On the off-diagonal Wick’s theorem and Onishi formula

Alternative and consistent approach to off-diagonal operator and norm kernels

A. Porro\textsuperscript{1,4}, T. Duguet\textsuperscript{1,2}

1 IRFU, CEA, Universit\'e Paris-Saclay, 91191 Gif-sur-Yvette, France
2 Department of Physics and Astronomy, Instituut voor Kern- en Stralingsfysica, KU Leuven, 3001 Leuven, Belgium

Received: 8 June 2022 / Accepted: 21 September 2022 / Published online: 18 October 2022
© The Author(s), under exclusive licence to Società Italiana di Fisica and Springer-Verlag GmbH Germany, part of Springer Nature 2022
Communicated by Michael Bender

Abstract The projected generator coordinate method based on the configuration mixing of non-orthogonal Bogoliubov product states, along with more advanced methods based on it, require the computation of off-diagonal Hamiltonian and norm kernels. While the Hamiltonian kernel is efficiently computed via the off-diagonal Wick theorem of Balian and Brezin, the norm kernel relies on the Onishi formula (or equivalently the Pfaffian formula by Robledo or the integral formula by Bally and Duguet). Traditionally, the derivation of these two categories of formulae relies on different formal schemes. In the present work, the formulae for the operator and norm kernels are computed consistently from the same diagrammatic method. The approach further offers the possibility to address kernels involving more general states in the future.

1 Introduction

The projected generator coordinate method (PGCM) is a popular and versatile many-body method based on the mixing of Bogoliubov vacua\textsuperscript{1} typically generated by solving constrained Hartree-Fock-Bogoliubov (HFB) mean-field equations [2]. The PGCM is traditionally employed with empirical effective interactions tailored to the full one-body Hilbert space [3–5] or to a so-called valence space [6–10]. However, the PGCM has recently been extended to the context of ab initio calculations aiming at approximating exact solutions of Schrödinger’s equation in the low-energy sector of the A-body Hilbert space starting from realistic nuclear Hamiltonians rooted into quantum chromodynamics. Possibly bined with a pre-processing of the Hamiltonian via a multi-reference in-medium similarity renormalization group transformation [11–13], the PGCM is either exploited as a stand-alone method for nuclear spectroscopy [14] or as a starting point of an expansion method towards the exact solution [13,15].

The PGCM is based on the wave-function ansatz

\[ |\Psi_\nu\rangle = \sum_r f_\nu(r)|\Phi(r)\rangle, \tag{1} \]

where \(|\Phi(r)\rangle\) denotes a set of non-orthogonal\textsuperscript{2} Bogoliubov states labelled by the collective coordinate\textsuperscript{3} \(r\). The unknown\textsuperscript{4} coefficients \(f_\nu(r)\) are determined on the basis of Ritz’ variational principle, the energy minimization associated with \(|\Psi_\nu\rangle\) leading to the well-known Hill-Wheeler-Griffin (HWG) secular equation

\[ \sum_r \left[ \langle \Phi(l)|H|\Phi(r)\rangle - E_\nu \langle \Phi(l)|\Phi(r)\rangle \right] f_\nu(r) = 0, \tag{2} \]

which can be rewritten as

\[ \sum_r \left[ \frac{\langle \Phi(l)|H|\Phi(r)\rangle}{\langle \Phi(l)|\Phi(r)\rangle} - E_\nu \right] \langle \Phi(l)|\Phi(r)\rangle f_\nu(r) = 0, \tag{3} \]

where \(H\) is the Hamiltonian and where \(E_\nu\) denotes the set of PGCM energies approximating a subset of its eigenvalues.

The key ingredients entering Eq. (3) and the computation of observables are the off-diagonal connected operator kernel

\textsuperscript{1} The simpler projected generator coordinate method based on non-orthogonal Slater determinants is denoted as the non-orthogonal configuration interaction (NOCI) method in quantum chemistry [1].

\textsuperscript{2} Some of the Bogoliubov states mixed in the PGCM ansatz may be either manifestly or accidentally orthogonal. This situation can be dealt with at the price of a generalization of the situation discussed in the present work where all pairs of Bogoliubov states entering Eq. (1) are considered to be non-orthogonal.

\textsuperscript{3} The collective coordinate is multi dimensional and contains the variable(s) parameterizing the transformations associated with the symmetry(ies) being restored via projection techniques.

\textsuperscript{4} The part of the coefficients fixed by the structure of the symmetry group does not have to be determined variationally.
and the norm kernel associated with two Bogoliubov states \(|\Phi(l)|\) and \(|\Phi(r)|\). Given a generic operator \(O\), the operator and norm kernels are respectively given by

\[
O(l, r) \equiv \langle \Phi(l) | O | \Phi(r) \rangle , \quad (4a)
\]
\[
\mathcal{N}(l, r) \equiv \langle \Phi(l) | \Phi(r) \rangle , \quad (4b)
\]

out of which the connected operator kernel \([16,17]\) is defined through

\[
o(l, r) \equiv \frac{O(l, r)}{\mathcal{N}(l, r)} . \quad (5)
\]

The connected operator kernel can be efficiently computed via the off-diagonal Wick theorem (ODWT) of Balian and Brezin \([18]\). The norm kernel relies on the Onishi formula \([19]\), on the Pfaffian formula by Robledo \([20]\) or the integral formula by Bally and Duguet \([17]\). Traditionally, the derivation of these two categories of formulae relies on different formal schemes that do not seem to share a common ground. One exception relies on the use of fermion coherent states based on Grassmann variables allowing one to express both the connected operator kernel \([21,22]\) and the norm kernel \([20]\) in terms of Pfaffians. The goal of the present work is to provide another consistent derivation of the connected operator kernel, i.e. of the ODWT, and of the norm kernel based on a common diagrammatic method.

The paper is organized as follows. Section 2 introduces the necessary elements of formalism. In Sect. 3, the diagrammatic method is used to derive both the ODWT for the connected operator kernel and the Onishi/Pfaffian formula for the norm kernel. Conclusions and perspectives are elaborated on in Sect. 4. The paper is complemented with several appendices providing necessary technical details, i.e. the normal-ordered representation of operators, the detailed diagrammatic rules and the standard derivation of the ODWT for completeness and comparison.

## 2 Basics of Bogoliubov algebra

The core of the present work involves three non-orthogonal Bogoliubov states\(^5\) denoted as \(|\Phi(l)|\), \(|\Phi(r)|\) and \(|\Phi|\).

### 2.1 Bogoliubov vacuum

Each of these three states is a vacuum for a set of associated quasi-particle operators. Taking \(|\Phi|\) as an example, this property reads as

\[
\beta_k |\Phi\rangle = 0 \quad \forall k , \quad (6)
\]

where the set of quasi-particle operators \(\{\beta^\dagger_k, \beta_k\}\) is related to particle operators \(\{c^\dagger_a, c_a\}\) associated with an arbitrary basis of the one-body Hilbert space \(\mathcal{H}_1\) via a unitary Bogoliubov transformation of the form

\[
\beta_k \equiv \sum_a (U_{ak}^* c_a + V_{ak}^* c_a^\dagger) , \quad (7a)
\]
\[
\beta_k^\dagger \equiv \sum_a (U_{ak} c_a^\dagger + V_{ak} c_a) . \quad (7b)
\]

This transformation can be written more compactly via a matrix representation

\[
\begin{pmatrix} \beta & \beta^\dagger \end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix} c & c^\dagger \end{pmatrix} , \quad (8)
\]

where the Bogoliubov matrix

\[
\mathcal{W} \equiv \begin{pmatrix} U^* & V^* \end{pmatrix} \quad (9)
\]

is unitary, such that the following relations hold

\[
\mathcal{W}^\dagger \mathcal{W} = \mathcal{W}^\dagger = 1 . \quad (10)
\]

This condition implies that the canonical fermionic anticommutation rules valid for the particle operators propagate to quasi-particle ones.

### 2.2 Thouless theorem

Starting from Bogoliubov transformations \(\mathcal{W}(l), \mathcal{W}(r)\) and \(\mathcal{W}\) defining the three sets of quasi-particle operators \(\{\beta^\dagger_k(l), \beta_k(l)\}, \{\beta^\dagger_k(r), \beta_k(r)\}\) and \(\{\beta^\dagger_k, \beta_k\}\), respectively, Thouless’ theorem \([23]\) allows one to connect the three vacua \(|\Phi(l)\rangle, |\Phi(r)\rangle\) and \(|\Phi\rangle\).

First, \(|\Phi(l)\rangle\) and \(|\Phi(r)\rangle\) are expressed with respect to \(|\Phi\rangle\). Taking \(|\Phi(r)\rangle\) as an example, the transformation connecting the two sets of quasi-particle operators is given by (see Appendix E.3 from Ref. \([2]\) for further details on the derivation)

\[
\begin{pmatrix} \beta(r) \\ \beta^\dagger(r) \end{pmatrix} = \mathcal{W}^\dagger(r) \mathcal{W} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \equiv \begin{pmatrix} U^T(r) & V^T(r) \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} , \quad (11)
\]

with

\[
U(r) \equiv \mathcal{V}^T \mathcal{U}(r) + \mathcal{U}^T(r) \mathcal{V}(r) , \quad (12a)
\]
\[
V(r) \equiv \mathcal{U}^T \mathcal{U}(r) + \mathcal{V}^T \mathcal{V}(r) . \quad (12b)
\]

Introducing the skew-symmetric matrix

\[
\mathcal{Z}(r) \equiv V^*(r) U^{*\dagger}(r) , \quad (13)
\]

\(^5\) While a generalization is possible, the reference state \(|\Phi\rangle\) is supposed to be non-orthogonal to both \(|\Phi(l)\rangle\) and \(|\Phi(r)\rangle\).
Thouless’ theorem allows one to write

\[ |\Phi(r)\rangle = \langle \Phi|\Phi(r)\rangle e^{Z^{20}(l,r)} |\Phi\rangle, \tag{14a} \]

where the one-body Thouless operator reads as

\[ Z^{20}(r) \equiv \frac{1}{2} \sum_{k_1k_2} z^{k_1k_2}(r) \beta^\dagger_{k_1} \beta_{k_2}. \tag{14b} \]

