Matrix elements of many-body operators and density correlations

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The matrix element of a general many-body operator between two Slater determinants is calculated explicitly. For this, a split-and-pair method is introduced that provides a convenient expression of Wick's theorem and simplifies many-body calculations. The same method is used to determine the generating function of the matrix elements of many-body operators. The split-and-pair method allows also for the diagonalization of the density correlation operators $:n(x_1)\cdots n(x_k):$, where $n(x)=\psi^\dagger(x)\psi(x)$ is the density operator. The relation between the split-and-pair method and quantum group theory is clarified.

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I. INTRODUCTION

Many-body calculations are often combinatorially complex. One of the causes of this complexity is the fact that Wick's theorem [1] is stated in combinatorial terms (taking all possible contractions). A new approach is introduced here to simplify such calculations: the split-and-pair method. It consists of two operations: the splitting of a normal product into all its possible pairs of factors and the pairing of two normal products u and v, which is simply $\langle 0|uv|0\rangle$ (i.e., the vacuum expectation value of the operator product of u and v). These two operations lead to a powerful expression of Wick's theorem because they replace its combinatorial structure by an algebraic structure.

Using the split-and-pair method, we first rederive a classical result: we calculate general matrix elements of the form $\langle K|O_k|L\rangle$, where O_k is a k-body operator and $|K\rangle$ and $|L\rangle$ are Slater determinants. Then the split-and-pair method is used to derive two new results: (i) a closed expression for the generating function of all matrix elements between $|K\rangle$ and $|L\rangle$, which is useful in nonequilibrium many-body theory; (ii) the eigenvalues and rank of the matrix obtained when O_k is a k-body density operator $:n(x_1)\cdots n(x_k):$, with $n(x)=\psi^\dagger(x)\psi(x)$. This last result can be used to calculate the k-point correlation function for a quantum system in a general state.

The paper starts with a definition of normal products and a description of how they can be split into two factors. The pairing of two normal products is introduced and calculated explicitly, and Wick's theorem is written in terms of the splitting and the pairing. Several simple examples are treated, in detail, to familiarize the reader with this new technique. Then three calculations are carried out as mentioned in the previous paragraph: $\langle K|O_k|L\rangle$, the generating function and the k-body density correlation function. Finally, the split-and-pair method is linked to general algebraic concepts.

II. SPLITTING OF NORMAL PRODUCTS

In this section, we show that the normal products of creation and annihilation operators can be split into factors in a useful way.

A. Normal products

The creation and annihilation operators of an electron in orbital i are denoted by $b_i^\dagger$ and b_i. We call $\mathcal{B}$ the set of linear combinations of terms of the form $u=b_{i_1}^\dagger\cdots b_{i_m}^\dagger b_{j_1}\cdots b_{j_n}$ for $m\geqslant 0$ and $n\geqslant 0$. The term corresponding to $n=m=0$ is denoted by 1. All $b_i^\dagger$ anticommute with all $b_j^\dagger$ and all b_i anticommute with all b_j. Thus, to define a basis of $\mathcal{B}$ we need to choose a definite order for the operators. It is convenient to choose the basis $u=b_{i_1}^\dagger\cdots b_{i_m}^\dagger b_{j_1}\cdots b_{j_n}$, where now $i_1<\cdots<i_m$ and $j_1<\cdots<j_n$. Such elements of $\mathcal{B}$ are said to be normally ordered and they are called the monomials of $\mathcal{B}$. The space $\mathcal{B}$ is convenient because Wick's theorem tells us that the product of operators can always be written in terms of normally ordered elements, so that products of operators are also defined in $\mathcal{B}$. Apart from the operator product, we can define now another product on $\mathcal{B}$: the *normal product*. If u and v are monomials of $\mathcal{B}$, the normal product of u and v is written $:uv:$ and it is calculated as follows: if u contains only creation operators and v only annihilation operators then $:uv:=uv$; otherwise, creation operators are brought to the left of annihilation operators by assuming that creation operators anticommute with annihilation operators. For example, if $u=b_i^\dagger b_k$ and $v=b_l^\dagger$, we have $:uv:=:(b_i^\dagger b_k)(b_l^\dagger):=-b_i^\dagger b_l^\dagger b_k$. The vector space $\mathcal{B}$ equipped with the normal product is an algebra. Of course, 1 is the unit of this algebra.

We define now the parity of a monomial u of $\mathcal{B}$. If $u=b_{i_1}^\dagger\cdots b_{i_m}^\dagger b_{j_1}\cdots b_{j_n}$, the parity of u is denoted by $|u|$ and is 0 if $n+m$ is even and 1 if $n+m$ is odd. The parity is useful because of the identity

$$:vu:=(-1)^{|u||v|}:uv:. \tag{1}$$

B. The splitting

We saw that for two monomials u and v, we can define a normal product $:uv:$. The trick that will be useful for explicit calculations is that we can also split any monomial w of $\mathcal{B}$ into two factors u and v such that $:uv:=w$. The splitting of w into all possible pairs of monomial factors will be called the coproduct of w.

To define more precisely the coproduct, we denote by a an operator that can be either an annihilation operator b_i or a creation operator $b_i^\dagger$ for some i, or, more generally, a linear combination of creation and annihilation operators: $a=\Sigma_i\alpha_i b_i+\beta_i b_i^\dagger$, where α_i and β_i are complex numbers. In the rest of the papers, all variables denoted by $a_1,a_2,\ldots,a_n$ will be such linear combinations.

For pedagogical reasons, we shall give three definitions of the coproduct. The coproduct of u will be denoted by Δu.

1. Elementary definition of the coproduct

As mentioned in the Introduction, the coproduct of u is the sum of all the ways to write u as a normal product of two monomials. For instance, $:a_1a_2:$ can be written as the normal product of a_1 and a_2 or of a_2 and a_1 (but with a minus sign) or of $:a_1a_2:$ and 1 or of 1 and $:a_1a_2:$. Therefore, we write

$$\Delta:a_1a_2:=a_1\otimes a_2-a_2\otimes a_1+:a_1a_2:\otimes 1+1\otimes:a_1a_2:. \tag{2}$$

The reader should not worry about the presence of the tensor symbol $\otimes$, which could be considered as just a way to separate the left-hand side of the product from its right-hand side [2]. The minus sign in the second term of $\Delta:a_1a_2:$ is due to the fact that $:a_1a_2:=-:a_2a_1:$.

Similarly, 1 can only be written as :11:, thus $\Delta 1=1\otimes 1$, a can only be written as $:a1:$ or $:1a:$, so that $\Delta a=a\otimes 1+1\otimes a$.

If we now have $u=:a_1\cdots a_n:$, let P_k by any subset of elements of the list $\{a_1,\ldots,a_n\}$. There are 2^n such subsets (the empty set being allowed) so that k runs from 1 to 2^n. Let v_1^k be the normal product of the elements of P_k and v_2^k be the normal product of the elements of $\{a_1,\ldots,a_n\}$, which are not in P_k. The coproduct of u is

$$\Delta u=\sum_{k=1}^{2^n}\pm v_1^k\otimes v_2^k, \tag{3}$$

where we replace v_1^k by 1 if P_k is the empty set and v_2^k by 1 if P_k is the full set $\{a_1,\ldots,a_n\}$ and where "$\pm$" is determined so that $u=\pm:v_1^kv_2^k:$. For $n=0$ to 3, we have

$$\Delta 1=1\otimes 1,$$

$$\Delta a=a\otimes 1+1\otimes a,$$

$$\Delta:a_1a_2:=:a_1a_2:\otimes 1+1\otimes:a_1a_2:+a_1\otimes a_2-a_2\otimes a_1,$$

$$\begin{aligned}\Delta:a_1a_2a_3:=&:a_1a_2a_3:\otimes 1+1\otimes:a_1a_2a_3:+:a_1a_2:\otimes a_3\\&-:a_1a_3:\otimes a_2+:a_2a_3:\otimes a_1+a_1\otimes:a_2a_3:-a_2\\&\otimes:a_1a_3:+a_3\otimes:a_1a_2:.\end{aligned}$$

This definition of the coproduct is elementary, but it looks very cumbersome. This will be improved with the second definition, which is recursive. Before leaving this section, we note that the coproduct was defined only for monomials. This definition is extended to the whole vector space $\mathcal{B}$ by linearity: if u and v are elements of $\mathcal{B}$ and λ is a complex number then $\Delta(u+v)=\Delta u+\Delta v$ and $\Delta(\lambda u)=\lambda\Delta u$.

2. Recursive definition of the coproduct

The first step is to find a nice notation for the coproduct of a monomial of $\mathcal{B}$. We shall write [3]

$$\Delta u=\sum u_{(1)}\otimes u_{(2)}.$$

Here $u_{(1)}$ stands for $\pm v_1^k$, $u_{(2)}$ stands for v_2^k, the sum means a sum over the subsets P_k, but k is implicit. This notation enables us to give a recursive definition of the coproduct as [4]

$$\Delta(:uv:)=\sum(-1)^{|u_{(2)}||v_{(1)}|}:u_{(1)}v_{(1)}:\otimes:u_{(2)}v_{(2)}:. \tag{4}$$

The meaning of this formula is the following: if you know the coproduct of u and v to be $\Delta u=\Sigma u_{(1)}\otimes u_{(2)}$ and $\Delta v=\Sigma v_{(1)}\otimes v_{(2)}$, then the coproduct of $:uv:$ is obtained by taking all terms $u_{(1)}\otimes u_{(2)}$ and $v_{(1)}\otimes v_{(2)}$ of each sum, set the normal product of $u_{(1)}$ and $v_{(1)}$ on the left of the tensor symbol, and the normal product of $u_{(2)}$ and $v_{(2)}$ on the right, and multiply by the sign $(-1)^{|u_{(2)}||v_{(1)}|}$, where $|u_{(2)}|$ is the parity of $u_{(2)}$ and $|v_{(1)}|$ the parity of $v_{(1)}$.

