Practical formulation of the extended Wick's theorem and the Onishi formula

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The extended Wick's theorem for fermion operators, which is used to compute matrix elements of an arbitrary operator between two different quasiparticle vacuums, is reformulated to deal with quasiparticle vacuums expanded in a finite single particle basis not closed under the canonical transformation relating them. A new expression for the overlap of those quasiparticle vacuums is also given.

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I. INTRODUCTION

The extended Wick's theorem for fermion operators [1,2] and the Onishi formula [3] are widely used tools in many body theories and more specifically in theoretical nuclear physics. They are the essential tools in projected mean field calculations and in the generator coordinate method (GCM).

Given a canonical transformation $\mathcal{T}$ preserving the commutation relations of fermion annihilation and creation operators (both single particle and quasiparticle) the extended Wick's theorem allows the calculation of general matrix elements of the form

$$\frac{\langle\varphi|\hat{A}\mathcal{T}|\varphi\rangle}{\langle\varphi|\mathcal{T}|\varphi\rangle}, \tag{1}$$

where $\hat{A}$ is some product of annihilation and creation operators and $|\varphi\rangle$ is an arbitrary product wave function of the Hartree-Fock-Bogoliubov (HFB) type. The matrix element can be computed as the sum of all possible contractions among two quasiparticle operators. The two quasiparticle contractions and the overlap $\langle\varphi|\mathcal{T}|\varphi\rangle$ are evaluated in terms of the matrix T defined as

$$\mathcal{T}^{-1}\gamma_i\mathcal{T} = \sum_{j=1}^{2N} T_{ij}\gamma_j \tag{2}$$

where γ_i is a shorthand notation for the set $(\alpha_1,\ldots,\alpha_k,\ldots,\alpha_1^\dagger,\ldots,\alpha_k^\dagger,\ldots)$ of quasiparticle operators associated with $|\varphi\rangle$ (i.e., $\alpha_k|\varphi\rangle = 0$). Writing T in block form with respect to the creation and annihilation operators

$$T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}, \tag{3}$$

it can be shown [1,2] that the only nontrivial contraction is given by

$$\frac{\langle\varphi|\alpha_k\alpha_l\mathcal{T}|\varphi\rangle}{\langle\varphi|\mathcal{T}|\varphi\rangle} = \left(T_{12}T_{22}^{-1}\right)_{lk}. \tag{4}$$

For the overlap we get the Onishi formula

$$\langle\varphi|\mathcal{T}|\varphi\rangle = \sqrt{\det(T_{22})}. \tag{5}$$

It is worth emphasizing here that $\mathcal{T}$ is only required to preserve the canonical commutation relations. It can be a Bogoliubov transformation ($\mathcal{T}|\varphi\rangle = |\varphi\,'\rangle$), an element of a symmetry group (the parity operator, the rotation operator, the translation operator, etc.), or just a transformation of the single particle basis.

In the derivation of the extended Wick's theorem there is no explicit mention of the single particle basis in which quasiparticle operators are expanded. However, it is important to explicitly consider the single particle basis (which is supposed to be finite) when it is not closed under the transformation $\mathcal{T}$ (that is, $\mathcal{T}^{-1}c^\dagger\mathcal{T}$ contains elements not belonging to the original basis). In this case the restriction of $\mathcal{T}$ to our finite single particle basis no longer preserves the canonical commutation relations and the extended Wick's theorem apparently cannot be used. Examples of such situations are the following: (i) The transformation $\mathcal{T}$ represents a spatial translation. The overlap between the translated and the original basis $\int d\vec{r}\,\phi_n^*(\vec{r})\phi_m(\vec{r}-\vec{a})$ is different from zero for any value of n, m unless we consider a plane wave basis. (ii) The transformation $\mathcal{T}$ represents a spatial rotation and the single particle basis is a harmonic oscillator basis with different oscillator lengths along the three axes. (iii) The transformation $\mathcal{T}$ transforms the original harmonic oscillator basis with oscillator lengths b_x, b_y, and b_z to a new oscillator basis with lengths b_x', b_y', and b_z'.

There is a simple solution to this problem: the single particle basis has to be made large enough as to make the $\mathcal{T}$ transformation closed. However, it might happen that the single particle basis has to be extended as to cover the full Hilbert space rendering this procedure impractical—as is the case in the examples mentioned above. To solve this problem there are two alternatives: truncate the extension of the basis—being very careful in estimating the effects of the truncation [4]—or restrict oneself to a single particle basis in which the $\mathcal{T}$ transformation is closed (this is the preferred alternative in most of the projected calculations carried out up to now). However, using a basis adapted to the canonical transformation $\mathcal{T}$ could be a poor alternative depending on the problem at hand. For example, if one has to deal with a spatial translation it is not very practical to describe a nucleus using a plane wave basis.

In the following a method to overcome the aforesaid problems will be presented. The single particle basis is formally extended as needed but then the $\mathcal{T}$ transformation is factorized in a way that makes it possible to express the final results (contractions and overlaps) in terms of quantities defined in the original (not extended) single particle basis.

II. DECOMPOSITION OF THE TRANSFORMATION

The purpose of the extended Wick's theorem is to compute the general overlap

$$\frac{\langle\varphi|\hat{A}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle}, \tag{6}$$

where $\hat{A}$ is a general product of creation and annihilation quasiparticle operators, $\mathcal{T}$ is a canonical transformation preserving commutation relations, and $|\varphi\rangle$, $|\varphi'\rangle$ are HFB wave functions related by a Bogoliubov transformation $\mathcal{T}_B$ such that $|\varphi'\rangle = \mathcal{T}_B|\varphi\rangle$.

Both HFB wave functions are supposed to be expanded in terms of the same finite single particle basis (the extension to different single particle bases for $|\varphi\rangle$ and $|\varphi'\rangle$ will be treated in Appendix B). This basis $\{|j\rangle_1, j = 1,\ldots,N\}$ will be referred to as basis 1. On the other hand, those states of the Hilbert space basis not present in basis 1 will be denoted by $|j\rangle_2$ (basis 2). In general, the $\mathcal{T}$ transformation will mix states of basis 1 with those of basis 2. This mixing means that $\mathcal{T}$ will no longer be a canonical transformation in the subspace generated by basis 1. Therefore, we are forced to use the full Hilbert space basis in order to apply the extended Wick's theorem for the calculation of the overlap of Eq. (6).