Similarly, the transformation

\[ \begin{pmatrix} \beta(r) \\ \beta^\dagger(r) \end{pmatrix} = W^\dagger(l) \begin{pmatrix} \beta(l) \\ \beta^\dagger(l) \end{pmatrix}, \]

\[ \equiv W^\dagger(l, r) \begin{pmatrix} \beta(l) \\ \beta^\dagger(l) \end{pmatrix}, \]

\[ \equiv \begin{pmatrix} B^\dagger(l, r) & A^\dagger(l, r) \\ A(l, r) & B(l, r) \end{pmatrix} \begin{pmatrix} \beta(l) \\ \beta^\dagger(l) \end{pmatrix}, \tag{15} \]

with

\[ A(l, r) \equiv V^T(l)U(r) + U^T(l)V(r), \tag{16a} \]

\[ B(l, r) \equiv U^\dagger(l)U(r) + V^\dagger(l)V(r), \tag{16b} \]

leads to defining the Thouless matrix

\[ \Phi(l, r) \equiv A^s(l, r)B^{s-1}(l, r), \tag{17} \]

thanks to which \(|\Phi(r)\rangle\) can be expressed with respect to \(|\Phi(l)\rangle\) according to

\[ |\Phi(r)\rangle = \langle \Phi|\Phi(r)\rangle e^{Z^{20}(l,r)} |\Phi(l)\rangle, \tag{18a} \]

where

\[ Z^{20}(l, r) \equiv \frac{1}{2} \sum_{k_1k_2} z^{k_1k_2}(l, r) \beta^\dagger_{k_1} \beta_{k_2}. \tag{18b} \]

### 2.3 Elementary contractions

Given \(|\Phi(l)\rangle\) and \(|\Phi(r)\rangle\), the four one-body off-diagonal elementary contractions are defined in the quasi-particle basis of \(|\Phi\rangle\) through

\[ \mathbf{R}_{k_1k_2}(l, r) = \begin{pmatrix} \langle \Phi(l)|\beta^\dagger_{k_2} \beta_{k_1} |\Phi(r)\rangle & \langle \Phi(l)|\beta^\dagger_{k_2} \beta_{k_1} |\Phi(r)\rangle \\ \langle \Phi(l)|\beta^\dagger_{k_2} \beta_{k_1} |\Phi(r)\rangle & \langle \Phi(l)|\beta^\dagger_{k_2} \beta_{k_1} |\Phi(r)\rangle \end{pmatrix}, \]

\[ \equiv \begin{pmatrix} +\rho_{k_1k_2}(l, r) +\kappa_{k_1k_2}(l, r) \\ -\tilde{\kappa}_{k_1k_2}(l, r) +\sigma_{k_1k_2}(l, r) \end{pmatrix}, \tag{19} \]

and satisfy, due to anticommutation rules and complex conjugation,

\[ \rho^*_{k_1k_2}(l, r) = +\rho_{k_2k_1}(r, l), \tag{20a} \]

\[ \kappa_{k_1k_2}(l, r) = -\kappa_{k_2k_1}(l, r), \tag{20b} \]

\[ \tilde{\kappa}_{k_1k_2}(l, r) = +\tilde{\kappa}_{k_2k_1}(l, r), \tag{20c} \]

\[ \sigma_{k_1k_2}(l, r) = +\sigma_{k_2k_1}(r, l) - \delta_{ab}. \tag{20d} \]

Setting \(|\Phi(l)\rangle = |\Phi(r)\rangle = |\Phi\rangle\), one can trivially obtain the diagonal contractions associated with \(|\Phi\rangle\) as

\[ \mathbf{R}_{k_1k_2}(l, l) = \begin{pmatrix} +\rho_{k_1k_2} + \kappa_{k_1k_2} \\ -\tilde{\kappa}_{k_1k_2} - \sigma_{k_1k_2} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \delta_{k_1k_2} \end{pmatrix}. \tag{21} \]

From this most simplistic case, one can easily infer the diagonal contractions associated with \(|\Phi(l)\rangle\) and \(|\Phi(r)\rangle\) in the quasi-particle basis of \(|\Phi\rangle\), e.g.

\[ \mathbf{R}_{k_1k_2}(l, l) = \begin{pmatrix} (V^*(l)V^T(l))_{k_1k_2} & (V^*(l)U^T(l))_{k_1k_2} \\ (U^*(l)V^T(l))_{k_1k_2} & (U^*(l)U^T(l))_{k_1k_2} \end{pmatrix}. \tag{22} \]

### 3 Computation of the kernels

The traditional way to compute the connected operator kernel, i.e. to derive the off-diagonal Wick theorem \[18\], invokes an asymmetric approach that consists of expressing, e.g., \(|\Phi(r)\rangle\) with respect to \(|\Phi(l)\rangle\) via Eq. (18). This delivers the connected operator kernel under the asymmetric form

\[ o(l, r) = \langle \Phi(l)|Oe^{Z^{20}(l,r)}|\Phi(l)\rangle. \tag{23} \]

The proof of the off-diagonal Wick theorem \[18\] based on Eq. (23) is recalled for reference in Appendix C. This constitutes the simplest derivation of the ODWT because the power series associated with the exponential appearing on one side of the operator \(O\) in Eq. (23) naturally terminates after a finite number of terms.

The asymmetric approach cannot provide access to the norm kernel and thus only delivers half of the needed ingredients. Typically, accessing the norm kernel relies on a symmetric approach\[6\] where \(|\Phi(l)\rangle\) and \(|\Phi(r)\rangle\) are both expressed with respect to a common reference state \(|\Phi\rangle\) according to Eq. (14).

In this context, it is of interest to consistently derive the connected operator kernel (i.e. the off-diagonal Wick theorem) and the norm kernel (i.e. the Onishi or Pfaffian formula) via a symmetric approach. While this was achieved starting from fermion coherent states based on Grassmann...
variables [21,22], this is presently realized using standard diagrammatic techniques. The symmetric approach leads to expressing the operator and norm kernels as

$$\frac{O(l,r)}{\langle \Phi | O \Phi \rangle} \equiv \langle \Phi | e^{Z_1(l)} O e^{Z_2(r)} | \Phi \rangle,$$  \hspace{1cm} (24a)

$$\frac{N(l,r)}{\langle \Phi | N \Phi \rangle} \equiv \langle \Phi | e^{Z_1(l)} | e^{Z_2(r)} | \Phi \rangle,$$  \hspace{1cm} (24b)

such that the connected operator kernel itself reads as

$$o(l,r) \equiv \langle \Phi | e^{Z_1(l)} O e^{Z_2(r)} | \Phi \rangle \langle \Phi | e^{Z_1(l)} e^{Z_2(r)} | \Phi \rangle.$$  \hspace{1cm} (25)

It is worth noting that the above expression resembles the expectation value at play in variational coupled cluster (vCC) theory [24–26]. On the one hand, it is more general because the two involved Thouless operators are not equal. On the other hand, it is more restricted given that the Thouless operators are one-body excitation operators, which essentially corresponds to the simplest vCC with singles (vCCS) approximation. Still, it is well known from vCC that, (i) while the norm overlap in the denominator can be exactly cancelled out in the numerator, (ii) the expansions of the two exponentials do not terminate and thus produce an infinite number of terms. It will thus have to be shown how the latter difficulty can be overcome to compute $N(l,r)$ and $o(l,r)$ exactly.

3.1 Operator kernel

Employing the simplified notations

$$R \equiv Z_2(r) = \frac{1}{2} \sum_{k_1 k_2} z_{k_1 k_2}(r) \beta_{k_1}^\dagger \beta_{k_2},$$ \hspace{1cm} (26a)

$$L \equiv Z_1(l) = \frac{1}{2} \sum_{k_1 k_2} z_{k_1 k_2}^\dagger(l) \beta_{k_2} \beta_{k_1},$$ \hspace{1cm} (26b)

for the Thouless operators fulfilling $\langle \Phi | R = L | \Phi \rangle = 0$, the operator kernel is expressed as

$$\frac{O(l,r)}{\langle \Phi | O \Phi \rangle} = \langle \Phi | e^L \Phi \rangle e^R \langle \Phi | e^R \Phi \rangle \langle \Phi | e^L \Phi \rangle \langle \Phi | e^{Z_1(l)} O e^{Z_2(r)} | \Phi \rangle \langle \Phi | e^{Z_1(l)} | e^{Z_2(r)} | \Phi \rangle \equiv \frac{N(l,r)}{\langle \Phi | N \Phi \rangle} \equiv \frac{N(l,r)}{\langle \Phi | N \Phi \rangle} \equiv \frac{N(l,r)}{\langle \Phi | N \Phi \rangle} \equiv \frac{N(l,r)}{\langle \Phi | N \Phi \rangle}.$$

where $O$ has been decomposed into normal-ordered contributions $\{O^{ij}\}$ with respect to $|\Phi\rangle$; see Appendix A. for details.\footnote{Given the chosen Bogoliubov reference state $|\Phi\rangle$, it is natural to normal order the operator $O$ with respect to that state as is presently done. While this is already very general, one can easily go one step further and express the operator in normal order with respect to yet another product state, e.g. the particle vacuum. The connection between both situations is straightforward.}
\[
\frac{1}{s! \ t!} \langle \Phi | L^s O^{42} R^t | \Phi \rangle = \sum \left[ \begin{array}{c}
\end{array} \right]
\]

Fig. 1 Diagrammatic representation of the matrix element \( \langle s | L^i O^j | t \rangle \), where \( s \) and \( t \) are positive integers, contributing to the operator kernel \( \langle \Phi (i) | O^{42} | \Phi (r) \rangle \). Each square (triangle) vertex represents an operator \( L (R) \), whereas the dot vertex denotes the operator \( O^{42} \). Whereas the vertex of \( L (R) \) displays two lines entering (leaving) it, two lines enter the vertex representing \( O^{42} \) and four lines leave it. See Appendix B for relevant details regarding the diagrammatic representation.

\[
\langle \Phi | e^L O^{ij} e^R | \Phi \rangle = \sum_{s,t=0}^{\infty} \frac{1}{s!(s-t)! t!} \langle \Phi | L \cdots L O^{ij} \cdots R \cdots R | \Phi \rangle
\]

where the index \( c \) stands for connected terms. Reshuffling the sums allows one to factorize in front of each connected contribution the infinite set of disjoint closed contributions making up the norm kernel according to

\[
\langle \Phi | e^L O^{ij} e^R | \Phi \rangle = \sum_{s,t=0}^{\infty} \sum_{s' = 0}^{\infty} \frac{1}{s'! (s-s')! t'! (t-t')!} \langle \Phi | L \cdots L O^{ij} \cdots R \cdots R | \Phi \rangle_c \langle \Phi | L \cdots L R \cdots R | \Phi \rangle
\]

The above equation demonstrates that the norm kernel exactly factorizes in the operator kernel\(^8\) such that the connected operator kernel is, hence the name, the sum of connected, necessarily joint, contributions

\[
o(l, r) = \langle \Phi | e^L O e^R | \Phi \rangle_c = \sum_{n=0}^{N} \sum_{i, j=0}^{2n} \sum_{s, t=0}^{\infty} \langle s | L^i O^j | t \rangle_c , \quad (30)
\]

where, for any \( O^{ij} \), the condition

\[
s - t = \frac{i - j}{2}
\]

is satisfied for each connected matrix element \( \langle s | L^i O^j | t \rangle_c \) given that \( L (R) \) contains two quasi-particle annihilation (creation) operators. In spite of the factorization of the norm kernel, the symmetric approach does not lead to a natural termination of the infinite number of terms making up the connected operator kernel\(^9\). The operators \( L \) and \( R \) being presently of one-body character, the infinite series thus generated can however be shown to be factorizable in terms of

\(^8\) Nothing in the proof depends on the character, e.g. rank, of the operators \( R \) and \( L \). Thus, the exact factorization of the norm kernel out of the operator kernel constitutes a general result going beyond the scope of the present study that constraints \( R (L) \) to be a one-body excitation (de-excitation) operator.