We can illustrate this rule with our favorite example. We want to calculate $\Delta(:uv:)$, where $u=a_1$ and $v=a_2$. We start from $\Delta u=a_1\otimes 1+1\otimes a_1$ and $\Delta v=a_2\otimes 1+1\otimes a_2$. Now we mix them using Eq. (4). Take first the first term of Δu, for which $u_{(1)}=a_1$ and $u_{(2)}=1$, and the first term of Δv, for which $v_{(1)}=a_2$ and $v_{(2)}=1$; the product in Eq. (4) gives us $(-1)^{|1||a_2|}:a_1a_2:\otimes 1$. If we repeat this for all terms of Δu and Δv, we obtain

$$\begin{aligned}\Delta:a_1a_2:=&(-1)^{|1||a_2|}:a_1a_2:\otimes 1+(-1)^{|1||1|}a_1\otimes a_2\\&+(-1)^{|a_1||a_2|}a_2\otimes a_1+(-1)^{|a_1||1|}1\otimes:a_1a_2:.\end{aligned}$$

Now we use the fact that $|1|=0$ and $|a_1|=|a_2|=1$ to conclude that

$$\Delta:a_1a_2:=:a_1a_2:\otimes 1+a_1\otimes a_2-a_2\otimes a_1+1\otimes:a_1a_2:.$$

The identity (4) is important because it is the basis of recursive proofs. This second definition is very useful, but it is not always explicit enough, therefore we give now the third definition in terms of permutations.

3. Definition in terms of permutations

A $(p,n-p)$-shuffle permutation is a permutation σ of the set $\{1,\ldots,n\}$ such that $\sigma(1)<\cdots<\sigma(p)$ and $\sigma(p+1)<\cdots<\sigma(n)$. The name comes from the fact that if you have a deck of n cards, p of them in the left hand and $n-p$ in the right hand, and if you shuffle these cards, then the shuffled deck is a $(p,n-p)$-shuffle permutation of the original deck. A precise definition of the coproduct of $u=:a_1\cdots a_n:$ can now be given as

$$\begin{aligned}\Delta u=u\otimes 1+1\otimes u+\sum_{p=1}^{n-1}\sum_{\sigma}(-1)^{\sigma}&:a_{\sigma(1)}\cdots a_{\sigma(p)}:\\&\otimes:a_{\sigma(p+1)}\cdots a_{\sigma(n)}:,\end{aligned} \tag{5}$$

where the sum over σ is the sum over $(p,n-p)$ shuffles and $(-1)^\sigma$ is the signature of the permutation σ. To simplify the

notation, we consider that the first and second terms on the right-hand side of Eq. (5) come from the $(n,0)$ shuffle and the $(0,n)$ shuffle, respectively, and we write

$$\Delta u = \sum_{\sigma} (-1)^{\sigma} :a_{\sigma(1)} \cdots a_{\sigma(p)}: \otimes :a_{\sigma(p+1)} \cdots a_{\sigma(n)}:,$$

where the sum is now over all shuffles. It must be stressed that this definition is exactly equivalent to Eq. (3). Its main advantage is that "±" in Eq. (3) is now given explicitly.

After these painful definitions, the reader can relax because the rest of the paper uses only standard concepts of many-body theory.

III. THE PAIRING

Up to now, we know only the normal product and the coproduct. To do quantum calculations, we need to also calculate the operator product, which is given by Wick's theorem in terms of normal products. To obtain a handy form of Wick's theorem, we define the pairing. If u and v are elements of $\mathcal{B}$, we can take their operator product uv. The *pairing* of u and v, denoted by $(u|v)$, is the vacuum expectation value of uv. In other words,

$$(u|v) = \langle 0|uv|0\rangle.$$

For example, from the standard results $\langle 0|b_i b_j^{\dagger}|0\rangle = \delta_{ij}$ and $\langle 0|b_i b_j|0\rangle = \langle 0|b_i^{\dagger} b_j|0\rangle = \langle 0|b_i^{\dagger} b_j^{\dagger}|0\rangle = 0$, we obtain the pairings

$$(b_i|b_j^{\dagger}) = \delta_{ij}, \quad (b_i|b_j) = (b_i^{\dagger}|b_j) = (b_i^{\dagger}|b_j^{\dagger}) = 0. \tag{6}$$

More generally, Grosshans *et al.* [5] proved the following important identity:

$$(:a_1 \cdots a_m:|:a_1' \cdots a_n':) = \delta_{mn}(-1)^{n(n-1)/2} \det(a_i|a_j'), \tag{7}$$

where $(a_i|a_j')$ denotes the matrix with matrix elements obtained by taking the pairing of a_i and a_j'. The possible values of $(a_i|a_j')$ are deduced from the values given in Eq. (6). Equation (7) is extended to the case $m=n=0$ by $(1|1) = \langle 0|1|0\rangle = 1$.

For instance, we have

$$(:b_i b_j:|:b_k^{\dagger} b_l^{\dagger}:) = -\det\begin{pmatrix} \delta_{ik} & \delta_{il} \\ \delta_{jk} & \delta_{jl} \end{pmatrix} = \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl}. \tag{8}$$

This explicit expression will prove quite powerful for the calculation of more general matrix elements. Note that because of Eqs. (6) and (7), $(u|v)$ is zero if u contains creation operators or v annihilation operators.

The right-hand side of Eq. (7) involves a determinant. In 1772, Laplace derived the so-called Laplace identities, which express the determinant of a matrix in terms of minors of this matrix (see Refs. 6 and 7, p. 26, and Ref. 8, p. 93). The Laplace identities take an elegant form in terms of the coproduct [4,5]

$$(:uv:|w) = \sum (-1)^{|v||w_{(1)}|} (u|w_{(1)})(v|w_{(2)}), \tag{9}$$

$$(u|:vw:) = \sum (-1)^{|u_{(2)}||v|} (u_{(1)}|v)(u_{(2)}|w), \tag{10}$$

for any monomials u, v, and w of $\mathcal{B}$. Equation (9) is called expansion by rows and Eq. (10) expansion by columns. Because of its relations with the Laplace identities, Rota called $(u|v)$ the Laplace pairing. For example, using Eqs. (9) and (10) we can check that

$$\begin{aligned}(:b_i b_j:|:b_k^{\dagger} b_l^{\dagger}:) &= -(b_i|b_k^{\dagger})(b_j|b_l^{\dagger}) + (b_i|b_l^{\dagger})(b_j|b_k^{\dagger}) \\ &= -\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk},\end{aligned}$$

and we recover Eq. (8).

Note that the definition of the Laplace pairing implies that it is bilinear

$$(u|v+w) = (u|v) + (u|w), \quad (u+v|w) = (u|w) + (v|w),$$

$$(\lambda u|v) = (u|\lambda v) = \lambda (u|v).$$

IV. WICK'S THEOREM

We now have all the concepts we need and can write Wick's theorem as: if u and v are two elements of $\mathcal{B}$ with a definite parity, then

$$uv = \sum (-1)^{|u_{(2)}||v_{(1)}|} (u_{(1)}|v_{(1)}) :u_{(2)} v_{(2)}:. \tag{11}$$

This formula is much easier to manipulate than the standard form of Wick's theorem where one must take all possible contractions between u and v. The fact that Eq. (11) is equivalent to Wick's theorem was proved in [4,9]. It is useful to get acquainted with this version of Wick's theorem by working out examples. The reader can check that

$$a_1 a_2 = :a_1 a_2: + (a_1|a_2),$$

$$(:a_1 a_2:) a_3 = :a_1 a_2 a_3: - (a_1|a_3) a_2 + (a_2|a_3) a_1,$$

$$a_1 (:a_2 a_3:) = :a_1 a_2 a_3: + (a_1|a_2) a_3 - (a_1|a_3) a_2,$$

$$\begin{aligned}(:a_1 a_2:)(:a_3 a_4:) = {} & :a_1 a_2 a_3 a_4: - (a_1|a_3) :a_2 a_4: + (a_1|a_4) :a_2 a_3: \\ & + (a_2|a_3) :a_1 a_4: - (a_2|a_4) :a_1 a_3: \\ & + (:a_1 a_2:|:a_3 a_4:).\end{aligned}$$

We prove the simple case: from Wick's theorem (11) and from the coproduct of a_1 and a_2, we have

$$\begin{aligned}a_1 a_2 = {} & (-1)^{|a_1||1|} (1|1) :a_1 a_2: + (-1)^{|a_1||a_2|} (1|a_2) :a_1 1: \\ & + (-1)^{|a_1||1|} (a_1|1) :1 a_2: + (-1)^{|1||a_2|} (a_1|a_2) :11:.\end{aligned}$$

a_1 and a_2 are odd and 1 is even, moreover 1 is the unit element; thus, we obtain

$$a_1 a_2 = (1|1) :a_1 a_2: - (1|a_2) a_1 + (a_1|1) a_2 + (a_1|a_2) 1.$$

Because of formula (7), the Laplace pairing is zero if both sides do not contain the same number of creation and annihilation operators. Thus, $(1|a_2) = (a_1|1) = 0$, and we obtain the desired result.