The effect of $\mathcal{T}$ on the single particle creation and annihilation operators of the full basis (basis 1 and 2) can be expressed through a mixing matrix R defined as

$$\mathcal{T}^{-1}\begin{pmatrix} c \\ c^{\dagger} \end{pmatrix}\mathcal{T} = R\begin{pmatrix} c \\ c^{\dagger} \end{pmatrix}. \tag{7}$$

The constraint on $\mathcal{T}$ of preserving the canonical commutation relations implies that the mixing matrix R has to satisfy

$$R\sigma R^T = \sigma, \tag{8}$$

where σ is the matrix

$$\sigma = [\gamma_i,\gamma_j]_+ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{9}$$

In the following we will assume that the transformation $\mathcal{T}$ does not mix single particle creation and annihilation operators.[1] This restriction allows us to write the matrix R in block diagonal form

$$R = \begin{pmatrix} \overline{R} & 0 \\ 0 & (\overline{R}^T)^{-1} \end{pmatrix}, \tag{10}$$

where $\overline{R}$ is the transformation matrix for the annihilation operators and the special form of the transformation matrix for creation operators is a direct consequence of Eq. (8). From the above definition it is clear that $\overline{R}_{ij}$ are the single particle matrix elements of the transformation operator $\mathcal{T}$

$$\overline{R}_{ij} = \langle i|\mathcal{T}|j\rangle, \tag{11}$$

provided that $\mathcal{T}|-\rangle = |-\rangle$. With the two restrictions imposed on $\mathcal{T}$ we can write it as (see Appendix A)

$$\mathcal{T} = \exp\left(\sum_{ij} q_{ij}c_i^{\dagger}c_j\right). \tag{12}$$

However, it is more convenient to rewrite the above expression as the exponential of an antisymmetric quadratic form of annihilation and creation operators

$$\mathcal{T} = C_{\mathcal{T}}\exp\left(\frac{1}{2}\sum_{ij}\gamma_i(Q_A)_{ij}\gamma_j\right), \tag{13}$$

where the antisymmetric matrix Q_A is given by

$$Q_A = \begin{pmatrix} 0 & -q^T \\ q & 0 \end{pmatrix} \tag{14}$$

and the constant $C_{\mathcal{T}}$ by

$$C_{\mathcal{T}} = \exp\left(\frac{1}{2}\mathrm{Tr}(q)\right). \tag{15}$$

In terms of Q_A the transformation matrix R is given by

$$R = \exp(\sigma Q_A). \tag{16}$$

From here it is easy to obtain the corresponding relation for $\overline{R}$

$$\overline{R} = \exp(q), \tag{17}$$

which also allows us to rewrite the constant $C_{\mathcal{T}}$ as

$$C_{\mathcal{T}} = \exp\left(\frac{1}{2}\mathrm{Tr}[\ln(\overline{R})]\right) \equiv \sqrt{\det(\overline{R})}. \tag{18}$$

Taking into account that we are dealing with two different bases it is convenient to decompose $\overline{R}$ in a block

[1] The generalization to a transformation mixing creation and annihilation operators is straightforward but seems to be of little interest.

form that makes explicit this fact,

$$\overline{R} = \begin{pmatrix} \mathcal{R}_1 & \mathcal{S}_1 \\ \mathcal{T}_1 & \mathcal{U}_1 \end{pmatrix}. \tag{19}$$

In the above expression $\mathcal{R}_1$ is the transformation matrix among the states of the single particle basis 1 (i.e., $(\mathcal{R}_1)_{ij} ={}_1 \langle i|\mathcal{T}|j\rangle_1$), $\mathcal{S}_1$ is the mixing matrix between basis 1 and 2 [i.e., $(\mathcal{S}_1)_{ij} ={}_1 \langle i|\mathcal{T}|j\rangle_2$], etc.

The key point in the argument is to decompose $\overline{R}$ as a product of three special transformations

$$\overline{R} = \begin{pmatrix} 1 & 0 \\ X_1 & 1 \end{pmatrix} \begin{pmatrix} Y_1 & 0 \\ 0 & \mathcal{Y}_1 \end{pmatrix} \begin{pmatrix} 1 & Z_1 \\ 0 & 1 \end{pmatrix}. \tag{20}$$

The first transformation does not mix elements of the basis 1 with those of basis 2 but it mixes elements of basis 2 with those of basis 1 through the mixing matrix X_1 (it is the sum of the unity matrix plus an idempotent matrix). The second does not mix elements of the two basis (i.e., it has block diagonal form), while the third one is the opposite to the first transformation as it mixes elements of basis 1 with those of basis 2 through a mixing matrix Z_1 but it does not mix elements of basis 2. Determining X_1, Y_1, $\mathcal{Y}_1$, and Z_1 is not a difficult task: the product of the three matrices appearing in Eq. (20) is carried out and equated to the expression appearing in Eq. (19). A little algebra yields the result $X_1 = \mathcal{T}_1\mathcal{R}_1^{-1}$, $Y_1 = \mathcal{R}_1$, $\mathcal{Y}_1 = \mathcal{U}_1 - \mathcal{T}_1\mathcal{R}_1^{-1}\mathcal{S}_1$, and $Z_1 = \mathcal{R}_1^{-1}\mathcal{S}_1$, provided that $\mathcal{R}_1$ can be inverted.

It is also possible to obtain an expression for X_1, Y_1, $\mathcal{Y}_1$, and Z_1 in terms of the matrix decomposition of $(\overline{R}^T)^{-1}$

$$(\overline{R}^T)^{-1} = \begin{pmatrix} \mathcal{R}_2 & \mathcal{S}_2 \\ \mathcal{T}_2 & \mathcal{U}_2 \end{pmatrix}. \tag{21}$$

The result is $X_1^T = -\mathcal{S}_2\mathcal{U}_2^{-1}$, $Y_1 = \mathcal{R}_2 - \mathcal{S}_2\mathcal{U}_2^{-1}\mathcal{T}_2$, $\mathcal{Y}_1 = (\mathcal{U}_2^T)^{-1}$, and $Z_1^T = -\mathcal{U}_2^{-1}\mathcal{T}_1$.