\(^9\) The asymmetric approach to the connected operator kernel detailed in Appendix C, including the natural termination of the exponential at play, can be recovered from the results obtained below by setting \( L \equiv 0 \) a posteriori.
off-diagonal elementary contractions such that the ODWT is recovered.

### 3.1.2 Off-diagonal Wick’s theorem

The connected operator kernel associated with the normal-order component $O^{ij}$ of arbitrary rank $n \equiv (i + j)/2$ reads as

$$
\langle \Phi | e^L O^{ij} e^R | \Phi \rangle_c = \sum_{s,t=0}^{\infty} \langle s | i^t j^s \rangle_c \\
= \sum_{s,t=0}^{\infty} \frac{1}{s!} \frac{1}{t!} \sum_{k_1 \cdots k_s} \sum_{l_1 \cdots l_t} O_{k_1 \cdots k_s} L_{l_1} \cdots L_{l_t} \beta_{k_1}^\dagger \cdots \beta_{k_s}^\dagger \beta_{l_1} \cdots \beta_{l_t} R \cdots R | \Phi \rangle_c.
$$

(32)

where Eq. (A. 7) has been used to express $O^{ij}$ in its second-quantized normal-ordered form.

The calculation of the connected operator kernel relies on the following considerations that are consistent with the diagrammatic rules detailed in Appendix B.

1. Each contribution to $\langle s | i^t j^s \rangle_c$ is made out of strings of contractions connected to quasi-particle operators belonging to $O^{ij}$. The characteristics of the operators $L$ and $R$ strongly constrains the topology of these connected strings.

(a) Starting from a quasi-particle operator belonging to $O^{ij}$, a connected string of contractions goes through a set of $L$ and $R$ operators until it reaches other quasi-particle operators of $O^{ij}$.

(b) Two successive contractions involving an operator $L$ ($R$) exhaust the two quasi-particle operators it contains. Consequently, a string necessarily forms a single loop connecting two $O^{ij}$ quasi-particle operators.

(c) There exist four types of closed loops joining two quasi-particle operators of $O^{ij}$. A so-called normal string of contractions starting from an operator $\beta^\dagger$ and ending at an operator $\beta$ is schematically indicated below by $[\beta^\dagger \beta]$ whenever the former operator is located to the left of the latter.11 Similarly, an anomalous string starting from an operator $\beta(\beta^\dagger)$ and ending at another operator $\beta(\beta^\dagger)$ is denoted as $[\beta \beta] ((\beta^\dagger \beta^\dagger))$.

2. The complete set of connected terms contributing to $\langle s | i^t j^s \rangle_c$ includes all possible combinations of $n$ normal and anomalous connected loops. This topological characteristic is responsible for the validity of the off-diagonal Wick’s theorem proven below, i.e. for the fact that the end result can be expressed in terms of products of off-diagonal elementary contractions12. Figure 2 displays one such contribution to $\langle 3 | 4^2 2^2 \rangle_c$.

3. The combinatorial associated with each contribution to $\langle s | i^t j^s \rangle_c$ is obtained from the following considerations.

(a) Among the $n$ strings, $k \leq \min(i, j)$ normal $[\beta^\dagger \beta]$ strings are formed, knowing that $k$ is even whenever $i$ and $j$ are even13 and odd otherwise.14 Once $k$ normal strings are formed, there remains an even number $i - k \ (j - k)$ of quasi-particle creation (annihilation) operators in $O^{ij}$ giving rise to $(i - k)/2 \ ((j - k)/2)$ anomalous $[\beta^\dagger \beta]$ $([\beta \beta])$ strings.

(b) There are $\binom{4}{i}$ different ways to pick $k$ operators out of the $i$ creation operators and, similarly, $\binom{4}{j}$ different ways to pick $k$ operators out of the $j$ annihilation operators. Once this done, there are $k!$ different ways to associate the $k$ creation to the $k$ annihilators to form the $k$ normal strings. Next, there are $(i - k - 1)!!$

10 Were $L$ and $R$ of higher rank, e.g. be two-body operators, this property would be lost. Indeed, an operator, e.g. $L$ belonging to a loop going through an alternate succession of $L$ and $R$ operators connecting two quasi-particle operators of $O^{ij}$ could further entertain a contraction with an operator $R$ belonging to another closed loop, thus forming a more elaborate closed string eventually involving more than two quasi-particle operators of $O^{ij}$.

11 Given that $O^{ij}$ is in normal-ordered form, no normal $[\beta \beta^\dagger]$ string may occur. This would however be the case if the present discussion were extended to the computation of the connected kernel associated with any product, e.g. $O^{ij} O^{kl}$, of normal-ordered operators. This happens for example when considering kernels involving elementary excitations of $\langle \Phi | \ell \rangle$ and/or $| \Phi (r) \rangle$ as in the multi-reference perturbation theory based on a PCGM unperturbed state [15]. Such an extension is straightforward.

12 If $L$ and/or $R$ are of higher rank, i.e. if $| \Phi (\ell) \rangle$ and/or $| \Phi (r) \rangle$ do not belong to the manifold of Bogoliubov states, the validity of the off-diagonal Wick’s theorem is lost.

13 The integers $i$ and $j$ always carry the same parity.

14 If this rule is not fulfilled, the operator cannot be fully contracted, thus providing a vanishing expectation value by virtue of its normal-ordered form.
((j – k – 1)!!) possible ways to form the (i – k)/2
((j – k)/2) anomalous [β†β], ([ββ]) strings.

(c) For a given k, all terms associated with the above
combinatorial contribute identically\(^\text{15}\) due to the anti-
symmetric character of the operator matrix elements
under the exchange of any pair of quasi-particle cre-
tion (i.e. upper) or annihilation (i.e. lower) indices;
see Eq. (A. 9).

(d) Combining the factor (i!/j!)\(^{-1}\) originating from the
operator with the above combinatorial\(^\text{16}\) one obtains
the overall factor
c(i, j, k) ≡ \(\frac{1}{k!} \frac{1}{(i – k)!} \frac{1}{(j – k)!} (j – k – 1)!!(j – k – 1)!!\)

for the diagram associated to k normal strings [β†β],
(i – k)/2 anomalous [β†β], and (j – k)/2 anomalous
strings [ββ].

4. So far, the focus has been on the nature and the num-
ber of closed strings that can be formed in Eq. (32) for a
given operator \(O^j\), while leaving the expansion of \(\exp(L)\)
(exp(R)) in the abstract. Let us now consider the specific
term of that expansion associated with the powers s (for
L) and t (for R), i.e. \(\langle \hat{s}^i \hat{t}^j \rangle\), and focus on the set of con-
tributions characterized by \(k \leq \min(i, j)\) normal strings.
Below, an index \(h \in [1, n]\) is artificially introduced to
label each string for bookkeeping purposes.

\[^{15}\] Instead of considering all possible strings, this is best seen by keeping
the contraction pattern fixed and by exchanging the position of the quasi-
particle operators within \(O^j\) in all ways consistent with that contraction
pattern and by employing the anti-symmetry of the operator matrix
elements to recover the original algebraic contribution.

\[^{16}\] Useful properties of the double factorial are

\[ n! = n!!(n – 1)!! \quad \forall n \]  \hspace{1cm} (33a)

\[ n!! = 2^k k! \quad \text{for} \ n = 2k \]  \hspace{1cm} (33b)

(a) Let us first concentrate on the k normal strings
[β†β] \(^{(h)}\). There are \(s^{(1)}\) operators L out of s involved
in the string [β†β] \(^{(1)}\) and \(c^{(1)}\) equivalent ways to choose them. Then, there are \(s^{(2)}\) such operators out of
\((s – s^{(1)})\) involved in [β†β] \(^{(2)}\) and so on, up to selecting
\(s^{(k)}\) out of \((s – \sum_{h=1}^{k-1} s^{(h)})\) operators L involved
in [β†β] \(^{(k)}\), such that \(s' \equiv \sum_{h=1}^{k} s^{(h)}\) operators out of
s are eventually involved in the k normal strings.

The overall associated combinatorial factor is given by

\[ \left( \begin{array}{c}
\frac{s}{s^{(1)}} \frac{s-s^{(1)}}{s^{(2)}} \frac{s-s^{(1)}-s^{(2)}}{s^{(3)}} \cdots \frac{s-s^{(1)}-s^{(2)}-\cdots-s^{(k-1)}}{s^{(k)}} \n\end{array} \right) \equiv \frac{s!}{s^{(1)}!s^{(2)}!\cdots s^{(k)}!} \]  \hspace{1cm} (34)

such that the initial \((s!)^{-1}\) factor is replaced by sim-
ilar factors for each normal contraction and for the
remaining \(s – s'\) operators L involved in anomalous
strings. The very same operation is considered for the
t' operators R involved in the k normal strings,
delivering the same combinatorial factor with s vari-
bles replaced by t ones. Because one is presently
dealing with normal strings, the additional factor
\(\prod_{h=1}^{k} \delta_{s^{(h)}},t^{(h)}\) must be included that as many
L and R operators must be involved in each of them.