V. EXAMPLES

In this section, we shall become familiar with this tool by calculating simples examples in detail. We first derive a useful identity

$$\sum (1|u_{(1)})u_{(2)} = \sum (u_{(1)}|1)u_{(2)} = u, \tag{12}$$

for any element u of $\mathcal{B}$. By linearity of the coproduct, it is enough to consider an element $u=:a_1\cdots a_n:$. The coproduct of u is given by Eq. (5), which gives us

$$\sum (1|u_{(1)})u_{(2)} = (1|u)1 + (1|1)u + \sum_{p=1}^{n-1}\sum_{\sigma} (-1)^{\sigma}(1|:a_{\sigma(1)}\cdots a_{\sigma(p)}:):a_{\sigma(p+1)}\cdots a_{\sigma(n)}:.$$

Equation (7) tells us that $(1|:a_{\sigma(1)},\ldots,a_{\sigma(p)}:)=0$ if $p>0$. Therefore, the only nonzero term of the right hand side is $(1|1)u=u$, which proves the result.

A. Action of the number operator

We call $N=\Sigma_i b_i^\dagger b_i$ the number operator and for any element u of $\mathcal{B}$ we show that

$$Nu = :Nu: + \mathcal{N}^+(u)u, \tag{13}$$

where $\mathcal{N}^+$ counts the number of creation operators in u. We first use Wick's theorem (11) to write

$$Nu = \sum (-1)^{|N_{(2)}||u_{(1)}|}(N_{(1)}|u_{(1)}):N_{(2)}u_{(2)}:.$$

From the definition of N and Eq. (2), we find that the coproduct of N is

$$\Delta N = N\otimes 1 + 1\otimes N + \sum_i b_i^\dagger \otimes b_i - \sum_i b_i \otimes b_i^\dagger.$$

According to identity (7), $(N_{(1)}|u_{(1)})=0$ for the first and third terms because $N_{(1)}$ contains a creation operator. Thus, we are left with

$$Nu = \sum (1|u_{(1)}):Nu_{(2)}: - \sum_i (-1)^{|u_{(1)}|}(b_i|u_{(1)}):b_i^\dagger u_{(2)}:.$$

From Eq. (12) we obtain $Nu=:Nu:+F(u)$ with

$$F(u) = \sum_i \sum (b_i|u_{(1)}):b_i^\dagger u_{(2)}:,$$

where we used the fact that, for $(b_i|u_{(1)})$ to be nonzero, $u_{(1)}$ must be a single creation operator so the parity of $u_{(1)}$ is 1 and $(-1)^{|u_{(1)}|}=-1$. We must now show that $F(u)=\mathcal{N}^+(u)u$. This will be proved recursively. If $\mathcal{N}^+(u)=0$, u does not contain creation operators, so that $(b_i|u_{(1)})=0$ and the identity is proved. Now assume that it is satisfied up to $\mathcal{N}^+(u)=k$ and take $u=:b_j^\dagger v:$, with $\mathcal{N}^+(v)=k$, so that $\mathcal{N}^+(u)=k+1$. Using the recursive definition of the coproduct, we have $\Delta u = \Sigma :b_j^\dagger v_{(1)}:\otimes v_{(2)} + \Sigma(-1)^{|v_{(1)}|}v_{(1)}\otimes :b_j^\dagger v_{(2)}:$ and

$$F(u) = \sum_i \sum (b_i|:b_j^\dagger v_{(1)}:):b_i^\dagger v_{(2)}: - (b_i|v_{(1)}):b_i^\dagger b_j^\dagger v_{(2)}:.$$

Using identity (7), we see that the first term on the right-hand side is nonzero only if $v_{(1)}=1$ and $i=j$. We interchange $b_i^\dagger$ and $b_j^\dagger$ in the second term and get

$$F(u) = :b_j^\dagger v: + \sum_i \sum (b_i|v_{(1)}):b_j^\dagger b_i^\dagger v_{(2)}: = :b_j^\dagger v: + :b_j^\dagger F(v):,$$

where we used the definition of F. We can now use the recursion hypothesis to conclude

$$F(u) = :b_j^\dagger v: + \mathcal{N}^+(v):b_j^\dagger v: = \mathcal{N}^+(u)u.$$

The identity is now proved.

The foregoing proof is not really shorter than the proof using standard methods, but it shows the main characteristics of the new approach: calculations are more algebraic and less combinatorial; general terms, such as u, are manipulated instead of explicit terms, such as $b_{i_1}^\dagger\cdots b_{i_k}^\dagger$.

B. Matrix elements

If we call $\mathcal{N}^-$ the operator that counts the number of annihiliation operator, a similar proof leads to the result

$$uN = :uN: + \mathcal{N}^-(u)u = :N\mathrm{u}: + \mathcal{N}^-(u)u. \tag{14}$$

The fact that $:uN:=:Nu:$ is showed using the parity equation (1) and the fact that the parity of N is zero. This will enable us to prove a classical but useful identity. Consider two states $|K\rangle=b_{i_1}^\dagger,\ldots,b_{i_m}^\dagger|0\rangle$ and $|L\rangle=b_{j_1}^\dagger,\ldots,b_{j_n}^\dagger|0\rangle$, so that $N|K\rangle=m|K\rangle$ and $N|L\rangle=n|L\rangle$ (the first term of Eq. (13) being annihilated by $|0\rangle$).

We want to calculate $\langle K|[N,u]|L\rangle$. By acting on the state vectors, we have

$$\langle K|[N,u]|L\rangle = \langle K|Nu|L\rangle - \langle K|uN|L\rangle = (m-n)\langle K|u|L\rangle.$$

On the other hand,

$$[N,u] = Nu - uN = [\mathcal{N}^+(u) - \mathcal{N}^-(u)]u.$$

Therefore

$$\langle K|[N,u]|L\rangle = (m-n)\langle K|u|L\rangle = [\mathcal{N}^+(u) - \mathcal{N}^-(u)]\langle K|u|L\rangle. \tag{15}$$

We conclude that, if $|K\rangle$ and $|L\rangle$ have the same number of particles (i.e., $m=n$) and if $\langle K|u|L\rangle\neq 0$, then u must have as many creation operators as annihilation operators. This result is physically clear and will be useful in the sequel.

VI. APPLICATIONS

In this section, we give some applications of the present approach to the calculation of matrix elements and generating functions. We consider matrix elements between two states $|K\rangle=b_{i_N}^\dagger,\cdots b_{i_1}^\dagger|0\rangle$ and $|L\rangle=b_{j_N}^\dagger\cdots,b_{j_1}^\dagger|0\rangle$, where N is the number of electrons in the system. We assume that the indices are ordered as $i_1<\cdots<i_N$ and $j_1<\cdots<j_N$.

A. Matrix elements

We want to calculate the general matrix element

$$A_{KL} = \langle K|b_{n_1}^\dagger\cdots b_{n_k}^\dagger b_{m_1}\cdots b_{m_k}|L\rangle.$$

Set $u=b_{i_1},\cdots,b_{i_N}$, $v=b^\dagger_{j_N},\cdots,b^\dagger_{j_1}$, $s=b^\dagger_{n_1},\cdots,b^\dagger_{n_k}$, and $t=b_{m_1},\cdots,b_{m_k}$. Now A_{KL} becomes $\langle 0|u(:st:)v|0\rangle$, and we can use Wick's theorem (11) to write

$$
\begin{aligned}
:st:v &= \sum (-1)^{|v_{(1)}|(|s_{(2)}|+|t_{(2)}|)}(:st:_{(1)}|v_{(1)}):(:st:_{(2)}v_{(2)}):\\
&= \sum (-1)^{|v_{(1)}||s_{(2)}|+|v_{(1)}||t_{(2)}|+|t_{(1)}||s_{(2)}|}\\
&\quad\times(:s_{(1)}t_{(1)}:|v_{(1)}):s_{(2)}t_{(2)}v_{(2)}:.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
A_{KL} &= (u|(:st:)v),\\
&= \sum (-1)^{|v_{(1)}||s_{(2)}|+|v_{(1)}||t_{(2)}|+|t_{(1)}||s_{(2)}|}(:s_{(1)}t_{(1)}:|v_{(1)})\\
&\quad\times(u|:s_{(2)}t_{(2)}v_{(2)}:).
\end{aligned}
$$