Using the above decomposition of $\overline{R}$ the full transformation matrix R can be decomposed as the product $R = R^{(1)}R^{(2)}R^{(3)}$

$$R = \begin{pmatrix} 1 & 0 & & \\ X_1 & 1 & & 0 \\ & & 1 & -X_1^T \\ & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Y_1 & 0 & & \\ 0 & \mathcal{Y}_1 & & 0 \\ & & (Y_1^T)^{-1} & 0 \\ & 0 & 0 & (\mathcal{Y}_1^T)^{-1} \end{pmatrix} \begin{pmatrix} 1 & Z_1 & & \\ 0 & 1 & & 0 \\ & & 1 & 0 \\ & 0 & -Z_1^T & 1 \end{pmatrix}, \tag{22}$$

where each of the transformations $R^{(i)}$ preserves the canonical commutation relations (i.e., $R^{(i)}\sigma R^{(i)^T} = \sigma$). The decomposition of R can also be expressed in terms of exponentials of quadratic forms of creation and annihilation operators (see Appendix A and [1])

$$\mathcal{T} = \exp\left\{c^\dagger_{(2)}\mathcal{T}_1\mathcal{R}_1^{-1}c_{(1)}\right\}\exp\left\{c^\dagger_{(1)}\ln Y_1 c_{(1)}\right\} \times \exp\left\{c^\dagger_{(2)}\ln \mathcal{Y}_1 c_{(2)}\right\}\exp\left\{c^\dagger_{(1)}\mathcal{R}_1^{-1}\mathcal{S}_1 c_{(2)}\right\}, \tag{23}$$

where the subscripts (1) and (2) stand for the operator of basis 1 and 2, respectively.

III. QUASIPARTICLE TRANSFORMATION

In the preceding section the $\mathcal{T}$ transformation for single particle states has been decomposed as a product of three simpler transformations. Now the effect of those transformations on the quasiparticle operators will be considered.

As we are dealing with two different HFB wave functions we have to consider not only the effect of $\mathcal{T}$ but also the effect of the Bogoliubov transformation $\mathcal{T}_B$ connecting $|\varphi'\rangle$ with $|\varphi\rangle$. Therefore, let us consider the total transformation operator $\mathcal{T}\mathcal{T}_B$. Let α_μ and β_μ be the quasiparticle annihilation operators associated with the quasiparticle vacuums $|\varphi\rangle$ and $|\varphi'\rangle = \mathcal{T}_B|\varphi\rangle$, respectively. The quasiparticle operators are linear combinations of the single particle annihilation and creation operators c_i, $c_i^\dagger$

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = W^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix}. \tag{24}$$

Taking into account that both set of quasiparticle operators are related through the $\mathcal{T}_B$ transformation

$$\mathcal{T}_B \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \mathcal{T}_B^{-1} = \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \tag{25}$$

and recalling that $\mathcal{T}$ and $\mathcal{T}_B$ are linear transformations, the effect of the transformation $\mathcal{T}\mathcal{T}_B$ in the $(\alpha, \alpha^\dagger)$ set is given by

$$\mathcal{T}_B^{-1}\mathcal{T}^{-1} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \mathcal{T}\mathcal{T}_B = W^\dagger R W' \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix}, \tag{26}$$

where W and W' are the Bogoliubov wave functions of Eq. (24) associated with the quasiparticle operators α, $\alpha^\dagger$ and β, $\beta^\dagger$, respectively. Denoting by T the product $W^\dagger R W'$ we decompose it as the product $T = T^{(1)}T^{(2)}T^{(3)}$, where the $T^{(i)}$ are given by

$$T^{(1)} = W^\dagger R^{(1)} W, \tag{27}$$

$$T^{(2)} = W^\dagger R^{(2)} W', \tag{28}$$

$$T^{(3)} = W'^\dagger R^{(3)} W'. \tag{29}$$

With the above definitions, and taking into account that $R^{(i)}$, W, and W' preserve canonical commutation relations, it can be shown that this is also the case for the $T^{(i)}$.

In order to compute the transformation matrices $T^{(i)}$ it is first necessary to consider what is the structure of the Bogoliubov wave functions U and V in terms of the two bases, 1 and 2. As only basis 1 is used to determine the HFB wave functions, the U and V matrices do not mix elements of basis 1 with those of basis 2. The structure of U and V in the basis 2 subspace is somewhat arbitrary, the only restriction being that the occupation probabilities in such subspace have to be zero (i.e., $v_\mu = 0$, $u_\mu = 1$). With the previous considerations we can write U and V in terms of basis 1 and basis 2 states as

$$U = \begin{pmatrix} \overline{U} & 0 \\ 0 & \overline{d} \end{pmatrix}, \quad V = \begin{pmatrix} \overline{V} & 0 \\ 0 & 0 \end{pmatrix}, \tag{30}$$

where $\overline{U}$ and $\overline{V}$ are the wave functions determining $|\varphi\rangle$ and $\overline{d}$ is an arbitrary unitary transformation among the basis 2 subspace. As $|\varphi\rangle$ and $|\varphi'\rangle$ are expanded in the same basis, the previous decomposition of U and V also holds for U' and V'.

In order to simplify the algebra and the expressions appearing in the following, $T^{(i)}$ is written as

$$T^{(i)} = \begin{pmatrix} T^{(i)}_{11} & T^{(i)}_{12} \\ T^{(i)}_{21} & T^{(i)}_{22} \end{pmatrix}, \tag{31}$$

where $T^{(i)}_{11}$ is the transformation matrix among annihilation operators, $T^{(i)}_{12}$ is the mixing matrix between annihilation and creation operators, etc.