(b) The same reasoning applies to both sets of anomalous
strings, knowing that the operators L and R must be
selected among the operators that have not been used
yet and that the condition \(\delta_{s^{(h)}},t^{(h)}\) \((\delta_{s^{(h)},t^{(h)}})\) must
be used for each string [β†β] \(^{(h)}\) ([ββ] \(^{(h)}\)).

5. Eventually summing over all possible values of s and t,
along with the subset of \(s^{(h)}\) and t \(^{(h)}\) values, taking into
account the Kronecker deltas generated through the
processes described above, each contribution to the operator
kernel containing k \(\leq \min(i, j)\) normal strings involves
intricate sums with the generic structure

\[ \sum_{a=0}^{\infty} \sum_{b=0}^{\infty} \sum_{c=0}^{\infty} \cdots \sum_{d=0}^{\infty} \]  \hspace{1cm} (35)

where, e.g. for normal strings, \(a \equiv n = s = t, b \equiv s^{(1)} =
t^{(1)}, c \equiv s^{(2)} = t^{(2)}, \) etc. These intricate sums are easily
shown to be equivalent to

\[ \sum_{a'=0}^{\infty} \sum_{b'=0}^{\infty} \sum_{c'=0}^{\infty} \cdots \]  \hspace{1cm} (36)
with \( a' = a - b - c - d - \cdots \). Each disentangled sum gathers an infinite set of contributions corresponding to closed strings connected to the same pair of quasiparticle operators and involving an increasing number of successive \( L \) and \( R \) operators. Weighted by the prefactor \( (s^{(h)})^{-1} (t^{(h)})^{-1} \) originating from the successive appropriate applications of Eq. (34), this set of terms exactly makes up the corresponding off-diagonal elementary contractions (Eq. (B.13)) according to the expansions\(^{17}\)

\[
\rho_{k_1 k_2}(l, r) = \sum_{s, t = 0}^{\infty} \frac{1}{s! t!} \langle \Phi \mid L^s L^t R^t R^s \mid \Phi \rangle_c
\]

\[
= \sum_{s, t = 0}^{\infty} \langle s_{k_2} | l_{k_1} \rangle_c , \tag{37a}
\]

\[
\kappa_{k_1 k_2}(l, r) = \sum_{s, t = 0}^{\infty} \frac{1}{s! t!} \langle \Phi \mid L^s L^t R^t R^s \mid \Phi \rangle_c
\]

\[
= \sum_{s, t = 0}^{\infty} \langle l_{k_2} | s_{k_1} \rangle_c , \tag{37b}
\]

\[
-k_{k_1 k_2}(l, r) = \sum_{s, t = 0}^{\infty} \frac{1}{s! t!} \langle \Phi \mid L^s L^t R^t R^s \mid \Phi \rangle_c
\]

\[
= \sum_{s, t = 0}^{\infty} \langle s_{k_2} | l_{k_1} \rangle_c , \tag{37c}
\]

\[
-\sigma_{k_1 k_2}(l, r) = \sum_{s, t = 0}^{\infty} \frac{1}{s! t!} \langle \Phi \mid L^s L^t R^t R^s \mid \Phi \rangle_c
\]

\[
= \sum_{s, t = 0}^{\infty} \langle l_{k_2} | s_{k_1} \rangle_c , \tag{37d}
\]

knowing that the diagrammatic rules applicable to the four connected\(^{18}\) matrix elements introduced through Eq. (37) are laid out in Appendix B.

Taking into account all multiplicative factors pointed out above and summing over all allowed numbers \( k \) of normal strings/contractions,\(^{19}\) one eventually obtains Eq. (32) under the final form

\[
\frac{\langle \Phi(l) | O^{ij} | \Phi(r) \rangle}{\langle \Phi(l) | \Phi(r) \rangle} = \sum_{k = 0}^{\text{parity}} c(i, j, k) a_{k_1 \cdots k_l}^{k_1 \cdots k_j}
\]

\( ^{17} \) The fourth contraction appearing in Eq. (37d) does not presently occur due to the normal-ordered character of \( O^{ij} \).

\( ^{18} \) The connected character of the presently introduced matrix elements is defined with respect to the two operators \( \beta_1^{(t)} \) and \( \beta_1^{(t)} \) that translate diagrammatically into two external lines; see Appendix B for details.

\( ^{19} \) The sum over \( k \) starts from 0 (1) and runs over even (odd) integers whenever \( i \) and \( j \) are even (odd).

which proves the off-diagonal Wick’s theorem \(^{18}\) by expressing the connected operator kernel in terms of off-diagonal elementary contractions. Applying Eq. (38) to the sum of \( O^{ij} \) operators characterized by \( n \leq 3 \), the expression of the connected operator kernel of a three-body operator \( (N = 3) \) is given in Appendix D.

While the ODWT has indeed been formally recovered, a full proof requires an explicit computation of the off-diagonal elementary contractions themselves via the symmetric approach. As clearly illustrated in Eq. (37), each of these contractions takes itself the form of an infinite, non-terminating, expansion. As demonstrated below, these expansions however happen to deliver known power series that are shown to be equal to the expressions obtained via the asymmetric approach in Appendix C.

### 3.1.3 Elementary contractions

The first elementary contraction \( \rho_{k_1 k_2}(l, r) \) (Eq. (37a)) sums the connected matrix elements \( \langle s_{k_2} | l_{k_1} \rangle_c \) over all \( s \) and \( t \) values, knowing in fact that both integers are constrained to be equal, i.e. \( s = t \equiv n \). The matrix element \( \langle n_{k_2} | k_1 \rangle_c \) is made out of a single unlabelled connected diagram with two external legs. Indeed, there is only one topologically distinct way to connect \( \beta_1^{(t)} \) to \( \beta_1^{(t)} \) via an alternate succession of \( n \) operators \( L \) and \( n \) operators \( R \). By virtue of Eq. (21), the term of order \( n = 0 \) is zero in the present case.

The corresponding diagrammatic expansion of \( \rho_{k_1 k_2}(l, r) \) is provided in Fig. 3. Diagrammatic rules deliver the algebraic expressions for each order \( n \), thus leading to

\[
\rho_{k_1 k_2}(l, r) = \sum_{n=0}^{\infty} \sum_{i_1h_1, \cdots, h_{2n-1}} k_{k_1k_2}^{h_1h_2} (r) z_{k_1k_2}^{h_1h_2} (r) \cdots
\]

\[
\times z_{k_1k_2}^{h_1h_2} (r) z_{k_1k_2}^{h_1h_2} (r) \cdots k_{k_1k_2}^{h_1h_2} (l) \cdots k_{k_1k_2}^{h_1h_2} (l), \tag{38}
\]

where the Taylor series

\[
\sum_{n=0}^{\infty} \varepsilon^n = \frac{1}{1 - \varepsilon} \tag{40}
\]

has been used to resum the infinite expansion.
The three other elementary contractions (Eqs. (37b–37d)) can be calculated similarly. Their diagrammatic expansions are also displayed in Fig. 3, where one notices that the fourth contraction contains a non-zero term of order $n = 0$. The corresponding algebraic expressions are given by

$$\kappa_{k_1k_2}^{l,r} = \sum_{n=0}^{\infty} \left[ z(r) \left( z^\dagger(l) z(r) \right)^n \right]_{k_1k_2}$$

$$= \left[ z(r) \frac{1}{1 - z^\dagger(l) z(r)} \right]_{k_1k_2}, \quad (41a)$$

$$-\kappa^*_{k_1k_2}^{l,r} = -\sum_{n=0}^{\infty} \left[ \left( z^\dagger(l) z(r) \right)^n z^\dagger(l) \right]_{k_1k_2}$$

$$= -\left[ \frac{1}{1 - z^\dagger(l) z(r)} \right]_{k_1k_2}, \quad (41b)$$

$$-\sigma^*_{k_1k_2}^{l,r} = \sum_{n=0}^{\infty} \left[ \left( z^\dagger(l) z(r) \right)^n \right]_{k_1k_2}$$

$$= \left[ \frac{1}{1 - z^\dagger(l) z(r)} \right]_{k_1k_2}. \quad (41c)$$

It is easy to check that the four properties listed in Eq. (20) are indeed satisfied by the off-diagonal contractions.

Eventually, the off-diagonal contractions have been expressed as a known power series in the variable $z^\dagger(l) z(r)$. It can be easily shown, as stipulated in Appendix C, that both sets of expressions are in fact identical.

### 3.2 Norm kernel

The norm kernel reads in the symmetric approach as

$$\frac{\langle \Phi(l) | \Phi(r) \rangle}{\langle \Phi(l) | \Phi \rangle \langle \Phi | \Phi(r) \rangle} = \sum_{s,t=0}^{\infty} \frac{1}{s!t!} \langle \Phi | L^s R^t | \Phi \rangle$$

$$\equiv \sum_{s,t=0}^{\infty} \langle s \| t \rangle \equiv \sum_{s=0}^{\infty} \langle s \| n \rangle, \quad (42)$$

where the condition $s = t \equiv n$ must be fulfilled.

#### 3.2.1 Exponentiation of closed diagrams

As already discussed, and as detailed in Appendix B, diagrams contributing to $\langle n \| n \rangle$ are composed of disjoint closed sub-diagrams. A closed$^{20}$ diagram involves an equal number of successively connected operators $L$ and $R$. For a given $n_i \geq 1$, there exists in fact a single topologically distinct unlabelled closed diagram$^{21}$

$$\Gamma_{cl}(n_i) \equiv \langle n_i \| n_i \rangle_{cl}, \quad (43)$$

$^{20}$The trivial diagram obtained for $n = 0$ is $\langle 0 \| 0 \rangle = \langle \Phi | \Phi \rangle = 1$. Since it contains neither vertices nor lines, it does not qualify as a closed diagram.

$^{21}$In the present discussion $\Gamma_{cl}(n_i)$ equally represents the closed diagram and its algebraic contribution.
where the index \( cl \) stands for \textit{closed}.