From identity (7), we know that $s_{(1)}$ cannot contain creation operators and $t_{(2)}$ cannot contain annihilation operators. Therefore, $s_{(1)}=t_{(2)}=1$, so that $s_{(2)}=s$ and $t_{(1)}=t$ and the expression becomes

$$
\begin{aligned}
A_{KL} &= \sum (-1)^{|v_{(1)}||s|+|t||s|}(t|v_{(1)})(u|:sv_{(2)}:),\\
&= \sum (-1)^{|v_{(1)}||s|+|t||s|+|u_{(2)}||s|}\\
&\quad\times(t|v_{(1)})(u_{(1)}|s)(u_{(2)}|v_{(2)}),
\end{aligned}
\tag{16}
$$

where we used the Laplace identity (10) to expand $(u|:sv_{(2)}:)$. We rewrite $v=(-1)^{N(N-1)/2}b^\dagger_{j_1}\ldots b^\dagger_{j_N}$ so

$$
\Delta u = \sum_{p=0}^{N}\sum_{\sigma}(-1)^{\sigma}b_{i_{\sigma(1)}}\cdots b_{i_{\sigma(p)}}\otimes b_{i_{\sigma(p+1)}}\cdots b_{i_{\sigma(N)}},
$$

$$
\Delta v = (-1)^{N(N-1)/2}\sum_{q=0}^{N}\sum_{\tau}(-1)^{\tau}b^\dagger_{j_{\tau(1)}}\cdots b^\dagger_{j_{\tau(q)}}\otimes b^\dagger_{j_{\tau(q+1)}}\cdots b^\dagger_{j_{\tau(N)}},
$$

where σ runs over the $(p,N-p)$ shuffles and τ over the $(q,N-q)$ shuffles. Equation (7) applied to (16) gives us $p=k$ and $q=k$ so that $|v_{(1)}|=|s|=|t|=k$, $|u_{(2)}|=N-k$ and

$$
\begin{aligned}
A_{KL} &= (-1)^{N(N-1)/2+(N-k)k+k(k-1)+(N-k)(N-k-1)/2}\\
&\quad\times\sum_{\sigma\tau}(-1)^{\sigma+\tau}\det(\delta_{m_p,j_{\tau(q)}})\det(\delta_{i_{\sigma(p)},n_q})\det(\delta_{i_{\sigma(p)},j_{\tau(q)}}),
\end{aligned}
\tag{17}
$$

where p and q run from 1 to k in the first two matrices and from $k+1$ to N in the last one.

The next transformation is first illustrated with the case $k=N-2$. The last factor of Eq. (17) becomes $\det(\delta_{i_{\sigma(p)},j_{\tau(q)}})=\delta_{i_{\sigma(N-1)},j_{\tau(N-1)}}\delta_{i_{\sigma(N)},j_{\tau(N)}}-\delta_{i_{\sigma(N)},j_{\tau(N-1)}}\delta_{i_{\sigma(N-1)},j_{\tau(N)}}$. The permutation τ is a $(N-2,2)$ shuffle, so that $j_{\tau(N-1)}<j_{\tau(N)}$. The δ functions of the second term give us $i_{\sigma(N)}=j_{\tau(N-1)}<j_{\tau(N)}=i_{\sigma(N-1)}$. Thus $i_{\sigma(N)}<i_{\sigma(N-1)}$, but this is impossible because σ is also a $(N-2,2)$ shuffle so that $i_{\sigma(N)}>i_{\sigma(N-1)}$. Therefore, the second term is zero and $\det(\delta_{i_{\sigma(p)},j_{\tau(q)}})=\delta_{i_{\sigma(N-1)},j_{\tau(N-1)}}\delta_{i_{\sigma(N)},j_{\tau(N)}}$.

A similar result can be proved for any value of k: The determinant of a $n\times n$ matrix a_{ij} is $\det(a)=\Sigma_\lambda(-1)^\lambda\Pi_{i=1}^n a_{i\lambda(i)}=\Sigma_\lambda(-1)^\lambda\Pi_{i=1}^n a_{\lambda(i)i}$, where λ runs over the permutations of n elements. Therefore, to calculate the last determinant in Eq. (17), we must sum over all permutations of $\tau(k+1),\ldots,\tau(N)$. By definition of the $(k,N-k)$ shuffles, we have $i_{\sigma(k+1)}<\cdots<i_{\sigma(N)}$ and $j_{\tau(k+1)}<\cdots<j_{\tau(N)}$; thus any permutation of $\tau(k+1),\ldots,\tau(N)$ would break this ordering and the only nonzero term of $\det(\delta_{i_{\sigma(p)},j_{\tau(q)}})$ is $\delta_{i_{\sigma(k+1)},j_{\tau(k+1)}}\cdots\delta_{i_{\sigma(N)},j_{\tau(N)}}$. This gives us the following expression for A_{KL}:

$$
\begin{aligned}
A_{KL} &= (-1)^{k(k-1)/2}\sum_{\sigma\tau}(-1)^{\sigma+\tau}\det(\delta_{m_p,j_{\tau(q)}})\\
&\quad\times\det(\delta_{i_{\sigma(p)},n_q})\prod_{p=k+1}^{N}\delta_{i_{\sigma(p)},j_{\tau(p)}},
\end{aligned}
\tag{18}
$$

where σ and τ run over the $(k,N-k)$ shuffles. Equation (18) is equivalent to the result obtained by Caianiello [10].

B. Generating function

In the nonequilibrium many-body theory of systems with initial correlations [11–13], the generating function Z of the Green's functions is written as

$$
Z = \exp(-iH^{\mathrm{int}})\exp(-i\bar{\eta}G^0\eta)Z_0,
\tag{19}
$$

where H^{int} is the interacting Hamiltonian (where fields are replaced by functional derivatives with respect to the anticommuting external sources $\bar{\eta},\eta$), G^0 is the free Green's function and Z_0 is the generating function of the correlations of the initial state of the system, before the interaction is switched on. If the initial state is described by the density matrix $\hat{\rho}=\Sigma_{KL}\rho_{LK}|L\rangle\langle K|$, where $|K\rangle$ and $|L\rangle$ are N-particle Slater determinants, then $Z_0=\Sigma_{KL}\rho_{LK}N^0_{KL}$, with

$$
N^0_{KL} = \langle K|:\exp\left(i\int\bar{\eta}(x)\psi(x)+\psi^\dagger(x)\eta(x)\mathrm{d}x\right):|L\rangle.
\tag{20}
$$

In Eq. (20), N^0_{KL} is the generating function of the matrix elements of the k-body operators and $\psi(x)$ is a field operator, which can be expanded over the eigenstates $\varphi_n(x)$ of the free Hamiltonian

$$
\psi(x)=\sum_n b_n\varphi_n(x),\quad \psi^\dagger(x)=\sum_n b^\dagger_n\varphi^*(x)
$$

and where $\bar{\eta}(x)$ and $\eta(x)$ are anticommuting sources. In the following, N^0_{KL} will be calculated for the first time.

The importance of N^0_{KL} comes from the fact that all matrix elements can be obtained by functional derivatives with respect to the sources. For instance, the matrix elements of the density are given by

$$
\langle K|:\psi^\dagger(x)\psi(x):|L\rangle = \left.\frac{\delta^2N^0_{KL}}{\delta\eta(x)\delta\bar{\eta}(x)}\right|_{\eta=\bar{\eta}=0}.
$$

We can rewrite N^0_{KL} as

$$N_{KL}^0 = \sum_{l=0}^{\infty} \frac{i^l}{l!}\langle K|:\left(\sum_n \int \bar{\eta}(x)\varphi_n(x)\mathrm{d}x b_n + b_n^\dagger \int \bar{u}(x)\eta(x)\mathrm{d}x\right)^l :|L\rangle$$

$$= \sum_{l=0}^{\infty} \frac{i^l}{l!}\langle K|:\left(\sum_n \bar{\alpha}_n b_n + b_n^\dagger \alpha_n\right)^l :|L\rangle,$$

where $\bar{\alpha}_n = \int \bar{\eta}(x)\varphi_n(x)dx$ and $\alpha_n = \int \varphi_n^*(x)\eta(x)dx$ are anticommuting variables. To calculate N_{KL}^0, we first note that the anticommutativity of b_n, $b_n^\dagger$, α_n, and $\bar{\alpha}_n$ for the normal product gives us the commutation rules $:\bar{\alpha}_i b_i \bar{\alpha}_j b_j: = :\bar{\alpha}_j b_j \bar{\alpha}_i b_i:$, $:\bar{\alpha}_i b_i b_j^\dagger \alpha_j: = :b_j^\dagger \alpha_j \bar{\alpha}_i b_i:$, and $:b_i^\dagger \alpha_i b_j^\dagger \alpha_j: = :b_j^\dagger \alpha_j b_i^\dagger \alpha_i:$. Thus, we can expand the power with the binomial formula

$$N_{KL}^0 = \sum_{l=0}^{\infty} \frac{i^l}{l!} \sum_{k=0}^{l} \binom{l}{k} \times \sum_{n_1 \cdots n_l} \langle K|b_{n_1}^\dagger \alpha_{n_1} \cdots b_{n_k}^\dagger \alpha_{n_k} \bar{\alpha}_{n_{k+1}} b_{n_{k+1}} \cdots \bar{\alpha}_{n_l} b_{n_l}|L\rangle$$

$$= \sum_{l=0}^{\infty} \frac{i^l}{l!} \sum_{k=0}^{l} \binom{l}{k} (-1)^{k+l(l-1)/2} \sum_{n_1 \cdots n_l} \alpha_{n_1} \cdots \alpha_{n_k} \bar{\alpha}_{n_{k+1}} \cdots \bar{\alpha}_{n_l} \langle K|b_{n_1}^\dagger \cdots b_{n_k}^\dagger b_{n_{k+1}} \cdots b_{n_l}|L\rangle.$$

As we saw in Sec. V B, the transition between $|K\rangle$ and $|L\rangle$ is zero if $l \neq 2k$ or $l > 2N$ because $|K\rangle$ and $|L\rangle$ contain N electrons. Thus, we obtain the finite sum

$$N_{KL}^0 = \sum_{k=0}^{N} \frac{(-1)^k}{(k!)^2} \sum_{n_1,\cdots,m_k} \alpha_{n_1} \cdots \alpha_{n_k} \bar{\alpha}_{m_1} \cdots \bar{\alpha}_{m_k} \times \langle K|b_{n_1}^\dagger \cdots b_{n_k}^\dagger b_{m_1} \cdots b_{m_k}|L\rangle. \quad (21)$$