The calculation of $T^{(i)}$ is straightforward. The results for $T^{(i)}_{nm}$, making explicit the terms corresponding to each basis, are

$$T^{(1)}_{11} = \begin{pmatrix} 1 & 0 \\ \overline{d}^\dagger X_1 \overline{U} & 1 \end{pmatrix}, \tag{32a}$$

$$T^{(1)}_{12} = \begin{pmatrix} 0 & -\overline{V}^\dagger X_1^T \overline{d}^* \\ \overline{d}^\dagger X_1 \overline{V}^* & 0 \end{pmatrix}, \tag{32b}$$

$$T^{(1)}_{21} = 0, \tag{32c}$$

$$T^{(1)}_{22} = \left(T^{(1)T}_{11}\right)^{-1}, \tag{32d}$$

for $T^{(1)}$,

$$T^{(2)}_{11} = \begin{pmatrix} \overline{A} & 0 \\ 0 & \overline{\mathcal{A}} \end{pmatrix}, \tag{33a}$$

$$T^{(1)}_{12} = \begin{pmatrix} B & 0 \\ 0 & 0 \end{pmatrix}, \tag{33b}$$

$$T^{(1)}_{21} = \begin{pmatrix} \overline{B} & 0 \\ 0 & 0 \end{pmatrix}, \tag{33c}$$

$$T^{(1)}_{22} = \begin{pmatrix} A & 0 \\ 0 & \mathcal{A} \end{pmatrix}, \tag{33d}$$

with

$$A = \overline{U}^T \left(\mathcal{R}_1^T\right)^{-1} \overline{U}'^* + \overline{V}^T \mathcal{R}_1 \overline{V}'^*, \tag{34a}$$

$$\mathcal{A} = \overline{d}^T \mathcal{U}_2 \overline{d}'^*, \tag{34b}$$

$$\overline{A} = \overline{U}^\dagger \mathcal{R}_1 \overline{U}' + \overline{V}^\dagger \left(\mathcal{R}_1^T\right)^{-1} \overline{V}', \tag{34c}$$

$$\overline{\mathcal{A}} = \overline{d}^\dagger \left(\mathcal{U}_2^T\right)^{-1} \overline{d}', \tag{34d}$$

$$B = \overline{U}^\dagger \mathcal{R}_1 \overline{V}'^* + \overline{V}^\dagger \left(\mathcal{R}_1^T\right)^{-1} \overline{U}'^*, \tag{34e}$$

$$\overline{B} = \overline{U}^T \left(\mathcal{R}_1^T\right)^{-1} \overline{V}' + \overline{V}^T \mathcal{R}_1 \overline{U}', \tag{34f}$$

for $T^{(2)}$ and

$$T^{(3)}_{11} = \begin{pmatrix} 1 & \overline{U}'^\dagger Z_1 \overline{d}' \\ 0 & 1 \end{pmatrix}, \tag{35a}$$

$$T^{(3)}_{21} = \begin{pmatrix} 0 & \overline{V}'^T Z_1 \overline{d}' \\ -\overline{d}'^T Z_1^T \overline{V}' & 0 \end{pmatrix}, \tag{35b}$$

$$T^{(3)}_{12} = 0, \tag{35c}$$

$$T^{(3)}_{22} = \left(T^{(1)T}_{11}\right)^{-1}, \tag{35d}$$

for $T^{(3)}$. At this point it is worth noting that both $T^{(1)}_{12}$ and $T^{(3)}_{21}$ are zero due to the special decomposition of $\overline{R}$, Eq. (20). This will be shown to be crucial in the calculation of the overlap and the proof of the extended Wick's theorem.

Resorting again to the relation between a transformation matrix and the corresponding operator (see Appendix A) it is possible to associate to each transformation matrix $T^{(i)}$ the corresponding operator $\mathcal{T}_T^{(i)}$

$$\mathcal{T}_T^{(i)^{-1}} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \mathcal{T}_T^{(i)} = T^{(i)} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \tag{36}$$

so that the total transformation $\mathcal{T}_T = \mathcal{T}\mathcal{T}_B$ can be decomposed as

$$\mathcal{T}_T = \sqrt{\det(\overline{R})}\,\mathcal{T}_T^{(1)}\mathcal{T}_T^{(2)}\mathcal{T}_T^{(3)}. \tag{37}$$

The general structure of the $\mathcal{T}_T^{(i)}$ operators is of the form

$$\mathcal{T}_T^{(i)} = \exp\left(\frac{1}{2}\sum_{\mu\nu} \gamma_\mu Q^{(i)}_{\mu\nu} \gamma_\nu\right), \tag{38}$$

where γ_μ is the μ^{th} element of the vector $(\alpha_1, \ldots, \alpha_1^\dagger, \ldots)$ and $Q^{(i)}_{\mu\nu}$ is an antisymmetric matrix such that $T^{(i)} = \exp(\sigma Q^{(i)})$. The explicit form of $Q^{(i)}$ is irrelevant of the arguments used in the following and, therefore, the operator $\mathcal{T}_T^{(i)}$ will be directly written in its factored form

$$\mathcal{T}_T^{(i)} = \exp\left(\frac{1}{2}\sum_{\mu\nu} \alpha_\mu^\dagger K^{(i)}_{\mu\nu} \alpha_\nu^\dagger\right) \exp\left(\sum_{\mu\nu} \alpha_\mu^\dagger L^{(i)}_{\mu\nu} \alpha_\nu\right) \times \exp\left(\frac{1}{2}\sum_{\mu\nu} \alpha_\mu M^{(i)}_{\mu\nu} \alpha_\nu\right) \exp\left(-\frac{1}{2}\mathrm{Tr}\left[L^{(i)}\right]\right). \tag{39}$$

The $K^{(i)}$, $L^{(i)}$, and $M^{(i)}$ matrices are expressed in terms of $T^{(i)}$ as (see Appendix A)

$$K^{(i)} = T^{(i)}_{12} T^{(i)^{-1}}_{22}, \tag{40a}$$

$$\exp\left(L^{(i)}\right) = \left(T^{(i)^T}_{22}\right)^{-1}, \tag{40b}$$

$$M^{(i)} = T^{(i)^{-1}}_{22} T^{(i)}_{21}. \tag{40c}$$

The only difficulty in the evaluation of these quantities seems to be the calculation of the inverse of the $T_{22}^{(i)}$ matrices. However, this calculation can be greatly simplified taking into account the following properties

$$\begin{pmatrix} 1 & 0 \\ X & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 \\ -X & 1 \end{pmatrix}, \tag{41a}$$

$$\begin{pmatrix} 1 & Z \\ 0 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & -Z \\ 0 & 1 \end{pmatrix}. \tag{41b}$$

Using them one can obtain the expressions for $K^{(1)}$, $L^{(1)}$, and $M^{(1)}$,

$$K^{(1)} = \begin{pmatrix} 0 & -\overline{V}^\dagger X_1^T \overline{d}^* \\ \overline{d}^\dagger X_1 \overline{V}^* & \overline{d}^\dagger X_1 \overline{V}^* \overline{U}^\dagger X_1^T \overline{d}^* \end{pmatrix}, \tag{42}$$

$$L^{(1)} = \begin{pmatrix} 0 & 0 \\ \overline{d}^\dagger X_1 \overline{U} & 0 \end{pmatrix}, \tag{43}$$

$$M^{(1)} = 0, \tag{44}$$

$$\mathrm{Tr}\left[L^{(1)}\right] = 0, \tag{45}$$

The fact that the $\mathcal{T}_T^{(1)}$ transformation does not have a two-quasiparticle annihilation operators part (i.e., $M^{(1)} = 0$) is due to the fact that $T_{12}^{(1)} = 0$.