A generic diagram \( \Gamma(n) \) contributing to \( \langle \Phi| |\Phi \rangle \) factorizes into \( m_1 \) identical closed subdiagrams \( \Gamma_{cl}(n_1) \), \( m_2 \) identical closed sub-diagrams \( \Gamma_{cl}(n_2) \), and so on. Obviously, a closed diagram \( \Gamma_{cl}(n_i) \) can only contribute whenever \( n \geq n_i \). Using the convention that a closed diagram occurs with multiplicity \( m_i = 0 \) whenever \( n < n_i \), a diagram contributing to \( \langle \Phi| |\Phi \rangle \) can be written as

\[
\Gamma(n) = \frac{[\Gamma_{cl}(n_1)]^{m_1} [\Gamma_{cl}(n_2)]^{m_2}}{m_1! m_2!} \cdots
\]

(44)

where the product runs over all possible closed strings \( \Gamma_{cl}(n_i) \) such that the condition

\[
\sum_{n_i=1}^{\infty} m_i n_i = n,
\]

(45)

is satisfied. According to the diagrammatic rules, the symmetry factor of \( \Gamma(n) \) must be worked out. In addition to the symmetry factors associated with each closed subdiagram (included into \( \Gamma_{cl}(n_i) \)), the symmetry factor \( S_{\Gamma(n)} \) incorporates the set of denominators in Eq. (44). Each such denominator \( m_i! \) denotes the number of permutations of the equivalent groups of \( L \) and \( R \) vertices in the labelled diagram \( \Gamma_{cl}(n_i) \) delivering topologically equivalent labelled diagrams. As illustrated in Fig. 5 for \( n = 4 \), there are \( S_{\Gamma_{cl}(n)} = 2n \) such permutations, made out of the convolution of

1. The identity plus 1 reflection inverting the clockwise ordering,
2. \( n \) clockwise circular permutations.

Summing over all closed diagrams, the final result is obtained as

\[
\sum_{n=1}^{\infty} \Gamma_{cl}(n) = -\frac{1}{2n} \text{Tr} \left\{ \left( z^*(l)z(r) \right)^n \right\},
\]

(47)

where the symmetry factor is \( S_{\Gamma_{cl}(n)} = 2n \). As visible from Fig. 4, the 1/2 factor obtained for \( n = 1 \) relates to the existence of a pair of equivalent lines. For \( n > 1 \), the symmetry factor relates to the number of permutations of the \( L \) and \( R \) vertices in the labelled diagram \( \Gamma_{cl}(n) \) delivering topologically equivalent labelled diagrams. As illustrated in Fig. 5 for \( n = 4 \), there are \( S_{\Gamma_{cl}(n)} = 2n \) such permutations, made out of the convolution of

1. The identity plus 1 reflection inverting the clockwise ordering,
2. \( n \) clockwise circular permutations.

Summing over all closed diagrams, the final result is obtained as

\[
\sum_{n=1}^{\infty} \Gamma_{cl}(n) = -\frac{1}{2n} \text{Tr} \left\{ \sum_{n=1}^{\infty} \frac{1}{n} \left( z^*(l)z(r) \right)^n \right\},
\]

(48)

thus demonstrating the exponentiation of closed diagrams in the expansion of the norm kernel. The above rationale is illustrated diagrammatically in Fig. 4.
Fig. 5 Permutations of the labelled diagram $\Gamma_{cl}(4)$ delivering topologically equivalent diagrams. a Labelled diagram in the original representation. b Same diagram but expanded in a way that makes permutations of the vertices more transparent. b’ Labelled diagram obtained from b via a reflection with respect to the diagonal $l_1 - l_4$ inverting the clockwise ordering of the labelled vertices. c, c’ One representative of the four clockwise circular permutations obtained from b, b’, respectively. There is thus a total of $S_{\Gamma_{cl}(4)} = 2 \times 4$ permutations out of which the original labelled diagram can be recovered by a mere translation of the vertices in the plane.

which is nothing but the well-celebrated Onishi formula \[19\]. It has often been stated that the Onishi formula\(^\text{22}\) is compromised by an undefined complex phase. In the derivation above based on the application of standard Wick’s theorem, there is no algebraic manipulation that can be responsible for a loss of phase. Thus, the loss of phase due to the apparent necessity to compute the square root originating from the factor $1/2$ in the exponent in Eq. (50) can only be fictitious. The same observation is at the heart of Ref. [29]. The key point relates to the fact that the eigenvalues of the matrix $\mathbf{z}^*(l)\mathbf{z}(r)$, which is the product of two skew-symmetric matrices, are doubly-degenerate [30,31]. This double degeneracy necessarily compensates for the factored in exponent $1/2$ in Eq. (50), thus demonstrating the fictitious character of the square root and of the apparent loss of phase [17,29].

\(^{22}\)Strickly speaking, the Onishi formula, as any formula based on the symmetric approach, can only deliver the phase of the overlap $\langle \Phi(l)|\Phi(r) \rangle$ modulo the knowledge of the phase associated with, i.e. initially fixed for, the overlaps $\langle \Phi(l)|\Phi \rangle$ and $\langle \Phi|\Phi(r) \rangle$ of the two involved states with respect to the reference Bogoliubov state $|\Phi\rangle$.

3.2.4 Pfaffian formula

The equivalence of the Onishi and Pfaffian [20] formulae for the norm kernel has been demonstrated in a pedestrian way in Ref. [29]. As a matter of fact, the two formulae can be directly connected by exploiting the generic identity [32]

$$ \text{pf}(A)\text{pf}(B) = \exp \left[ \frac{1}{2} \text{Tr} \ln(A^T B) \right], $$

(51)

where $A$ and $B$ are two skew-symmetric matrices such that $A^T B$ is itself a positive-definite matrix. Rewriting the argument of the logarithm in Eq. (50) as

$$ 1 - \mathbf{z}^*(l)\mathbf{z}(r) = \mathbf{z}^*(l)(\mathbf{z}^*(l)^{-1} - \mathbf{z}(r)), $$

(52)

Equation (51) is applied for

$$ A \equiv \mathbf{z}^*(l), $$

(53a)

$$ B \equiv \mathbf{z}^*(l)^{-1} - \mathbf{z}(r). $$

(53b)

This leads to expressing the norm overlap as

$$ \frac{\langle \Phi(l)|\Phi(r) \rangle}{\langle \Phi(l)|\Phi \rangle \langle \Phi|\Phi(r) \rangle} = \text{pf}\left(\mathbf{z}^*(l)\right)\text{pf}( \mathbf{z}^*(l)^{-1} - \mathbf{z}(r)) $$

$$ = (-1)^{n/2} \text{pf}\left(\mathbf{z}^*(l)\right)\text{pf}( \mathbf{z}^*(l)^{-1} + \mathbf{z}^T(r)), $$

(54)
where the last equivalence makes use of the property
\[ pf(A^T) = (-1)^npf(A), \]
with 2\(n\) the size of the matrix \(A\), i.e. the (even) dimension \(n_1\) of the (truncated) one-body Hilbert space \(\mathcal{H}_1\) in the present context. The last useful identity for the pfaffian of a skew-symmetric matrix displaying the structure
\[ S = \begin{pmatrix} M & Q \\ -Q^T & N \end{pmatrix}, \]
with \(M\) an invertible matrix, is given by \[ pf(S) = pf(M)pf(N + Q^T M^{-1} Q). \]
Identifying
\[ M = z^t(l), \]
\[ N = z^t(r), \]
\[ Q = 1, \]
the pfaffian formulation of the norm overlap
\[ \frac{\langle \Phi(l) | \Phi(r) \rangle}{\langle \Phi(l) | \Phi \rangle \langle \Phi | \Phi(r) \rangle} = (-1)^{n_1/2} pf \left[ \begin{pmatrix} z^t(l) & 1 \\ -1 & z^t(r) \end{pmatrix} \right], \]
is eventually obtained from the Onishi formula, thus bypassing the intermediate apparent phase undetermination.

4 Discussion and conclusions

The interest of the present work is primarily formal and conceptual. The main goal has been to offer a novel perspective on the off-diagonal Wick theorem and the Onishi formula by consistently computing the off-diagonal operator and norm kernels at play in, e.g., the projected generator coordinate method via a single formal approach. The method expresses the two Bogoliubov states at play with respect to a third reference state \(|\Phi\rangle\) via Thouless’ theorem such that the kernels of interest read as
\[ \frac{\langle \Phi(l) | O | \Phi(r) \rangle}{\langle \Phi(l) | \Phi \rangle \langle \Phi | \Phi(r) \rangle} = \frac{\langle \Phi | e^{Z_{20}(l)}^t O e^{Z_{20}(r)} | \Phi \rangle}{\langle \Phi | e^{Z_{20}(l)}^t e^{Z_{20}(r)} | \Phi \rangle}, \]
\[ \frac{\langle \Phi(l) | \Phi \rangle \langle \Phi | \Phi(r) \rangle}{\langle \Phi(l) | \Phi \rangle \langle \Phi | \Phi(r) \rangle} = \langle \Phi | e^{Z_{20}(l)}^t e^{Z_{20}(r)} | \Phi \rangle. \]

While the exponentials of the Thouless one-body operators \(Z_{20}(l)^t\) and \(Z_{20}(r)\) do not naturally terminate, a diagrammatic method was used to demonstrate that the infinite set of terms can be resummed exactly.

Interestingly, the diagrammatic technique and the associated infinite resumptions leading to the exact computation of the above kernels can be used to design non-trivial approximations to more complex kernels of interest. As the simplest example, replacing the two Thouless one-body operators by a two-body cluster amplitude into Eq. \((59a)\) leads to
\[ E^{\text{CCD}} = \frac{\langle \Phi | e^{T_2^T} H e^{T_2} | \Phi \rangle}{\langle \Phi | e^{T_2^T} e^{T_2} | \Phi \rangle} = \langle \Phi | e^{T_2^T} H e^{T_2} | \Phi \rangle, \]
which is nothing but the energy at play in the variational coupled cluster with doubles method \([24]\). Because \(T_2\) is now a two-body operator, the equivalent to the off-diagonal Wick theorem and the associated resummation of the infinite expansion of the exponentials do not hold. As a result, approximation schemes have to be set up \([25,26]\) such that designing more advanced truncation schemes than existing ones can be of interest. Because the diagrammatic does not require the operators in the two exponentials to be the same, addressing even more general kernels (including the corresponding norm kernels) than the one displayed in Eq. \((60)\) can be envisioned.

Acknowledgements The authors wish to thank V. Somà and P. Arthuis for proofreading the manuscript. A.P. is supported by the CEA NUMER-ICS program, which has received funding from the European Union’s Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 809945.

Data availability statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: This is a theoretical work and neither experimental nor numerical data were generated.]