In the last term, we recognize the matrix element that we calculated in Sec. VI A Therefore, we introduce Eq. (18) into Eq. (21).

$$N_{KL}^0 = \sum_{k=0}^{N} \frac{(-1)^{k(k+1)/2}}{(k!)^2} \sum_{n_1 \cdots m_k} \alpha_{n_1} \cdots \alpha_{n_k} \bar{\alpha}_{m_1} \cdots \bar{\alpha}_{m_k} \times \sum_{\sigma\tau} (-1)^{\sigma+\tau} \det(\delta_{m_p, j_{\tau(q)}}) \det(\delta_{i_{\sigma(p)}, n_q}) \times \prod_{p=k+1}^{N} \delta_{i_{\sigma(p)}, j_{\tau(p)}}. \quad (22)$$

To calculate $\det(\delta_{m_p, j_{\tau(q)}})$, we write

$$\det(\delta_{m_p, j_{\tau(q)}}) = \sum_{\lambda} (-1)^{\lambda} \delta_{m_{\lambda(1)}, j_{\tau(1)}} \cdots \delta_{m_{\lambda(k)}, j_{\tau(k)}},$$

where λ runs over the permutations of $\{1, \ldots, k\}$ and we obtain

$$\sum_{m_1, \ldots, m_k} \bar{\alpha}_{m_1} \cdots \bar{\alpha}_{m_k} \det(\delta_{m_p, j_{\tau(q)}}) = k! \bar{\alpha}_{j_{\tau(1)}} \cdots \bar{\alpha}_{j_{\tau(k)}}$$

because the anticommutation of the variables α_i and $\bar{\alpha}_j$ implies that all permutations λ give the same contribution. Hence,

$$N_{KL}^0 = \sum_{k=0}^{N} (-1)^{k(k+1)/2} \sum_{\sigma\tau} (-1)^{\sigma+\tau} \alpha_{i_{\sigma(1)}} \cdots \alpha_{i_{\sigma(k)}} \bar{\alpha}_{j_{\tau(1)}} \cdots \bar{\alpha}_{j_{\tau(k)}} \times \prod_{p=k+1}^{N} \delta_{i_{\sigma(p)}, j_{\tau(p)}}.$$

Therefore, our final result is

$$N_{KL}^0 = \sum_{k=0}^{N} (-1)^{k(k-1)/2} \sum_{\sigma\tau} (-1)^{\sigma+\tau} \times \prod_{p=1}^{k} \bar{\alpha}_{j_{\tau(p)}} \prod_{p=1}^{k} \alpha_{i_{\sigma(p)}} \prod_{p=k+1}^{N} \delta_{i_{\sigma(p)}, j_{\tau(p)}},$$

$$= \sum_{k=0}^{N} \sum_{\sigma\tau} (-1)^{\sigma+\tau} \prod_{p=1}^{k} (\bar{\alpha}_{j_{\tau(p)}} \alpha_{i_{\sigma(p)}}) \prod_{p=k+1}^{N} \delta_{i_{\sigma(p)}, j_{\tau(p)}}, \quad (23)$$

where we recall that σ and τ run over the $(k, N-k)$ shuffles. We see that the generating function is rather simple. In the Appendix, we show that a still simpler formula can be obtained for N_{KL}^0.

$$N_{KL}^0 = \exp\left(\sum_n \frac{\partial^2}{\partial \alpha_n \partial \bar{\alpha}_n}\right)(\bar{\alpha}_{i_1}\alpha_{j_1}, \ldots, \bar{\alpha}_{i_N}\alpha_{j_N}). \quad (24)$$

C. Diagonal matrix elements

It is interesting to consider the case where $|K\rangle = |L\rangle$. This implies that $i_p = j_p$ for all $p = 1, \ldots, N$. We consider first the diagonal elements of A_{KL}. According to Eq. (18), they are given by

$$A_{KK} = (-1)^{k(k-1)/2} \sum_{\sigma\tau} (-1)^{\sigma+\tau} \times \det(\delta_{m_p, i_{\tau(q)}}) \det(\delta_{i_{\sigma(p)}, n_q}) \prod_{p=k+1}^{N} \delta_{i_{\sigma(p)}, i_{\tau(p)}},$$

The last product implies that $\sigma(p) = \tau(p)$ for $p = k+1, \ldots, N$. The $(k, N-k)$ shuffles are entirely determined by their last $N-k$ values; thus, $\sigma = \tau$ and we get

$$A_{KK} = (-1)^{k(k-1)/2} \sum_{\sigma} \det(\delta_{m_p, i_{\sigma(q)}}) \det(\delta_{i_{\sigma(p)}, n_q}),$$

where p and q run from 1 to k and σ runs over the $(k, N-k)$ shuffles. To simplify this expression, we consider the case where an m_p does not belong to the set $\{i_1, \ldots, i_N\}$, then $\delta_{m_p, i_{\sigma(q)}}$ is zero for all q and $\det(\delta_{m_p, i_{\sigma(q)}}) = 0$. Therefore, A_{KK} is zero unless the set $\{m_1, \ldots, m_k\}$ is included in $\{i_1, \ldots, i_N\}$.

If this condition is satisfied, there is a unique $(k,N-k)$ shuffle such that $\det(\delta_{m_p,i_{\sigma(q)}})$ is not zero. To see this, consider the permutation λ of $\{1,\ldots,k\}$ that orders $\{m_1,\ldots,m_k\}$ (i.e., $m_{\lambda(1)}<\cdots<m_{\lambda(k)}$). We also have $i_{\sigma(1)}<\cdots<i_{\sigma(k)}$ so the determinant is nonzero if and only if $m_{\lambda(q)}=i_{\sigma(q)}$ for $q=1,\ldots,k$. This fully determines the shuffle σ. For a general ordering of $\{m_1,\ldots,m_k\}$ we have $\delta_{m_p,i_{\sigma(q)}}$ nonzero if and only if $p=\lambda(q)$. To conclude, we use the fact that the product of the determinant of two matrices is the determinant of the matrix product [i.e., $\det(\delta_{m_p,i_{\sigma(q)}})\det(\delta_{i_{\sigma(p)},n_q})=\det(\delta_{m_p,n_q})$]:

$$A_{KK}=(-1)^{k(k-1)/2}\det(\delta_{m_p,n_q}) \quad \text{if } \{m_1,\ldots,m_k\}\subset\{i_1,\ldots,i_N\},$$

$$=0 \quad \text{otherwise}. \tag{25}$$

We now consider the diagonal matrix elements of the generating function N^0_{KL}. The Kronecker δ functions in Eq. (23) yields $\sigma=\tau$ and

$$N^0_{KK}=\sum_{k=0}^{N}\sum_{\sigma}\prod_{p=1}^{k}(\bar{\alpha}_{i_{\sigma(p)}}\alpha_{i_{\sigma(p)}})$$
$$=\sum_{k=0}^{N}\sum_{j_1<\cdots<j_k}(\bar{\alpha}_{j_1}\alpha_{j_1})\cdots(\bar{\alpha}_{j_k}\alpha_{j_k}),$$

where $j_1,\ldots,j_k$ are k numbers taken in $i_1,\ldots,i_N$. We recognize here [14] the definition of the elementary symmetric polynomials e_k, so that

$$N^0_{KK}=\sum_{k=0}^{N}e_k(\bar{\alpha}_{i_1}\alpha_{i_1},\ldots,\bar{\alpha}_{i_N}\alpha_{i_N}).$$

The generating function for elementary symmetric polynomials is well known [14]. It yields

$$N^0_{KK}=\prod_{p=1}^{N}(1+\bar{\alpha}_{i_p}\alpha_{i_p}).$$

Another expression can be obtained if we note that

$$\ln\left(\prod_{p=1}^{N}(1+\bar{\alpha}_{i_p}\alpha_{i_p})\right)=\sum_{p=1}^{N}\ln(1+\bar{\alpha}_{i_p}\alpha_{i_p})$$
$$=\sum_{i=1}^{N}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}(\bar{\alpha}_{i_p}\alpha_{i_p})^n.$$

The variables $\bar{\alpha}_{i_p}$ and α_{i_p} are fermionic, thus $\bar{\alpha}^2_{i_p}=\alpha^2_{i_p}=0$ and $(\bar{\alpha}_{i_p}\alpha_{i_p})^2=\bar{\alpha}_{i_p}\alpha_{i_p}\bar{\alpha}_{i_p}\alpha_{i_p}=-\bar{\alpha}_{i_p}\bar{\alpha}_{i_p}\alpha_{i_p}\alpha_{i_p}=0$. Consequently, only the term $n=1$ remains in the sum and

$$\ln\left(\prod_{i=1}^{N}(1+\bar{\alpha}_{i_p}\alpha_{i_p})\right)=\sum_{i=1}^{N}\bar{\alpha}_{i_p}\alpha_{i_p}.$$

In other words,

$$N^0_{KK}=\exp\left(\sum_{p=1}^{N}\bar{\alpha}_{i_p}\alpha_{i_p}\right). \tag{26}$$

The diagonal generating function N^0_{KK} arises when the initial state of the system (without interaction) can be described by a single Slater determinant. This is the situation met in standard many-body theory [15,16]. Equation (26) shows that, in this case, Z_0 is the exponential of a term linear in the external sources $\bar{\eta}$ and η. Thus, the free Green's function G^0 is modified by adding $\Sigma_{p=1}^{N}\bar{\alpha}_{i_p}\alpha_{i_p}$, i.e., by filling all the orbitals up to the Fermi energy. This is exactly the standard way to calculate the free Green's function in many-body theory. In other words, the reasoning leading to Eq. (26) can be considered as a complete proof of the standard electron-hole transormation [15].