For $\mathcal{T}_T^{(2)}$ the following expressions are obtained:

$$K^{(2)} = \begin{pmatrix} BA^{-1} & 0 \\ 0 & 0 \end{pmatrix}, \tag{46}$$

$$\exp\left(L^{(2)}\right) = \begin{pmatrix} \left(A^T\right)^{-1} & 0 \\ 0 & \left(\mathcal{A}^T\right)^{-1} \end{pmatrix}, \tag{47}$$

$$M^{(2)} = \begin{pmatrix} A^{-1}\overline{B} & 0 \\ 0 & 0 \end{pmatrix}, \tag{48}$$

$$\exp(-\tfrac{1}{2}\mathrm{Tr}[L^{(2)}]) = \sqrt{\det(A)\det(\mathcal{A})}, \tag{49}$$

where the matrices A, $\mathcal{A}$, B, and $\overline{B}$ are those of Eqs. (34a), (34b), (34e), and (34f).

Using the decomposition of $\overline{R}$ it is easy to show that $\det(\overline{R}) = \det(Y_1)\det(\mathcal{Y}_1) = \det(\mathcal{R}_1)\det\left[\left(\mathcal{U}_2^T\right)^{-1}\right]$. Taking into account the expression for $\mathcal{A}$ and the previous relation, we can write $\det(\mathcal{A}) = \det(\mathcal{U}_2) = \det(\mathcal{R}_1)/\det(\overline{R})$. This allows one to write the constant term appearing in the expression of $\mathcal{T}_T^{(2)}$ solely in terms of quantities defined in the basis 1 subspace,

$$\exp(-\tfrac{1}{2}\mathrm{Tr}[L^{(2)}]) = \sqrt{\frac{\det(A)\det(\mathcal{R}_1)}{\det \overline{R}}}. \tag{50}$$

Finally, for $\mathcal{T}_T^{(3)}$ we get

$$K^{(3)} = 0, \tag{51}$$

$$L^{(3)} = \begin{pmatrix} 0 & \overline{U}'^\dagger Z_1 \overline{d}' \\ 0 & 0 \end{pmatrix}, \tag{52}$$

$$M^{(3)} = \begin{pmatrix} 0 & \overline{V}'^T Z_1 \overline{d}' \\ -\overline{d}^T Z_1^T \overline{V}' & \overline{d}'^T Z_1^T \overline{U}'^* \overline{V}'^T Z_1 \overline{d}' \end{pmatrix}, \tag{53}$$

$$\mathrm{Tr}\left[L^{(3)}\right] = 0. \tag{54}$$

Here, $K^{(3)} = 0$ is a direct consequence of having $T_{21}^{(3)} = 0$.

IV. WICK'S THEOREM AND ONISHI FORMULA

In the preceding section the transformation operator $\mathcal{T}_T$ has been decomposed as the product [Eq. (37)] of three special transformations $\mathcal{T}_T^{(i)}$ having the properties

$$\mathcal{T}_T^{(3)}|\varphi\rangle = |\varphi\rangle, \tag{55}$$

$$\langle\varphi|\mathcal{T}_T^{(1)} = \langle\varphi|, \tag{56}$$

$$\langle\varphi|\mathcal{T}_T^{(2)}|\varphi\rangle = \exp(-\tfrac{1}{2}\mathrm{Tr}[L^{(2)}]). \tag{57}$$

The first two properties stem directly from the fact that both $K^{(3)}$ and $M^{(1)}$ are zero and this is a consequence of the special decomposition of $\mathcal{T}$.

With the above properties the calculation of the overlap $\langle\varphi|\mathcal{T}|\varphi'\rangle$ (Onishi formula) is straightforward:

$$\begin{aligned}\langle\varphi|\mathcal{T}|\varphi'\rangle &= \langle\varphi|\mathcal{T}_T|\varphi\rangle = \sqrt{\det(\overline{R})}\langle\varphi|\mathcal{T}_T^{(2)}|\varphi\rangle \\ &= \sqrt{\det(A)\det(\mathcal{R}_1)}.\end{aligned} \tag{58}$$

The above result gives us an expression of the overlap solely in terms of quantities defined in the basis 1 subspace. It differs from the usual one in the definition of the matrix A, Eq. (34a), and the extra $\det(\mathcal{R}_1)$ [for the definition of $\mathcal{R}_1$ see Eq. (19)].

To prove the extended Wick's theorem and to compute the contractions, the property of $\mathcal{T}_T^{(3)}$ given in Eq. (55) is used to write the overlap of the operator $\hat{A}$ as

$$\begin{aligned}\frac{\langle\varphi|\hat{A}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} &= \langle\varphi|\hat{A}\mathcal{T}_T^{(1)}\exp(\tfrac{1}{2}\alpha^\dagger K^{(2)}\alpha^\dagger)|\varphi\rangle \\ &\equiv \langle\varphi|\hat{A}\mathcal{T}_W|\varphi\rangle.\end{aligned} \tag{59}$$

This shows that the only relevant part of the transformation is given by $\mathcal{T}_W = \mathcal{T}_T^{(1)}\exp\left(\tfrac{1}{2}\alpha^\dagger K^{(2)}\alpha^\dagger\right)$.