Appendix A: Normal-ordered operator

An arbitrary rank-\(N\) particle-number-conserving fermionic operator \(O\) can be written as
\[ O \equiv \sum_{n=0}^{N} O^{mn}, \]
where
\[ O^{mn} \equiv \frac{1}{m!n!} \sum_{a_1\cdots a_m \atop b_1\cdots b_n} c_{a_1} \cdots c_{a_m} e^{b_1} \cdots c_{b_n}, \]
contains \(m(n)\) particle creation (annihilation) operators. The zero-body part \(O^{00}\) is the scalar obtained as the expectation value of \(O\) in the particle vacuum
\[ O^{00} = \langle 0 | O | 0 \rangle. \]

In Eq. \((A.2)\), matrix elements are fully anti-symmetric under the exchange of any pair of upper or lower indices, i.e.
\[ o_{a_1\cdots a_m}^{b_1\cdots b_n} = \epsilon(\sigma_m) \epsilon(\sigma_n) o_{\sigma(\sigma_1\cdots\sigma_m)}^{\sigma(\sigma_1\cdots\sigma_n)}, \]
where \(\epsilon(\sigma_m) (\epsilon(\sigma_n))\) refers to the signature of the permutation \(\sigma_m(\cdots) (\sigma_n(\cdots))\) of the \(m\) \((n)\) upper \((lower)\) indices. In case
the particle-number conserving operator is hermitian, each term \( O^{nn} \) is hermitian with its matrix elements fulfilling

\[
o_{b_1 \cdots b_n} = (o_{a_1 \cdots a_n})^*. \tag{A.5}
\]

By virtue of standard Wick’s theorem [34], the operator \( O \) can be normal ordered with respect to the Bogoliubov vacuum \( |\Phi\rangle \)

\[
O \equiv \sum_{n=0}^{N} O^{[2n]} = \sum_{n=0}^{N} \sum_{i,j=0}^{2n} O^{ij} \tag{A.6}
\]

where the component

\[
O^{ij} = \frac{1}{i!j!} \sum_{k_1 \cdots k_i} \sum_{l_1 \cdots l_j} \epsilon(\sigma_i) \epsilon(\sigma_j) c_{i}^{k_1 \cdots k_i} c_{j}^{l_1 \cdots l_j}. \tag{A.7}
\]

contains \((i\ j)\) quasi-particle creation (annihilation) operators. The zero-body part \( O^{00} \) is the scalar obtained as the expectation value of \( O \) in the Bogoliubov vacuum

\[
O^{00} = \langle \Phi | O | \Phi \rangle. \tag{A.8}
\]

In Eq. (A.7), matrix elements are fully anti-symmetric under the exchange of any pair of upper or lower indices, i.e.

\[
o_{i_1 \cdots i_j}^{k_1 \cdots k_i} = \epsilon(\sigma_i) \epsilon(\sigma_j) o_{\sigma_i(k_1 \cdots k_i)}^{a_1 \cdots a_n}. \tag{A.9}
\]

These matrix elements are functionals of the Bogoliubov matrices \((U, V)\) associated with \( |\Phi\rangle \) and of the matrix elements \(\{o_{a_1 \cdots a_n}\} \) initially defining the operator \( O \). As such, the content of each operator \( O^{ij} \) depends on the rank \( N \) of \( O \). For more details about the normal ordering procedure and for explicit expressions of the matrix elements up to \( N = 3 \), see Refs. [16,35–37].

In case the operator is hermitian, each component \( O^{[2n]} \) is itself hermitian with \( O^{ij} = O^{ji} \) such that matrix elements satisfy

\[
o_{i_1 \cdots i_j}^{k_1 \cdots k_i} = (o_{k_1 \cdots k_i}^{i_1 \cdots i_j})^*. \tag{A.10}
\]

**Appendix B: Diagrammatic rules**

The present appendix is dedicated to setting up the diagrammatic rules allowing one to compute matrix elements of the form

\[
\langle s' | j' | t' \rangle = \frac{1}{s! t!} \langle \Phi | L' O^{ij} R' | \Phi \rangle, \tag{B.11a}
\]

\[
\langle s | t' \rangle = \frac{1}{s! t!} \langle \Phi | L' R' | \Phi \rangle, \tag{B.11b}
\]

where \( O^{ij} \) takes the form given in Eq. (A.7) and where \( R \) (\( L \)) is a one-body\(^{23}\) excitation (de-excitation) operator as defined in Eqs. (26a, 26b).

The diagrammatic rules are also worked out to compute a second category of matrix elements of present interest

\[
\langle s | k' | t' \rangle = \frac{1}{s! t!} \langle \Phi | L' \beta k' \beta k \ R' | \Phi \rangle, \tag{B.11c}
\]

\[
\langle s | k' | t' \rangle = \frac{1}{s! t!} \langle \Phi | L' \beta k' \beta k \ R' | \Phi \rangle. \tag{B.11d}
\]

These matrix elements differ from the two introduced in Eq. (B.11) by the presence of two “external/fixed” quasi-particle operators, i.e. quasi-particle operators whose indices are not summed over.

The diagrammatic rules derive from the straight application of standard Wick’s theorem with respect to the Bogoliubov vacuum \( |\Phi\rangle \). The application of Wick’s theorem delivers the complete set of fully contracted terms associated with the operator product entering the matrix element of interest. Given that the operators at play are all conveniently expressed in the quasi-particle basis associated with the Bogoliubov vacuum \( |\Phi\rangle \), the four possible elementary contractions take the simplest possible form

\[
R_{k' k} = \begin{pmatrix}
\langle \Phi | L' \beta k' \beta k | \Phi \rangle & \langle \Phi | L' \beta k' \beta k | \Phi \rangle \\
\langle \Phi | L' \beta k' \beta k | \Phi \rangle & \langle \Phi | L' \beta k' \beta k | \Phi \rangle
\end{pmatrix}
\]

\[
= \begin{pmatrix}
R_{k' k}^+ & R_{k' k}\, \delta_{k' k} \\
0 & \delta_{k' k}
\end{pmatrix}, \tag{B.13}
\]

such that the sole non-zero contraction \( R_{k' k}^+ \) needs to be considered.

**Appendix B.1: Diagrammatic representation**

The diagrammatic representation of the various contributions to the matrix elements of interest relies on the definition of the following building blocks

1. As illustrated in Fig. 6, the normal-ordered operator \( O^{ij} \) entering the matrix element \( \langle s' | j' | t' \rangle \) is represented by a Hugenholtz vertex with \( i \) (\( j \)) lines traveling out of (into)
3. The only non-zero contraction $R_{k_1k_2}$ corresponds to the up-down reading of the diagram. The convention is that the left-to-right reading of a matrix element corresponds to the up-down reading of the diagram.

2. As illustrated in Fig. 7, the operator $\mathbf{L}$ (R) entering all matrix elements of present interest is represented by a vertex of the $O^{02}$ ($O^{20}$) type and carry the associated algebraic factor $z^*_{l_1l_2} (l)$ ($z_{k_1k_2} (r)$).

3. The only non-zero contraction $R^+_{k_1k_2} = \delta_{k_1k_2}$ is represented in Fig. 8 and connects two up-going lines associated with one annihilation and one creation operator, both carrying the same quasi-particle index. For simplicity, one can eventually represent the contraction as a line carrying a single up-going arrow along with one quasi-particle index.

**Appendix B.2: Diagrams generation**

With these building blocks at hand, one can construct the diagrams gathering all contributions to the matrix elements introduced in Eq. (B.11) and (B.12). The basic rules to do so are as follows

1. Diagrams contain $s$ square vertices ($\mathbf{L}$) and $t$ triangle vertices ($\mathbf{R}$), the former being located above the latter. This is consistent with the convention that the left-to-right reading of a matrix element corresponds to the up-down reading of the diagram.

2. Diagrams making up the two matrix elements introduced in Eq. (B.11) are vacuum-to-vacuum diagrams with no line leaving the diagram. In $\langle s | f | l \rangle$, a dot vertex ($O^{ij}$) is located in between the square and triangle vertices. This is consistent with the convention that the left-to-right reading of a matrix element corresponds to the up-down reading of the diagram.

3. Diagrams making up the four matrix elements introduced in Eq. (B.12) are linked with two external lines associated with the operators $\beta^{\dagger}_{k_1}$ and $\beta_{k_2}$. The two lines leave the diagram on the same side to the, e.g., left such that (i) both lines are asymptotically in between the square ($\mathbf{L}$) and triangle ($\mathbf{R}$) vertices and such that (ii) the line carrying index $k_2$ is asymptotically located above the line carrying index $k_1$. This is consistent with the convention that the left-to-right reading of a matrix element corresponds to the up-down reading of the diagram. The arrow carried by each of the two lines points towards the interior (exterior) of the diagram if it is associated with a quasi-particle creation (annihilation) operator.

4. The fact that $R^+_{k_1k_2}$ is the sole non-zero contraction implies that the number of quasi-particle creation operators involved in a given matrix element is equal to the number of quasi-particle annihilation operators. Given that each operator $\mathbf{L}$ (R) contains two quasi-particle annihilation (creation) operators, this property require the following conditions to be fulfilled

(a) $\langle s | f | l \rangle$ demands $t = s + (i - j)/2$ ,
(b) $\langle s | f | l \rangle$ demands $t = s$ ,
(c) $\langle s | k^1 | k^2 \rangle$ demands $t = s$ ,
(d) $\langle s | k^1 | k^2 \rangle$ demands $t = s + 1$ ,
(e) $\langle s | k^2 | k^1 \rangle$ demands $t = s - 1$ ,
(f) $\langle s | k^2 | k^1 \rangle$ demands $t = s$ .

such that $t \geq (i - j)/2$, $t \geq s$ and $s \geq 1$ in case (a), (d) and (e), respectively.

5. Given the above considerations, one must construct all possible topologically distinct unlabelled diagrams from the building blocks; i.e., contract together the lines belonging to the $s$ square ($\mathbf{L}$) vertices and to the $t$ triangle ($\mathbf{R}$) vertices, along with those belonging to the dot
7. The diagrams making up the various matrix elements of interest display different typical topologies. Indeed, each contribution generated via the application of Wick’s theorem can be expressed as a product of strings of contractions, each of which involves a subset of the \( L \) and \( R \) operators at play. As for \( \langle i' | j' \rangle \) with \( (i + j) \geq 4 \), several such strings actually involve quasi-particle operators belonging to \( O^{ij} \), thus forming an overall closed string that is said to be connected to \( O^{ij} \). Translated into diagrammatic language, closed strings correspond to topologically disjoint closed sub-diagrams. In the case of \( \langle i' | j' \rangle \), any given diagram is thus made out of disjoint closed sub-diagrams, one of which is connected. As for the matrix elements introduced in Eq. (B.12), one set of contractions must form a connected string involving the operators \( \beta_{k_2}^{(1)} \) and \( \beta_{k_1}^{(1)} \). These two operators cannot belong to two disjoint strings given that any string necessarily involves an even number of quasi-particle operators. Eventually, the diagrams making up the matrix elements introduced in Eq. (B.12) are made out of disjoint closed sub-diagrams, one of which is connected to the external lines. Last but not least, each diagram contributing to \( \langle i' | j' \rangle \) is made out of disjoint closed sub-diagrams, none of which is connected.

