed without JW strings using Eq. (50).

VII. CONCLUDING REMARKS

In quantum mechanical calculations with nonorthogonal basis, negligible overlaps do not necessarily imply negligible interactions, as one might erroneously infer from the nonorthogonal Wick’s theorem in Eq. (3), where the matrix element is proportional to the overlap $\langle \Phi_0 | \Phi_1 \rangle$. The fallacy originates from the fact that Eq. (3) is ill-defined when $\langle \Phi_0 | \Phi_1 \rangle = 0$, as shown by our formal and numerical analyses. Accurate computation of the matrix element requires evaluating the limit of Eq. (3) as $\langle \Phi_0 | \Phi_1 \rangle \rightarrow 0$, which is always well-defined and can be nonzero in general.

The idea of taking the limit before numerical evaluation is a recurring theme of this paper. It underlies how we resolve the two major limitations of the standard formulation of the nonorthogonal Wick’s theorem:

- First, when $\langle \Phi_0 | \Phi_1 \rangle$ vanishes, the Pfaffian in Eq. (3) develop poles even after self-interaction is

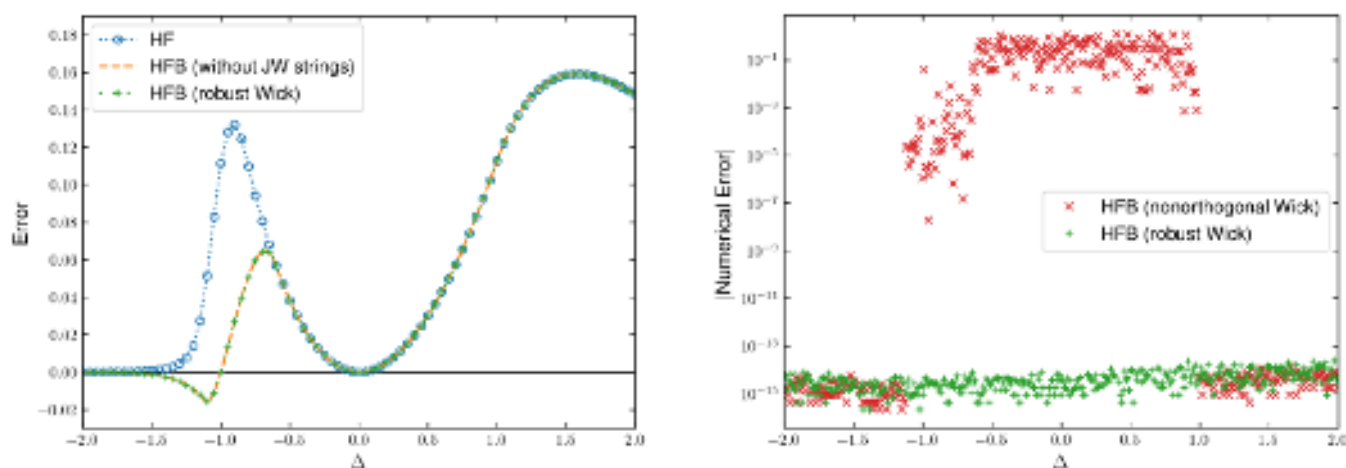


FIG. 1. Energy errors for the 8-site XXZ chain with $\langle S^z \rangle = 0$. Left panel: Errors with respect to the full configuration interaction (FCI) energy. Hartree–Fock (HF) results are plotted to show symmetry breaking. Right panel: Numerical errors in absolute value with respect to the Hartree–Fock–Bogoliubov (HFB) energy computed without Jordan–Wigner (JW) strings according to Eq. (50).

eliminated. We have addressed this issue in Sec. III by cancelling these poles with the zeros of the overlap. The resulting robust formulation of Wick’s theorem is universally applicable and numerically stable for computing matrix elements between HFB wavefunctions. And it remains amenable to efficient implementation as shown in Sec. IV.

- Second, the normalization factors for $|\Phi_0\rangle$ and $|\Phi_1\rangle$ may become divergently large. We have addressed this issue in Sec. V by introducing a robust normalization procedure. This is achieved by formally viewing normalized HFB wavefunctions as vacuum states of unnormalized quasiparticles. Although the coefficients defining these unnormalized quasiparticles are unbounded in general, the S' and V' matrices entering the final expressions for the matrix elements remains bounded.

We expect the present work to have a broad impact in quantum many-body theories, facilitating future developments of methods based on quasiparticle vacuum states. One promising area of application is HFB-based NOCI or generator coordinate method (GCM) in general.^{30,31} Not only do these methods recover important ground-state correlations,^{6,12} but they are also expected to be suitable for describing excited states, particularly those of charge transfer or double excitation character.^{80–82} Moreover, PHFB is closely related to geminal theories.^{6,83–85} Our formalism can be applied to compute matrix elements between number-projected HFB (NHFB) or antisymmetrized geminal power (AGP) states, especially for ones that do not share the same set of canonical orbitals. Another potential application is correlated methods using HFB or PHFB as the reference state.^{18,24,86–88} Reduced transition matrices encountered in these methods are typically of high order, for which the low-scaling ver-

sion of our robust Wick’s theorem becomes useful.

SUPPLEMENTARY MATERIAL

The supplementary material contains definitions of the Pfaffian and hyper-Pfaffian along with detailed proofs of equations and theorems in main text. We also show therein how our robust formulation of Wick’s theorem reduces to the RTM expressions in Ref. 43 in the Hartree–Fock limit.

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