Now a new set of quasiparticle operators $(d_\mu, \overline{d}_\mu)$ satisfying canonical commutation relations (but not necessarily being Hermitian conjugated) is defined as

$$\begin{pmatrix} d \\ \overline{d} \end{pmatrix} = \mathcal{T}_W^{-1}\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix}\mathcal{T}_W. \tag{60}$$

Using the transformation properties of $\mathcal{T}_T^{(1)}$ [see Eq. (36)] and those of $\exp\left(\tfrac{1}{2}\alpha^\dagger K^{(2)}\alpha^\dagger\right)$ (see Appendix A), we establish the linear relation between the $(d_\mu, \overline{d}_\mu)$ and the $(\alpha_\mu, \alpha_\mu^\dagger)$ sets

$$\begin{aligned}\begin{pmatrix} d \\ \overline{d} \end{pmatrix} &= \begin{pmatrix} T_{11}^{(1)} & T_{12}^{(1)} \\ 0 & T_{22}^{(1)} \end{pmatrix}\begin{pmatrix} 1 & K^{(2)} \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \\ &= \begin{pmatrix} T_{11}^{(1)} & T_{11}^{(1)}K^{(2)} + T_{12}^{(1)} \\ 0 & T_{22}^{(1)} \end{pmatrix}\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix},\end{aligned} \tag{61}$$

where the matrices $T_{11}^{(1)}$, $T_{12}^{(1)}$, $T_{22}^{(1)}$ have been defined in Eq. (32) and $K^{(2)}$ in Eqs. (46), (34a), (34e).

Noting that

$$\langle\varphi|\mathcal{T}_W = 0 \tag{62}$$

and inserting in the expression of $\hat{A}(\alpha,\alpha^\dagger)$ as many $\mathcal{T}_W\mathcal{T}_W^{-1}$ as needed, we express the general overlap of Eq. (6) as a mean field value of d and $\overline{d}$ quasiparticle operators

$$\frac{\langle\varphi|\hat{A}(\alpha,\,\alpha^\dagger)\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \langle\varphi|\hat{A}(d,\,\overline{d})|\varphi\rangle. \tag{63}$$

As d_μ, $\overline{d}_\mu$ are linear combinations of the quasiparticle operators α, $\alpha^\dagger$ associated with $|\varphi\rangle$, the matrix element

$$\langle\varphi|\hat{A}(d,\,\overline{d})|\varphi\rangle \tag{64}$$

can be computed using the usual Wick's theorem as the sum of all possible contractions of the d and $\overline{d}$ operators. Using the definition of d and $\overline{d}$ we obtain for the contractions

$$\langle\varphi|d_\mu\overline{d}_\nu|\varphi\rangle = \delta_{\mu\nu}, \tag{65}$$

$$\langle\varphi|d_\mu d_\nu|\varphi\rangle = \left[T_{11}^{(1)}\left(T_{12}^{(1)^T} + K^{(2)^T}T_{11}^{(1)^T}\right)\right]_{\mu\nu}, \tag{66}$$

$$\langle\varphi|\overline{d}_\mu\overline{d}_\nu|\varphi\rangle = 0, \tag{67}$$

$$\langle\varphi|\overline{d}_\mu d_\nu|\varphi\rangle = 0. \tag{68}$$

Using the relation of Eq. (63) and taking into account that the matrix element of Eq. (64) can be computed as the sum of the contractions given in Eqs. (65)–(68) the proof of the extended Wick's theorem is complete.

Finally, the structure of the only nontrivial contraction $\langle\varphi|d_\mu d_\nu|\varphi\rangle$ can be determined by using the explicit form of $T_{11}^{(1)}$, $T_{12}^{(1)}$ [Eqs. (32)] and $K^{(2)}$ [see Eqs. (46), (34a), (34e)] in terms of the 1 and 2 subspaces. However, the final result involves rather lengthy expressions and therefore it is convenient to use the relation

$$\overline{V}^*A + \overline{U}B = \mathcal{R}_1\overline{V}'^*, \tag{69}$$

which can be obtained using the explicit expression of the A and B matrices and the unitarity relations of the Bogoliubov wave functions, to simplify the final result,

$$\langle\varphi|d_\mu d_\nu|\varphi\rangle = \begin{pmatrix} -BA^{-1} & (A^T)^{-1}\overline{V}'^\dagger\mathcal{T}_1^T\overline{d}^* \\ -\overline{d}^\dagger\mathcal{T}_1\overline{V}'^*A^{-1} & -\overline{d}^\dagger X_1\overline{U}(A^T)^{-1}\overline{V}'^\dagger\mathcal{T}_1^T\overline{d}^* \end{pmatrix}_{\mu\nu}. \tag{70}$$

The result for the subspace spanned by the basis 1 is identical to the usual expression for this contraction except for the different definition of the A and B matrices [Eqs. (34a), (34e)]. On the other hand, the contractions for those pairs of indices containing at least one index of basis 2 cannot be compared with any previous result. They show the peculiarity of containing the arbitrary transformation $\overline{d}$ [see Eq. (30)]. At a first glance this seems rather suspicious but, as it will be shown in the next section, the $\overline{d}$ matrix never appears in the calculation of overlaps of operators.

For unitary transformations not mixing basis 1 with basis 2 ($\mathcal{S}_1 = \mathcal{T}_1 = 0$ in $\overline{R}$), $\mathcal{R}_1$ has to be an unitary matrix [i.e., $(\mathcal{R}_1^T)^{-1} = \mathcal{R}_1^*$]. In this case the A and B matrices of Eqs. (34a), (34e) are given by

$$A = \overline{U}^T\mathcal{R}_1^*\overline{U}'^* + \overline{V}^T\mathcal{R}_1\overline{V}'^*, \tag{71a}$$

$$B = \overline{U}^\dagger\mathcal{R}_1\overline{V}'^* + \overline{V}^\dagger\mathcal{R}_1^*\overline{U}'^*, \tag{71b}$$

which are the usual expressions previously found in the literature [2]. Moreover, if one takes into account that the unitarity of $\mathcal{R}_1$ implies that its determinant is a phase, it is clear that the overlap of Eq. (58) reduces to the usual Onishi formula [3]. The $\langle\varphi|d_\mu d_\nu|\varphi\rangle$ contraction is in this case only different from zero if both indexes μ and ν belong to the basis 1 set thus reducing to the usual contraction [1,2].