When the initial state is not described by a single Slater determinant (i.e., for many-body theory with initial correlations), the orbitals are not either full or empty and partial occupation is allowed. The probability of hoppping between two partially occupied orbitals is also required. All this information is contained in $Z_0=\Sigma_{KL}\rho_{LK}N^0_{KL}$, where the general expression (24) must be used for N^0_{KL}. The logarithm of Z_0 is no longer linear in the external sources [11,17–19]. This is the main source of the complexity of the many-body theory with initial correlations [11,20,21].

VII. DENSITY CORRELATION FUNCTIONS

The density operator is given by $n(x)=\psi^\dagger(x)\psi(x)$, where $\psi(x)$ is a field operator. The k-density correlation operator is

$$n^k(x_1,\ldots,x_k)=:n(x_1)\cdots n(x_k):$$
$$=:\psi^\dagger(x_1)\cdots\psi^\dagger(x_k)\psi(x_k)\cdots\psi(x_1):. \tag{27}$$

A general N-particle state of the system can be described by the density matrix $\hat{\rho}=\Sigma_{KL}\rho_{LK}|L\rangle\langle K|$, where $|K\rangle$, $|L\rangle$ are N-particle Slater determinants and where ρ_{LK} is a positive Hermitian matrix with unit trace. Thus, the k-density correlation in state $\hat{\rho}$ can be calculated once we know the matrix elements $\langle K|n^k(x_1,\ldots,x_k)|L\rangle$. We are going to find the eigenvalues of this matrix. In this calculation, the power and elegance of the split-and-pair method will be clear.

A. General case

We can rewrite the operators $n^k(x_1,\ldots,x_k)$ defined in Eq. (27) as $n^k(x_1,\ldots,x_k)=u^\dagger u$, where $u=\psi(x_k)\cdots\psi(x_1)$.

We start with a proof of the important identity

$$(u^\dagger u)^2=u^\dagger uu^\dagger u=(u|u^\dagger)u^\dagger u. \tag{28}$$

We first use Wick's theorem (11) to get

$$uu^\dagger=\sum(-1)^{|u_{(2)}||u^\dagger_{(1)}|}(u_{(1)}|u^\dagger_{(1)}|:u_{(2)}u^\dagger_{(2)}:.$$

We interchange $u_{(2)}$ and $u^\dagger_{(2)}$ in the normal product, using Eq. (1) and also use $|u^\dagger_{(1)}|+|u^\dagger_{(2)}|=|u^\dagger|=|u|$ to rewrite

$$uu^\dagger=\sum(-1)^{|u||u_{(2)}|}(u_{(1)}|u^\dagger_{(1)})u^\dagger_{(2)}u_{(2)}. \tag{29}$$

The normal order symbols of $:u^\dagger_{(2)}u_{(2)}:$ were removed because $u^\dagger_{(2)}$ contains only creation operators and $u_{(2)}$ annihila-

tion operators, so that $:u^\dagger_{(2)}u_{(2)}: = u^\dagger_{(2)}u_{(2)}$. We multiply both members of Eq. (29) by $u^\dagger$ on the left and u on the right and obtain

$$(u^\dagger u)^2 = \sum (-1)^{|u||u_{(2)}|}(u_{(1)}|u^\dagger_{(1)})u^\dagger u^\dagger_{(2)}u_{(2)}u.$$

Now we use the fact that $u_{(2)}u=0$ except when $u_{(2)}=1$. To see this, we consider the coproduct of u given by Eq. (5)

$$\Delta u = u\otimes 1 + 1\otimes u + \sum_{p=1}^{k-1}\sum_{\sigma}(-1)^\sigma \psi(x_{\sigma(k)})\cdots\psi(x_{\sigma(p+1)}) \otimes \psi(x_{\sigma(p)})\cdots\psi(x_{\sigma(1)}).$$

If $u_{(2)}$ contains an operator $\psi(x_i)$, then $u_{(2)}u=0$ because $\psi(x_i)$ is also contained in u and $\psi(x_i)^2=0$. The only term of Δu where $u_{(2)}$ does not contain any operator $\psi(x_i)$ is the term $u\otimes 1$. Similarly, the only term of $u^\dagger u^\dagger_{(2)}$ that is not zero is the term $u^\dagger_{(2)}=1$, so that $u^\dagger_{(1)}=u$. Therefore, the sum has only one term and we obtain $u^\dagger u u^\dagger u=(u|u^\dagger)u^\dagger u$, which is the desired result.

From Eq. (28) we deduce that $P=u^\dagger u/(u|u^\dagger)$ satisfies $P^2=P$. Moreover, $P^\dagger=P$ because $(u|u^\dagger)=\langle 0|uu^\dagger|0\rangle$ is real. Therefore, P is a projection operator and the density operator $n(x_1,\ldots,x_k)=(u|u^\dagger)P$ is proportional to a projection operator. As a projection operator, P has the only eigenvalues 0 and 1. The number of eigenvalues 1, which is also the rank of P, is given by tr$P$ that we calculate now.

To obtain a finite result, we consider the *projected* density of states, which is often used in physics and chemistry. So we select a number M of orbitals $\varphi_1(x),\ldots,\varphi_M(x)$ and define projected fields

$$\psi_p(x) = \sum_{i=1}^{M}\varphi_i(x)b_i.$$

For instance, we can be interested in the density of d electrons in a system, then $M=10$ and $\varphi_1(x),\ldots,\varphi_M(x)$ are the spin-orbitals of the d shell. We also assume that the Slater determinants $|K\rangle$ and $|L\rangle$ contain only these orbitals (plus possible closed shells that are common to all $|K\rangle$ and $|L\rangle$, so that the correlation functions concern only the valence electrons). If the system contains N electrons chosen among the M orbitals, there are $\binom{M}{N}$ possible states $|K\rangle$.

If we sum over a complete set of states $|J\rangle$ and use Eq. (28), we obtain

$$\begin{aligned}\langle K|(u^\dagger u)^2|L\rangle &= \sum_J \langle K|u^\dagger u|J\rangle\langle J|u^\dagger u|L\rangle \\ &= \sum_J \langle K|n^k_p(x_1,\ldots,x_k)|J\rangle\langle J|n^k_p(x_1,\ldots,x_k)|L\rangle \\ &= (u|u^\dagger)\langle K|u^\dagger u|L\rangle = \lambda^k_p(x_1,\ldots,x_k) \\ &\quad\times\langle K|n^k_p(x_1,\ldots,x_k)|L\rangle,\end{aligned}$$

where

$$\lambda^k_p(x_1,\ldots,x_k) = (\psi_p(x_k)\cdots\psi_p(x_1)|\psi^\dagger_p(x_1)\cdots\psi^\dagger_p(x_k)).$$

From $\psi_p(x_k)\cdots\psi_p(x_1)=(-1)^{k(k-1)/2}\psi_p(x_1)\cdots\psi_p(x_k)$, Eq. (7) gives us

$$\lambda^k_p(x_1,\ldots,x_k) = \det(\psi_p(x_i)|\psi^\dagger_p(x_j)),$$

with

$$(\psi_p(x_i)|\psi^\dagger_p(x_j)) = \langle 0|\psi_p(x_i)\psi^\dagger_p(x_j)|0\rangle = \sum_{n=1}^{M}\varphi_n(x_i)\varphi^*_n(x_j).$$

The sum over the intermediate states $|J\rangle$ can be much reduced because the projected density correlation operators use only the orbitals from 1 to M. The reasoning leading equation (15) shows that matrix elements with $|J\rangle$ can be nonzero only if $|J\rangle$ is a N-body Slater determinant formed from the orbitals $\varphi_1,\ldots,\varphi_M$. In other words, the sum over J can be restricted to the finite sum over the $\binom{M}{N}$ states obtained by choosing N electrons among the M orbitals.

We showed that $n^k_p(x_1,\ldots,x_k)$ is proportional to a projection operator. To know the number of nonzero eigenvalues of $n^k_p(x_1,\ldots,x_k)$, we just have to calculate its trace. We expand the field operators

$$\begin{aligned}\mathrm{tr}[n^k_p(x_1,\ldots,x_k)] &= \sum_K \langle K|n^k_p(x_1,\ldots,x_k)|K\rangle \\ &= \sum_{m_1,\ldots,n_k}\varphi_{m_1}(x_k)\cdots\varphi_{m_k}(x_1) \\ &\quad\times\varphi^*_{n_1}(x_1)\ldots\varphi^*_{n_k}(x_k)\sum_K A_{KK}.\end{aligned}$$

According to Eq. (25), A_{KK} is nonzero if and only if $\{m_1,\ldots,m_k\}\subset\{i_1,\ldots,i_N\}$. This means that k elements of $\{i_1,\ldots,i_N\}$ are fixed, and it remains to choose $N-k$ elements among $M-k$ orbitals. In other words,

$$\begin{aligned}\sum_K A_{KK} &= (-1)^{k(k-1)/2}\binom{M-k}{N-k}\det(\delta_{m_p,n_q}) \\ &= \binom{M-k}{N-k}(b_{m_1}\cdots b_{m_k}|b^\dagger_{n_1}\cdots b^\dagger_{n_k}).\end{aligned}$$

Therefore,

$$\mathrm{tr}[n^k_p(x_1,\ldots,x_k)] = \binom{M-k}{N-k}\lambda^k_p(x_1,\ldots,x_k),$$

and the rank of the projected density correlation operator is $\binom{M-k}{N-k}$.