Appendix B.3: Diagrams evaluation

Once all the diagrams are drawn, one must compute their expressions. The rules to do so are the following

1. Label all quasi-particle lines and associate the appropriate factor to each vertex, i.e. a factor \( z_{k_1k_2}(l) (z^{k_1k_2}(r)) \) to each vertex \( L \) (\( R \)) and a factor \( \Phi_{\ell_1\cdots\ell_j}^{(1)} \) to the vertex \( O^{ij} \), respectively.

2. Sum over all internal line labels.

3. Include a factor \( (n_c!)^{-1} \) for each set of \( n_c \) equivalent internal lines. Equivalent internal lines are those connecting identical vertices.

4. For any topologically distinct unlabelled diagram \( \Gamma \), a symmetry factor \( S_{\Gamma}^{-1} \) must be considered. Given a labelled version of \( \Gamma \), i.e. a version in which each operator \( L \) and \( R \) carries a specific label, \( S_{\Gamma} \) is equal to the number of permutations of the \( L \) and \( R \) operators delivering a topologically equivalent labelled diagram. The most obvious cases correspond to equivalent subgroups of \( L \) and \( R \) operators whose overall permutations lead to topologically equivalent labelled diagrams. The simplest example concerns two \( L \) (\( R \)) operators that are doubly connected to \( O^{ij} \) or singly connected to \( O^{ij} \) and to the same operator \( R \) (\( L \)). These \( n_o \equiv 2 \) operators \( L \) (\( R \)) are equivalent and contribute a factor \( l! \) to \( S_{\Gamma} \). The next simplest example corresponds to \( n_o > 2 \) operators \( L \) (\( R \)) fully connected to \( O^{ij} \). These \( n_o > 2 \) operators are indeed equivalent such that their permutations contribute a factor \( n_o! \) to \( S_{\Gamma} \).

5. Provide the diagram with a sign \( (-1)^{\ell_c} \), where \( \ell_c \) is the number of line crossings in the diagram. For diagrams containing external lines, their potential crossing must be counted.

Appendix C: Asymmetric approach

The asymmetric approach constitutes the standard path to the off-diagonal Wick theorem at play in the computation of the connected operator kernel [2,18]. Employing the simplified notation

\[
R \equiv Z^{20}(l, r) = \frac{1}{2} \sum_{k_1k_2} z^{k_1k_2}(l, r) \beta_{k_1}^{\dagger}(l) \beta_{k_2}^{\dagger}(l),
\]

for the Thouless operator introduced in Eq. (18b) and satisfying \( \langle \Phi(l) \rangle R = 0 \), the connected operator kernel reads as

\[24\] Note that \( n_o > 2 \) operators \( L \) (\( R \)) cannot be equivalent if any of them is connected to an operator \( R \) (\( L \)) given that the latter cannot entertain the same contraction pattern with \( n_o > 2 \) operators \( L \) (\( R \)). More general patterns would however occur if \( L \) and \( R \) were of higher ranks.

\[25\] There is no general rule to identify them such that the symmetry factor associated with each topologically distinct unlabelled diagram must be identified on a case by case basis.
\[
\begin{align*}
\langle \Phi(l)|O|\Phi(r) \rangle &= \sum_{n=0}^{N-1} \sum_{i,j=0}^{2n} \langle \Phi(l)| O^{ij} e^R |\Phi(l) \rangle , \\
&= N \sum_{n=0}^{N-1} \sum_{i,j=0}^{2n} \langle \Phi(l)| R O^{ij} |\Phi(l) \rangle , \quad \text{(C.15)}
\end{align*}
\]

where the operator
\[
R O^{ij} \equiv e^{-R} O^{ij} e^R
\]
formally reads as \( O^{ij} \) but with the quasi-particle operators replaced by their similarity-transformed partners
\[
\left( \begin{array}{cc}
R \beta_k \\
R \beta^+_k
\end{array} \right) \equiv e^{-R} \left( \begin{array}{cc}
\beta_k \\
\beta^+_k
\end{array} \right) e^R . \quad \text{(C.17)}
\]

Given that the similarity-transformed quasi-particle operators satisfy anticommutation relations
\[
\begin{align*}
\{ R \beta^+_k , R \beta^+_l \} &= e^{-R} \{ \beta^+_k , \beta^+_l \} e^R = 0 , \\
\{ R \beta_k , R \beta^+_l \} &= e^{-R} \{ \beta_k , \beta^+_l \} e^R = 0 , \\
\{ R \beta_k , R \beta^+_k \} &= e^{-R} \{ \beta_k , \beta^+_k \} e^R = \delta_{kk} , \quad \text{(C.18c)}
\end{align*}
\]

standard Wick’s theorem with respect to \( |\Phi(l) \rangle \) applies and can be used to compute the matrix elements entering the right-hand side of Eq. (C.15). This results into the standard set of fully contracted terms, except that the elementary contractions at play do not involve the original quasi-particle operators but rather the similarity-transformed ones. The latter are related to the former via a non-unitary Bogoliubov transformation that is now detailed to compute the relevant elementary contractions.

Using Baker-Campbell-Hausdorff (BCH) identity, one first evaluates Eq. (C.17) according to
\[
R \beta^+_k = R \beta^+_k [ R \beta_k ] + \frac{1}{2} [ R, [ R, \beta^+_k ] ] + \cdots . \quad \text{(C.19)}
\]

Given the two elementary commutators
\[
\begin{align*}
\left[ \begin{array}{c}
\beta^+_k (l) \\
\beta_k (l)
\end{array} \right] \left( \begin{array}{c}
\beta^+_l (l) \\
\beta_l (l)
\end{array} \right) &= \beta^+_k (l) \delta_{kk} - \beta^+_l (l) \delta_{kl} , \\
\left[ \begin{array}{c}
\beta^+_k (l) \\
\beta_k (l)
\end{array} \right] \left( \begin{array}{c}
\beta^+_l (l) \\
\beta_l (l)
\end{array} \right) &= 0 , \quad \text{(C.20b)}
\end{align*}
\]
it is straightforward to prove
\[
\left[ \begin{array}{c}
R, \beta_k
\end{array} \right] = - \sum_{k_1, k_2} \left[ U(l) z(l, r) \right]_{k_1 k_2} \beta^+_k (l) , \quad \left[ \begin{array}{c}
R, \beta^+_k
\end{array} \right] = \sum_{k_1, k_2} \left[ V(l) z(l, r) \right]_{k_1 k_2} \beta^+_k (l) ,
\]
\[
\sum_{k_1, k_2} \left[ V(l) z(l, r) \right]_{k_1 k_2} \beta^+_k (l) = 0 ,
\]
\[
\left[ \begin{array}{c}
R, \beta_k
\end{array} \right] = 0 ,
\]
\[
\left[ \begin{array}{c}
R, \beta^+_k
\end{array} \right] = 0 ,
\]
\[
\sum_{k_1, k_2} \left[ V(l) z(l, r) \right]_{k_1 k_2} \beta^+_k (l) = 0 .
\]

As Eqs. (C.21–C.22) testify, the infinite expansion in Eq. (C.19), originating from the presence of \( e^R \) in Eq. (23), naturally terminates, i.e. it stops after two terms. Eventually, the four elementary contractions read as
\[
\begin{align*}
\rho_{k_1 k_2} (l, r) &= \langle \Phi(l)| R \beta^+_k R \beta_k | \Phi(l) \rangle \\
&= \left[ V^*(l) V^T (l) + U(l) z(l, r) V^T (l) \right]_{k_1 k_2} , \\
&= + \rho_{k_1 k_2} (l, l) + \left[ U(l) z(l, r) V^T (l) \right]_{k_1 k_2} , \quad \text{(C.23a)}
\end{align*}
\]
\[
\begin{align*}
\kappa_{k_1 k_2} (l, r) &= \langle \Phi(l)| R \beta_k R \beta^+_k | \Phi(l) \rangle \\
&= \left[ V^*(l) U^T (l) + U(l) z(l, r) U^T (l) \right]_{k_1 k_2} , \\
&= + \kappa_{k_1 k_2} (l, l) + \left[ U(l) z(l, r) U^T (l) \right]_{k_1 k_2} , \quad \text{(C.23b)}
\end{align*}
\]
\[
\begin{align*}
- \tilde{\kappa}_{k_1 k_2}^* (l, r) &= \langle \Phi(l)| R \beta^+_k R \beta^+_k | \Phi(l) \rangle \\
&= \left[ U^*(l) V^T (l) + V(l) z(l, r) V^T (l) \right]_{k_1 k_2} , \\
&= - \tilde{\kappa}_{k_1 k_2}^* (l, l) + \left[ V(l) z(l, r) V^T (l) \right]_{k_1 k_2} , \quad \text{(C.23c)}
\end{align*}
\]
\[
\begin{align*}
- \sigma_{k_1 k_2}^* (l, r) &= \langle \Phi(l)| R \beta_k R \beta^+_k | \Phi(l) \rangle \\
&= \left[ U^*(l) U^T (l) + V(l) z(l, r) U^T (l) \right]_{k_1 k_2} .
\end{align*}
\]
\[ \langle \Phi(l) | O(r) | \Phi(r) \rangle = O[0] + \frac{1}{2} \sum_{k_1 k_2} o_{k_1 k_2}^\ast \sigma_{k_1 k_2}^\ast (l, r) + \sum_{k_1 l_1} o_{k_1 l_1}^\ast \rho_{l_1 k_1} (l, r) + \frac{1}{2} \sum_{l_1 l_2} o_{l_1 l_2} \kappa_{l_1 l_2} (l, r) \]

where Eqs. (C.21–C.22) have been used. This completes the derivation of the off-diagonal Wick theorem where the explicit form of the elementary off-diagonal contractions in Eq. (C.23) reflects the asymmetric character of the approach, i.e. the expressions are anchored on the bra state |\Phi(l)| and are a functional of the Thouless matrix z(l, r) associated with the transition Bogoliubov transformation of Eqs. (15–17).