V. SOME APPLICATIONS

In this section the Hartree-Fock limit for the overlap $\langle\varphi|\mathcal{T}|\varphi\rangle$ and the calculation of the overlap of one body operators will be presented.

In the Hartree-Fock (HF) limit we can consider that basis 1 is the self-consistent single particle basis of the occupied states. Therefore, the $\overline{U}$ matrix is zero and $\overline{V}$ is equal to the unity matrix. The A matrix of Eq. (34a) is simply $\mathcal{R}_1$ and then the expression of the overlap Eq. (58) reduces to

$$\langle\varphi|\mathcal{T}|\varphi\rangle = \det(\mathcal{R}_1). \tag{72}$$

Taking into account that $\mathcal{R}_1$ are the matrix elements of the transformation operator $\mathcal{T}$ in the basis 1 (i.e., the self-consistent basis), it is clear that the previous result coincides with the well-known Lowdin formula [5]. The generalization of the previous limit to the more general overlap $\langle\varphi|\mathcal{T}|\varphi'\rangle$ requires the use of two different single particle basis for $|\varphi\rangle$ and $|\varphi'\rangle$ and the reader is referred to Appendix B for further details.

Now we turn to the calculation of the overlap

$$\frac{\langle\varphi|\hat{Q}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle}, \tag{73}$$

where $\hat{Q}$ is a single particle operator

$$\hat{Q} = \sum_{ij} Q_{ij}c_i^\dagger c_j. \tag{74}$$

Using the inverse Bogoliubov transformation, we can express the creation and annihilation single particle operators in terms of the quasiparticles associated with $|\varphi\rangle$

$$\frac{\langle\varphi|\hat{Q}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \sum_{ij} Q_{ij} V_{i\mu} \frac{\langle\varphi|\alpha_\mu \left(V^*_{j\nu}\alpha^\dagger_\nu + U_{j\nu}\alpha_\nu\right)\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle}. \tag{75}$$

Using now the contractions

$$\frac{\langle\varphi|\alpha_\mu\alpha^\dagger_\nu\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \langle\varphi|d_\mu d^\dagger_\nu|\varphi\rangle = \delta_{\mu\nu}, \tag{76}$$

$$\frac{\langle\varphi|\alpha_\mu\alpha_\nu\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \langle\varphi|d_\mu d_\nu|\varphi\rangle = C_{\mu\nu}, \tag{77}$$

we obtain

$$\frac{\langle\varphi|\hat{Q}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \mathrm{Tr}\left[V^T Q(V^* + UC^T)\right]. \tag{78}$$

Using the explicit form of the matrices entering the above expression as well as known properties of the trace, we obtain after some algebra

$$\frac{\langle\varphi|\hat{Q}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \mathrm{Tr}[\overline{V}^T Q_{11}(\overline{V}^* + \overline{U}BA^{-1}) + \overline{V}^T Q_{12}\mathcal{T}_1(\overline{V}'^* A^{-1})], \tag{79}$$

where Q_{11} and Q_{12} refer to the matrix elements of $\hat{Q}$ in the basis 1 subspace and to the overlap of $\hat{Q}$ between basis 1 and 2, respectively. The previous trace can be simplified by using the property of Eq. (69) to

$$\mathrm{Tr}\left[\overline{V}^T(Q_{11}\mathcal{R}_1 + Q_{12}\mathcal{T}_1)\overline{V}'^* A^{-1}\right]. \tag{80}$$

The matrix $(Q_{11}\mathcal{R}_1 + Q_{12}\mathcal{T}_1)_{ij}$ can be written as

$$\sum_m {}_1\langle i|\hat{Q}|m\rangle_{11}\langle m|\mathcal{T}|j\rangle_1 + {}_1\langle i|\hat{Q}|m\rangle_{22}\langle m|\mathcal{T}|j\rangle_1 = {}_1\langle i|\hat{Q}\mathcal{T}|m\rangle_1 \equiv (Q\mathcal{T})_{11}, \tag{81}$$

which allows us to finally write the overlap of Q as

$$\frac{\langle\varphi|\hat{Q}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \mathrm{Tr}\left[\overline{V}^T(Q\mathcal{T})_{11}\overline{V}'^* A^{-1}\right]. \tag{82}$$

As it was said before, the overlap of Q can be expressed solely in terms of quantities defined in the basis 1 subspace.

VI. CONCLUSIONS

In this paper the extended Wick's theorem and the Onishi formula have been reformulated to consider the situation where the single particle basis is not complete under the transformation operator appearing in the calculation of the overlaps. It has been shown that the overlap can be expressed in terms of quantities defined in the noncomplete single particle basis. Although the contractions appearing in the application of the extended Wick's theorem are different from zero for those indexes not belonging to the original basis, it has been shown that in the calculation of overlaps of operators the final result does only depend on quantities defined in the original basis. The results obtained are of great importance in the practical application of the angular momentum or center of mass (among others) projection of HFB wave functions.

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APPENDIX A

In this appendix we present some well-known results concerning the effect of a linear canonical transformation operator on a given set of creation and annihilation operators. Although we have closely followed the approach of Balian and Brezin [1] the main results of their work are summarized here for convenience of the reader. The reader interested in further details should consult the original reference.

Given a set of fermion annihilation and creation operators obeying canonical commutation relations $\{c, \bar{c}\}$ (the notation $\bar{c}$ is used for creation operators as they do not necessarily have to be the hermitian conjugates of the annihilation operators) the operator

$$\mathcal{T} = \exp\left[\frac{1}{2}\sum_{ij}\gamma_i Q_{ij}\gamma_j\right], \tag{A1}$$

where γ_i is a shorthand notation for the vector $(c_1, \ldots, c_N, \ldots, \bar{c}_1, \ldots, \bar{c}_N, \ldots)$ and Q is an antisymmetric matrix, transform the annihilation and creation operators in the following way:

$$\mathcal{T}^{-1}\begin{pmatrix} c \\ \bar{c} \end{pmatrix}\mathcal{T} = T\begin{pmatrix} c \\ \bar{c} \end{pmatrix}. \tag{A2}$$

The transformation matrix T is related to Q through the relation

$$T = \exp\left[\sigma Q\right], \tag{A3}$$

where σ is the anticommutator of the γ_i operators

$$\sigma_{ij} = [\gamma_i, \gamma_j]_+ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

With the above definition of T it is easy to show that this matrix satisfies the relation

$$T\sigma T^T = \sigma. \tag{A4}$$

which is equivalent to say that $\mathcal{T}$ preserves the canonical commutation relations $\{c_i, \bar{c}_j\} = \delta_{ij}$.