We can summarize our results as follows: the kth projected density correlation operator is a matrix of dimension $\binom{M}{N}$ with two eigenvalues $\lambda^k_p(x_1,\ldots,x_k)$ and 0, with multiplicity $\binom{M-k}{N-k}$ and $\binom{M}{N}-\binom{M-k}{N-k}$, respectively. As a consequence, there exists a unitary matrix $U_{K\alpha}(x_1,\ldots,x_k)$ such that

$$\langle K|n^k_p(x_1,\ldots,x_k)|L\rangle = \lambda^k_p(x_1,\ldots,x_k)\sum_{\alpha=1}^{\binom{M-k}{N-k}}U_{K\alpha}(x_1,\ldots,x_k) \times U^*_{L\alpha}(x_1,\ldots,x_k). \quad (30)$$

B. Electron density

The simplest example is the case $k=1$, for which

$$\lambda_p^1(x) = \sum_{i=1}^{M} |\varphi_i(x)|^2.$$

The nonzero eigenvalue of $n_p(x)$ is therefore the charge density of the closed valence shell. The reason that we have to consider a projected density is now clear; if we take all possible orbitals (i.e., $M=\infty$), we obtain $\lambda_p^1(x)=\delta(0)$, which is infinite.

We can illustrate this result with the case $N=2$ and $M=3$. There are three Slater determinants for the two-particle states: $|1\rangle=\{\varphi_1,\varphi_2\}$, $|2\rangle=\{\varphi_1,\varphi_3\}$, and $|3\rangle=\{\varphi_2,\varphi_3\}$, where $\{\varphi_i,\varphi_j\}$ is the Slater determinant

$$\{\varphi_i,\varphi_j\}(x,y) = \frac{1}{\sqrt{2}}[\varphi_i(x)\varphi_j(y) - \varphi_j(x)\varphi_i(y)].$$

From the result (18) for A_{KL}, we can calculate the projected density matrix $\langle K|n(x)|L\rangle$

$$n = \begin{pmatrix} |\varphi_1|^2 + |\varphi_2|^2 & \varphi_2^*\varphi_3 & -\varphi_1^*\varphi_3 \\ \varphi_3^*\varphi_2 & |\varphi_1|^2 + |\varphi_3|^2 & \varphi_1^*\varphi_2 \\ -\varphi_3^*\varphi_1 & \varphi_2^*\varphi_1 & |\varphi_2|^2 + |\varphi_3|^2 \end{pmatrix},$$

where we omitted the argument x for notational convenience. It can be checked that $nn=\lambda n$, with $\lambda=|\varphi_1|^2+|\varphi_2|^2+|\varphi_3|^2$.

There is a one-parameter family of solutions for the unitary matrix $U_{K\alpha}$ that diagonalizes n. A simple particular solution is

$$U_{K1} = \frac{1}{\sqrt{\lambda(|\varphi_2|^2 + |\varphi_3|^2)}}(-\varphi_1^*\varphi_3, \varphi_1^*\varphi_2, |\varphi_2|^2 + |\varphi_3|^2),$$

$$U_{K2} = \frac{1}{\sqrt{|\varphi_2|^2 + |\varphi_3|^2}}(\varphi_2^*, \varphi_3^*, 0).$$

C. Density-density correlation

Let us consider now the density-density correlation $n_p^2(x,y)$. According to the general result, this is $\lambda_p^2(x,y)$ times a projection operator, where

$$\lambda_p^2(x,y) = \lambda_p^1(x)\lambda_p^1(y) - \left| \sum_{n=1}^{M} \varphi_n(x)\varphi_n^*(y) \right|^2.$$

Note that by Schwartz' inequality $\lambda_p^2(x,y) \geqslant 0$ and that $\lambda_p^2(x,y)=0$ if and only if $\varphi_n(x)=\alpha\varphi_n(y)$ for all n. This is a general result. The matrix $M_{ij}=(\psi_p(x_i)|\psi_p^\dagger(x_j))$ is positive definite because for any complex numbers α_i we have $\Sigma_{ij}\alpha_i^* M_{ij}\alpha_j=(v^*|v)=\langle 0|v^* v|0\rangle=|v|0\rangle|^2 \geqslant 0$, where $v=\Sigma_i\alpha_i\psi_p^\dagger(x_i)$. Therefore, its determinant is positive and $\lambda_p^k(x_1,\ldots,x_k) \geqslant 0$.

Note that the structure of the density correlation function given by Eq. (30) might be relevant to solve the ensemble N-representability problem for the second-order mixed-state density matrix [22].

VIII. CONCLUSION

The split-and-pair method was introduced to express Wick's theorem and simplify many-body calculations. It was used to calculate the matrix elements of many-body operators between two Slater determinants and to derive a compact expression for the generating function of many-body matrix elements. It provided an elegant determination of the eigenvalues of the density correlation functions.

The reader might wonder why the splitting of a normal product and the pairing of two normal products can lead to Wick's theorem and provide a powerful calculation tool. The key to this mystery is the fact that many-body theory has the structure of a quantum group. Quantum groups have been used for some time in molecular spectroscopy (see Ref. 23 for a review and Ref. 24 for recent developments). They also play a role in solid-state physics [25–28]. In particular, they are the basic symmetry of the quantum-Hall effect [29,30]. These quantum groups are q deformations of Lie algebras. Recently, it was observed that more general quantum groups provide a powerful tool for many-body calculations in molecular and solid-state physics, as well as in quantum-field theory [4,31,32]. In particular, it was shown that many-body theory has a natural quantum group structure [4]. The coproduct that we defined is indeed the coproduct of the Hopf algebra of normal products. The pairing $(1|u)$ is the counit of this algebra. The Laplace pairing is also called a coquasitriangular structure [33] because it is the dual of the quasitriangular structure of a quantum group. Wick's theorem becomes an instance of the Drinfled twist of the comodule algebra of normal products. The idea of using quantum group concepts to write Wick's theorem is due to Fauser [34]. The quantum group structure was used to derive a general expression for the time-ordered product of any number of Wick polynomials in quantum-field theory [4]. The hidden purpose of the present paper was to show that the quantum group approach to many-body calculations can be introduced at an elementary level without explicit reference to the considerable conceptual apparatus of Hopf algebra.

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APPENDIX: ALTERNATIVE FORMULA

In this appendix, we are going to derive the alternative formula for N_{KL}^0. But we first need to be able to calculate derivatives with respect to anticommuting variables.

1. Derivations of $\alpha_1\cdots\alpha_n$

We want to calculate

$$\frac{\partial^k}{\partial\beta_1\cdots\partial\beta_k}(\alpha_1\cdots\alpha_n), \tag{A1}$$

where α_i and β_j are anticommuting variables. We first state the Leibniz rule when u is the product of m α_i and v the product of any number of α_i

$$\frac{\partial uv}{\partial\beta}=\frac{\partial u}{\partial\beta}v+(-1)^m u\frac{\partial v}{\partial\beta}. \tag{A2}$$

Now we consider Eq. (A1) for $k=1$, and we use the Leibniz rule (A2)

$$\frac{\partial(\alpha_1\cdots\alpha_n)}{\partial\beta_1}=\sum_{p=1}^{n}(-1)^{p-1}\alpha_1\cdots\alpha_{p-1}\frac{\partial\alpha_p}{\partial\beta_1}\alpha_{p+1}\cdots\alpha_n,$$

$$=\sum_{p=1}^{n}(-1)^{p-1}\alpha_1\cdots\alpha_{p-1}\alpha_{p+1}\cdots\alpha_n\frac{\partial\alpha_p}{\partial\beta_1},$$

$$=(-1)^{n-1}\sum_{\sigma}(-1)^{\sigma}\alpha_{\sigma(1)}\cdots\alpha_{\sigma(n-1)}\frac{\partial\alpha_{\sigma(n)}}{\partial\beta_1},$$

where the permutations σ are such that $\sigma(1)<\cdots<\sigma(n-1)$. The second line is obtained from the first line by noting that $\partial\alpha_p/\partial\beta_1$ is a commuting variable. At the next order we have

$$\frac{\partial^2(\alpha_1\cdots\alpha_n)}{\partial\beta_1\partial\beta_2}=(-1)^{n-1}\sum_{\sigma}(-1)^{\sigma}\frac{\partial(\alpha_{\sigma(1)}\cdots\alpha_{\sigma(n-1)})}{\partial\beta_1}\frac{\partial\alpha_{\sigma(n)}}{\partial\beta_2},$$

$$=-\sum_{\sigma\tau}(-1)^{\sigma+\tau}(\alpha_{\tau\sigma(1)}\cdots\alpha_{\tau\sigma(n-2)})\frac{\partial\alpha_{\tau\sigma(n-1)}}{\partial\beta_1}\frac{\partial\alpha_{\sigma(n)}}{\partial\beta_2}.$$