Starting from Eq. (C.23) and using repeatedly relations associated with the unitarity of W(l) (Eq. (10)), one can symmetrize the elementary contractions by expressing them in terms of the Thouless matrices z(l, r) and z(r) associated with right states, respectively. Doing so, one recovers exactly Eqs. (39) and (41) obtained directly via the symmetric approach.

**Appendix D: Connected kernel of a rank-3 operator**

According to Eq. (38), the connected kernel associated with a rank-3 operator \( O \equiv O[0] + O[2] + O[4] + O[6] \) reads in terms of the off-diagonal elementary contractions as

\[ \langle \Phi(l) | O[0] | \Phi(r) \rangle = \sum_{k_1 k_2 k_3} o_{k_1 k_2}^\ast \sigma_{k_1 k_2}^\ast (l) + \sum_{k_1 k_2} o_{k_1 k_2} \sigma_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \rho_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \kappa_{k_1 k_2} (l) \]

\[ + \sum_{k_1 k_2} o_{k_1 k_2}^\ast \sigma_{k_1 k_2}^\ast \sigma_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \sigma_{k_1 k_2} \sigma_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \rho_{k_1 k_2} \rho_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \kappa_{k_1 k_2} \kappa_{k_1 k_2} (l) \]

\[ + \sum_{k_1 k_2} o_{k_1 k_2}^\ast \sigma_{k_1 k_2}^\ast \rho_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \sigma_{k_1 k_2} \rho_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \rho_{k_1 k_2} \kappa_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \kappa_{k_1 k_2} \kappa_{k_1 k_2} (l) \]

\[ + \sum_{k_1 k_2} o_{k_1 k_2}^\ast \rho_{k_1 k_2} \rho_{k_1 k_2} (l) + \sum_{k_1 k_2} o_{k_1 k_2} \kappa_{k_1 k_2} \kappa_{k_1 k_2} (l) \]
References

1. A.J.W. Thom, M. Head-Gordon, J. Chem. Phys. 131, 124113 (2009)
2. P. Ring, P. Schuck, The Nuclear Many-Body Problem (Springer, New York, 1980)
3. M. Bender, P.-H. Heenen, P.-G. Reinhard, Self-consistent mean-field models for nuclear structure. Rev. Mod. Phys. 75, 121 (2003). https://doi.org/10.1103/RevModPhys.75.121
4. T. Niksic, D. Vretenar, P. Ring, Relativistic nuclear energy density functionals: mean-field and beyond. Prog. Part. Nucl. Phys. 66, 519–548 (2011). arXiv:1102.4193, https://doi.org/10.1016/j.ppnp.2011.01.055
5. L.M. Robledo, T.R. Rodríguez, R.R. Rodríguez-Guzmán, Mean field and beyond description of nuclear structure with the Gogny force: a review. J. Phys. G 46(1), 013001 (2019). arXiv:1807.02518, https://doi.org/10.1088/1361-6471/aadebd
6. Z.-C. Gao, M. Horoi, Y.S. Chen, Variation after projection with a triaxially deformed nuclear mean field. Phys. Rev. C 92(6), 064310 (2015). arXiv:1509.03058, https://doi.org/10.1103/PhysRevC.92.064310
7. C.F. Jiao, J. Engel, J.D. Holt, Neutrinoless double-beta decay matrix elements in large shell-model spaces with the generator-coordinate method. Phys. Rev. C 96(5), 054310 (2017). arXiv:1707.03940, https://doi.org/10.1103/PhysRevC.96.054310
8. B. Bally, A. Sánchez-Fernández, T.R. Rodríguez, Variational approximations to exact solutions in shell-model valence spaces: calcium isotopes in the pf-shell. Phys. Rev. C 100(4), 044308 (2019). arXiv:1907.05493, https://doi.org/10.1103/PhysRevC.100.044308
9. N. Shimizu, T. Mizusaki, K. Kaneko, Y. Tsumoda, Generator-coordinate methods with symmetry-restored Hartree–Fock–Bogoliubov wave functions for large-scale shell-model calculations. Phys. Rev. C 103(6), 064302 (2021). https://doi.org/10.1103/PhysRevC.103.064302
10. A. Sánchez-Fernández, B. Bally, T.R. Rodríguez, Variational approximations to exact solutions in shell-model valence spaces: systematic calculations in the sd-shell. arXiv:2106.08841
11. J.M. Yao, B. Bally, J. Engel, R. Wirth, T.R. Rodríguez, H. Hergert, Ab Initio treatment of collective correlations and the neutrinoless double beta decay of 48Ca. Phys. Rev. Lett. 124(23), 232501 (2020). arXiv:1908.05424, https://doi.org/10.1103/PhysRevLett.124.232501
12. J.M. Yao, J. Engel, L. J. Wang, C.F. Jiao, H. Hergert, Generator-coordinate reference states for spectra and ννββ decay in the in-medium similarity renormalization group. Phys. Rev. C 98(5), 054311 (2018). arXiv:1807.11053, https://doi.org/10.1103/PhysRevC.98.054311
13. M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, H. Hergert, T.R. Rodríguez, R. Roth, J. Yao, V. Somá, Multi-reference many-body perturbation theory for nuclei: III. Ab initio calculations at second order in PGCM-PT. Eur. Phys. J. A 58(4), 64 (2022). arXiv:2111.01461, https://doi.org/10.1140/epja/s10050-022-00694-x
14. M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, T. Mongelli, T.R. Rodríguez, R. Roth, V. Somá, Multi-reference many-body perturbation theory for nuclei: II. Ab initio study of neon isotopes via PGCM and IM-NCSM calculations. Eur. Phys. J. A 58(4), 63 (2022). arXiv:2111.00797, https://doi.org/10.1140/epja/s10050-022-00693-y
15. M. Frosini, T. Duguet, J.-P. Ebran, V. Somá, Multi-reference many-body perturbation theory for nuclei: I. Novel PGCM-PT formalism. Eur. Phys. J. A 58(4), 62 (2022). arXiv:2110.15737, https://doi.org/10.1140/epja/s10050-022-00692-z
16. T. Duguet, A. Signoracci, Symmetry broken and restored coupled-cluster theory. II. Global gauge symmetry and particle number. J. Phys. G 44(1), 015103 (2017). [Erratum: J.Phys.G 44, 049601 (2017)]. arXiv:1512.02878, https://doi.org/10.1088/0954-3899/44/1/015103
17. B. Bally, T. Duguet, Norm overlap between many-body states: uncorrelated overlap between arbitrary Bogoliubov product states. Phys. Rev. C 97(2), 024304 (2018). arXiv:1704.05324, https://doi.org/10.1103/PhysRevC.97.024304
18. R. Balian, E. Brezin, Nonunitary Bogoliubov transformations and extension of Wick’s theorem. Il Nuovo Cimento B 64(1), 37–55 (1969)
19. N. Onishi, S. Yoshida, Nucl. Phys. 80, 367 (1966)
20. L.M. Robledo, The sign of the overlap of HFB wave functions. Phys. Rev. C 79, 021302 (2009)
21. T. Mizusaki, M. Oi, A new formulation to calculate general HFB matrix elements through Pfaffian. Phys. Lett. B 715, 219–224 (2012). arXiv:1204.6531, https://doi.org/10.1016/j.physletb.2012.07.023
22. T. Mizusaki, M. Oi, F.-Q. Chen, Y. Sun, Grassmann integral and Balian–Brézin decomposition in Hartree–Fock–Bogoliubov matrix elements. Phys. Lett. B 725, 175–179 (2013). arXiv:1305.1682, https://doi.org/10.1016/j.physletb.2013.07.005
23. D.J. Thouless, Perturbation theory in statistical mechanics and the theory of superconductivity. Ann. Phys. 10, 553 (1960)
24. R.J. Bartlett, J. Noga, Chem. Phys. Lett. 150, 29 (1988)
25. J.B. Robinson, P.J. Knowles, J. Chem. Phys. 136, 054114 (2012)
26. R. Roth, J. Yao, J.D. Holt, Neutrinoless double-beta decay of 48Ca. Phys. Rev. Lett. 124, 232501 (2020). arXiv:1908.05424, https://doi.org/10.1103/PhysRevLett.124.232501
27. J.M. Yao, J. Engel, L. J. Wang, C.F. Jiao, H. Hergert, Generator-coordinate reference states for spectra and ννββ decay in the in-medium similarity renormalization group. Phys. Rev. C 98(5), 054311 (2018). arXiv:1807.11053, https://doi.org/10.1103/PhysRevC.98.054311
28. J.M. Yao, J. Engel, L. J. Wang, C.F. Jiao, H. Hergert, Generator-coordinate reference states for spectra and ννββ decay in the in-medium similarity renormalization group. Phys. Rev. C 98(5), 054311 (2018). arXiv:1807.11053, https://doi.org/10.1103/PhysRevC.98.054311
29. M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, H. Hergert, T.R. Rodríguez, R. Roth, J. Yao, V. Somá, Multi-reference many-body perturbation theory for nuclei: III. Ab initio calculations at second order in PGCM-PT. Eur. Phys. J. A 58(4), 64 (2022). arXiv:2111.01461, https://doi.org/10.1140/epja/s10050-022-00694-x
30. M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, T. Mongelli, T.R. Rodríguez, R. Roth, V. Somá, Multi-reference many-body perturbation theory for nuclei: II. Ab initio study of neon isotopes via PGCM and IM-NCSM calculations. Eur. Phys. J. A 58(4), 63 (2022). arXiv:2111.00797, https://doi.org/10.1140/epja/s10050-022-00693-y
36. P. Arthuis, T. Duguet, A. Tichai, R.D. Lasseri, J.P. Ebran, ADG: automated generation and evaluation of many-body diagrams I. Bogoliubov many-body perturbation theory. Comput. Phys. Commun. 240, 202–227 (2019). arXiv:1809.01187, https://doi.org/10.1016/j.cpc.2018.11.023

37. J. Ripoche, A. Tichai, T. Duguet, Normal-ordered k-body approximation in particle-number-breaking theories. Eur. Phys. J. A 56(2). https://doi.org/10.1140/epja/s10050-020-00045-8. http://dx.doi.org/10.1140/epja/s10050-020-00045-8

Springer Nature or its licensor holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.