The opposite is also true: Given a transformation matrix satisfying Eq. (A4) there is an operator, exponential of an antisymmetric quadratic form of creation and annihilation operators, which produces the desired transformation. The operator is unique if we restrict it to be the exponential of an antisymmetric form; otherwise it is defined within a multiplicative constant. The origin of this constant can be easily understood if a general matrix Q is considered in Eq. (A2) instead of an antisymmetric matrix. The quadratic form $\gamma Q \gamma$ can be decomposed as the sum of two terms $\gamma Q_S \gamma$ and $\gamma Q_A \gamma$ which are the symmetric and antisymmetric parts of Q, respectively. Using the commutation relations $[\gamma_i, \gamma_j]_+ = \sigma_{ij}$ it is straightforward to show that the symmetric part reduces to a constant $\frac{1}{2}\mathrm{Tr}(Q_S\sigma)$.

Now we will consider some useful transformations (see [1] for further details)

$$T^{(1)} = \begin{pmatrix} 1 & X \\ 0 & 1 \end{pmatrix} \to \mathcal{T}^{(1)} = \exp\left[\frac{1}{2}\bar{c}X\bar{c}\right], \tag{A5}$$

$$T^{(2)} = \begin{pmatrix} e^Y & 0 \\ 0 & e^{-Y^T} \end{pmatrix} \to \mathcal{T}^{(2)} = \exp\left[\bar{c}Yc\right]\exp\left[-\frac{1}{2}\mathrm{Tr}Y\right], \tag{A6}$$

$$T^{(3)} = \begin{pmatrix} 1 & 0 \\ Z & 1 \end{pmatrix} \to \mathcal{T}^{(3)} = \exp\left[\frac{1}{2}cZc\right], \tag{A7}$$

where X and Z must be antisymmetric matrices so that the corresponding T satisfies Eq. (A4). In Ref. [1] it was shown that any transformation operator $\mathcal{T}$ exponential of an antisymmetric quadratic form of fermion annihilation and creation operators can be decomposed as the product of three elemental transformations of the type mentioned above Eqs. (A5), (A6), and (A7),

$$\mathcal{T} = \mathcal{T}^{(1)}\mathcal{T}^{(2)}\mathcal{T}^{(3)}. \tag{A8}$$

The X, Y, and Z matrices are related to the transformation matrix

$$T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = T^{(1)}T^{(2)}T^{(3)} \tag{A9}$$

of $\mathcal{T}$ through the relations $X = T_{12}(T_{22})^{-1}$, $\exp(-Y) = T_{22}^T$, and $Z = (T_{22})^{-1}T_{21}$. For a general operator $\mathcal{T}$ [i.e., the matrix Q in Eq. (A1) not having any symmetry property] one has to write it first as the product of the constant $\exp[\frac{1}{2}\mathrm{Tr}(\sigma Q_S)]$ times the operator $\mathcal{T}_A = \exp[\frac{1}{2}\sum_{ij}\gamma_i(Q_A)_{ij}\gamma_j]$ and apply the decomposition to $\mathcal{T}_A$.

APPENDIX B

In this appendix we consider the situation in which the two quasiparticle vacuums $|\varphi\rangle$ and $|\varphi'\rangle$ are expanded in two different single particle bases.

Let us denote by $c^\dagger$ and $a^\dagger$ the creation operators of the bases in which the quasiparticle operators of $|\varphi\rangle$ and $|\varphi'\rangle$ are expanded. Both bases are related through a unitary transformation $\mathcal{T}_{ac}$ such that

$$\mathcal{T}_{ac}^{-1}\begin{pmatrix} a \\ a^\dagger \end{pmatrix}\mathcal{T}_{ac} = \begin{pmatrix} c \\ c^\dagger \end{pmatrix}. \tag{B1}$$

The effect of $\mathcal{T}_{ac}$ on the quasiparticle operators associated with $|\varphi'\rangle$

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U'^\dagger & V'^\dagger \\ V'^T & U'^T \end{pmatrix}\begin{pmatrix} a \\ a^\dagger \end{pmatrix} = W'^\dagger\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \tag{B2}$$

is to transform them into a new set

$$\mathcal{T}_{ac}^{-1}\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix}\mathcal{T}_{ac} = \begin{pmatrix} \tilde{\beta} \\ \tilde{\beta}^\dagger \end{pmatrix} = \begin{pmatrix} U'^\dagger & V'^\dagger \\ V'^T & U'^T \end{pmatrix}\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = W'^\dagger\begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \tag{B3}$$

which has the same Bogoliubov wave functions U' and V' but is expanded in the single particle basis of $|\varphi\rangle$. The quasiparticle vacuum of the $(\tilde{\beta}, \tilde{\beta}^\dagger)$ set, $|\tilde{\varphi}'\rangle$ is therefore related to $|\varphi'\rangle$ through the same transformation

$$|\varphi'\rangle = \mathcal{T}_{ac}|\tilde{\varphi}'\rangle. \tag{B4}$$

Using the previous relation we can write

$$\frac{\langle\varphi|\hat{A}\mathcal{T}|\varphi'\rangle}{\langle\varphi|\mathcal{T}|\varphi'\rangle} = \frac{\langle\varphi|\hat{A}\mathcal{T}\mathcal{T}_{ac}|\tilde{\varphi}'\rangle}{\langle\varphi|\mathcal{T}\mathcal{T}_{ac}|\tilde{\varphi}'\rangle}, \tag{B5}$$

so that we have reduced the problem to the one treated in this paper but using instead of $\mathcal{T}$ the transformation operator $\mathcal{T}_N = \mathcal{T}\mathcal{T}_{ac}$. The transformation matrix $\overline{R}$ associated with $\mathcal{T}_N$ is given by

$$\overline{R}_{ij} = {}_0\langle i|\mathcal{T}|j\rangle_1 \tag{B6}$$

where $|i\rangle_0$ and $|j\rangle_1$ stand for those states associated with the creation operators $c_i^\dagger$ and $a_j^\dagger$, respectively.

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