Here τ is a permutation of $\{\sigma(1),\ldots,\sigma(n-2)\}$ such that $\tau(\sigma(1))<\cdots<\tau(\sigma(n-2))$. We extend τ to a permutation τ' of n numbers by $\tau'(\sigma(i))=\tau(\sigma(i))$ for i different from n and $\tau'(\sigma(n))=\sigma(n)$. The signature of τ' is the signature of τ. We call σ' the composition of τ' and σ

$$\frac{\partial^2(\alpha_1\cdots\alpha_n)}{\partial\beta_1\partial\beta_2}=-\sum_{\sigma'}(-1)^{\sigma'}\alpha_{\sigma'(1)}\cdots\alpha_{\sigma'(n-2)}\frac{\partial\alpha_{\sigma'(n-1)}}{\partial\beta_1}\frac{\partial\alpha_{\sigma'(n)}}{\partial\beta_2},$$

where σ' is a permutation of $\{1,\ldots,n\}$ such that $\sigma'(1)<\cdots<\sigma'(n-2)$. A recursive argument gives us

$$\frac{\partial^k(\alpha_1\cdots\alpha_n)}{\partial\beta_1\cdots\partial\beta_k}=(-1)^{kn-k(k+1)/2}\sum_{\sigma}(-1)^{\sigma}\times\alpha_{\sigma(1)}\cdots\alpha_{\sigma(n-k)}\frac{\partial\alpha_{\sigma(n-k+1)}}{\partial\beta_1}\cdots\frac{\partial\alpha_{\sigma(n)}}{\partial\beta_k},$$

where the permutations σ are such that $\sigma(1)<\cdots<\sigma(n-k)$. For further application, it is useful to decompose the permutations σ as the product of a $(n-k,k)$ shuffle σ' and a permutation τ of $\{\sigma'(n-k+1),\ldots,\sigma'(n)\}$. Since the factors $\partial\alpha_{\sigma(n-k+i)}/\partial\beta_i$ commute we can rewrite this as

$$\frac{\partial^k(\alpha_1\cdots\alpha_n)}{\partial\beta_1\cdots\partial\beta_k}=(-1)^{kn-k(k+1)/2}\sum_{\sigma,\tau}(-1)^{\sigma+\tau}(\alpha_{\sigma(1)}\cdots\alpha_{\sigma(n-k)})\frac{\partial\alpha_{\sigma(n-k+1)}}{\partial\beta_{\tau(1)}}\cdots\frac{\partial\alpha_{\sigma(n)}}{\partial\beta_{\tau(k)}}, \tag{A3}$$

where σ is a $(n-k,k)$ shuffle and τ is a permutation of $\{1,\ldots,k\}$.

2. Alternative formula for N^0_{KL}

With the above result, we can obtain an alternative expression

$$N^0_{KL}=\exp\left(\sum_n\frac{\partial^2}{\partial\alpha_n\partial\bar{\alpha}_n}\right)(\bar{\alpha}_{i_1}\alpha_{j_1}\cdots\bar{\alpha}_{i_N}\alpha_{j_N}). \tag{A4}$$

To get this result, we reorder the anticommuting variables and we expand the exponential in (A4)

$$N^0_{KL}=(-1)^{N(N-1)/2}\sum_{k=0}^{\infty}\frac{1}{k!}\prod_{i=1}^{k}\frac{\partial^2}{\partial\alpha_{n_i}\partial\bar{\alpha}_{n_i}}(\bar{\alpha}_{i_1}\cdots\bar{\alpha}_{i_N}\alpha_{j_1}\cdots\alpha_{j_N}),$$

$$=(-1)^{N(N-1)/2}\sum_{k=0}^{\infty}\frac{(-1)^{k(k+1)/2}}{k!}\sum_{n_1\ldots n_k}\frac{\partial^k}{\partial\bar{\alpha}_{n_1}\cdots\partial\bar{\alpha}_{n_k}}\frac{\partial^k}{\partial\alpha_{n_1}\cdots\partial\alpha_{n_k}}(\bar{\alpha}_{i_1}\cdots\bar{\alpha}_{i_N}\alpha_{j_1}\cdots\alpha_{j_N}).$$

Using now the Leibniz rule, we obtain

$$N^0_{KL}=(-1)^{N(N-1)/2}\sum_{k=0}^{\infty}\frac{(-1)^{k(k+1)/2+kN}}{k!}\sum_{n_1\ldots n_k}\frac{\partial^k}{\partial\bar{\alpha}_{n_1}\cdots\partial\bar{\alpha}_{n_k}}\times(\bar{\alpha}_{i_1}\cdots\bar{\alpha}_{i_N})\frac{\partial^k}{\partial\alpha_{n_1}\cdots\partial\alpha_{n_k}}(\alpha_{j_1}\cdots\alpha_{j_N}).$$

We use now equation (A3) to expand the derivations

$$N^0_{KL}=(-1)^{N(N-1)/2}\sum_{k=0}^{N}\frac{(-1)^{k(k+1)/2+kN}}{k!}\sum_{\sigma\sigma'}(-1)^{\sigma+\sigma'}\bar{\alpha}_{i_{\sigma(1)}}\cdots\bar{\alpha}_{i_{\sigma(N-k)}}\alpha_{j_{\sigma'(1)}}\cdots\alpha_{j_{\sigma'(N-k)}}\sum_{n_1\ldots n_k}\sum_{\tau\tau'}(-1)^{\tau+\tau'}\times\frac{\partial\bar{\alpha}_{i_{\sigma(N-k+1)}}}{\partial\bar{\alpha}_{n_{\tau(1)}}}\cdots\frac{\partial\bar{\alpha}_{i_{\sigma(N)}}}{\partial\bar{\alpha}_{n_{\tau(k)}}}\frac{\partial\alpha_{j_{\sigma'(N-k+1)}}}{\partial\alpha_{n_{\tau'(1)}}}\cdots\frac{\partial\alpha_{j_{\sigma'(N)}}}{\partial\alpha_{n_{\tau'(k)}}}.$$

The functional derivative of $\alpha_{j_{\sigma'(N-k+i)}}$ with respect to $\alpha_{n_{\tau'(i)}}$ is $\delta_{j_{\sigma'(N-k+i)},n_{\tau'(i)}}$. Thus, the last partial sum can be rewritten

$$X=\sum_{n_1\ldots n_k}\sum_{\tau\tau'}(-1)^{\tau+\tau'}\delta_{i_{\sigma(N-k+1)},n_{\tau(1)}}\cdots\delta_{i_{\sigma(N)},n_{\tau(k)}}\times\delta_{j_{\sigma'(N-k+1)},n_{\tau'(1)}}\cdots\delta_{j_{\sigma'(N)},n_{\tau'(k)}}.$$

For each τ, we define $m_i=n_{\tau(i)}$, so that $n_{\tau'(i)}=m_{\tau^{-1}\tau'(i)}$. If we call $\rho=\tau^{-1}\tau'$, we see that $(-1)^{\tau+\tau'}=(-1)^{\rho}$ and the variable τ disappears. Therefore, the sum becomes

$$X = k! \sum_{m_1 \cdots m_k} \sum_{\rho} (-1)^{\rho} \delta_{i_{\sigma(N-k+1)},m_1} \cdots \delta_{i_{\sigma(N)},m_k} \times \delta_{j_{\sigma'(N-k+1)},m_{\rho(1)}} \cdots \delta_{j_{\sigma'(N)},m_{\rho(k)}}.$$

Then we use the fact that $i_{\sigma(N-k+1)} < \cdots < i_{\sigma(N)}$ and $j_{\sigma'(N-k+1)} < \cdots < j_{\sigma'(N)}$ to deduce that the only permutation ρ which can give a nonzero result is the identity and

$$X = k! \delta_{i_{\sigma(N-k+1)},j_{\sigma'(N-k+1)}} \cdots \delta_{i_{\sigma(N)},j_{\sigma'(N)}}.$$

Finally, we reorder

$$\bar{\alpha}_{i_{\sigma(1)}} \cdots \bar{\alpha}_{i_{\sigma(N-k)}} \alpha_{j_{\sigma'(1)}} \cdots \alpha_{j_{\sigma'(N-k)}} = (-1)^{(N-k)(N-k-1)/2} \bar{\alpha}_{i_{\sigma(1)}} \alpha_{j_{\sigma'(1)}} \cdots \bar{\alpha}_{i_{\sigma(N-k)}} \alpha_{j_{\sigma'(N-k)}},$$

and we obtain

$$N_{KL}^0 = \sum_{k=0}^{N} \sum_{\sigma\sigma'} (-1)^{\sigma+\sigma'} \prod_{p=1}^{N-k} \bar{\alpha}_{i_{\sigma(p)}} \alpha_{j_{\sigma'(p)}} \times \delta_{i_{\sigma(N-k+1)},j_{\sigma'(N-k+1)}} \cdots \delta_{i_{\sigma(N)},j_{\sigma'(N)}},$$

which is indeed the expression for N_{KL}^0 found in Eq. (23), once we replace k by $N-k$.

It must be admitted that the present derivation does not share the elegance of the proofs using the split-and-pair method. In fact, the split-and-pair method can be applied to partial derivatives, and this yields a much shorter proof of our last result [35]. However, the present proof was chosen because it does not require the introduction of still more concepts of quantum group theory.

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