Multiphonon theory: Generalized Wick's theorem and recursion formulas

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Overlaps and matrix elements of one- and two-body operators are calculated in a space spanned by multiphonons of different types taking the Pauli principle properly into account. Two methods are developed: a generalized Wick's theorem dealing with new contractions and recursion formulas well suited for numerical applications.

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I. INTRODUCTION

In atomic nuclei, many excited states show a vibrational nature. To explain the properties of these states, phenomenological bosons or "microscopic" quasibosons were first introduced. With these intermediate quantities, assumed to be pure bosons, matrix elements of the Hamiltonian and of electromagnetic transition operators are easily calculated with the help of the Wick's theorem for bosons that leads to harmonic features. However, the observation of anharmonicities in the nuclear vibrations demonstrates the importance of the Pauli principle in building higher excited states.

One way to solve the problem would be to start with many quasiparticle excitations. The corresponding Fock space would then be tremendously large and the Wick's theorem for fermions rapidly inapplicable. To take advantage of the collective nature of the vibrational states it appears to be better to introduce new entities: the phonons $Q_i^\dagger$, which are defined as a superposition of two quasiparticles

$$Q_i^\dagger=\frac{1}{2}\sum_{\mu,\nu}(Z_i)_{\mu\nu}\alpha_\mu^\dagger\alpha_\nu^\dagger\,, \tag{1.1}$$

where $(Z_i)_{\mu\nu}=-(Z_i)_{\nu\mu}$ is chosen to be an antisymmetric matrix, and $\alpha_\mu^\dagger$ creation operators of fermions (quasiparticles). These phonons are no longer considered as bosons since their commutation rules are now

$$[Q_1,Q_2^\dagger]=-\frac{1}{2}\mathrm{tr}(Z_1Z_2)+\sum_{\mu,\nu}(Z_1Z_2)_{\mu\nu}\alpha_\nu^\dagger\alpha_\mu\,. \tag{1.2}$$

Among the theories developed to deal with the problem of anharmonicities, the following two are of special interest:

(a) The boson expansion (BE) techniques[1] aim to return to pure bosons by expanding fermion pairs like $\alpha_\mu^\dagger\alpha_\nu^\dagger$ and $\alpha_\nu^\dagger\alpha_\mu$ in terms of pure bosons. The matrix elements of H (or of other operators) are then again easy to calculate. But one is faced with difficulties concerning the convergence of the expansion. Furthermore, the Pauli principle is only approximatively taken into account and some spurious states may appear (see Ref. 3).

(b) The multiphonon method (MPM), where the phonons (1.1) are piled up, takes the Pauli principle fully into account. This method has been developed previously[2] for *one type* of phonon, compared to boson expansions[3] and checked in a simple model[4] where an exact solution can be obtained. The main problem in this method is the calculation of the exact norms of the multiphonon states and of the matrix elements of H in the subspace spanned by these states. Simple recursion formulas[2] were obtained which allowed easy numerical evaluation of the matrix elements.

The aim of this paper is to extend the MPM to cases where phonons of different types are involved. Two methods are given. In Sec. II we formulate a Wick's theorem for phonons where we define "new contractions." In Sec. III we generalize the approach with recursion formulas. Illustrative examples are given in Sec. IV where the two approaches are compared. Finally, conclusions are drawn in the last section.

II. A WICK'S THEOREM FOR PHONONS

We first write the commutation rules of the phonon operator $Q^\dagger$ defined in (1.1) with pairs of fermion operators

$$[\alpha_\nu\alpha_\mu, Q^\dagger]=Z_{\mu\nu}+\sum_\lambda (Z_{\nu\lambda}\alpha_\lambda^\dagger\alpha_\mu - Z_{\mu\lambda}\alpha_\lambda^\dagger\alpha_\nu)\ ,$$
$$[\alpha_\mu^\dagger\alpha_\nu, Q^\dagger]=\sum_\lambda Z_{\nu\lambda}\alpha_\mu^\dagger\alpha_\lambda^\dagger\ . \tag{2.1}$$

From these relations one deduces the double commutator

$$[[Q_1,Q_2^\dagger],Q_4^\dagger]=\sum_{\mu\nu}(Z_4Z_1Z_2)_{\mu\nu}\alpha_\mu^\dagger\alpha_\nu^\dagger\ .$$

According to the antisymmetry of the Z matrices one has

$$(Z_4Z_1Z_2)_{\mu\nu}=-(Z_2Z_1Z_4)_{\nu\mu}\ ,$$

which allows us to write

$$[[Q_1,Q_2^\dagger],Q_4^\dagger]=\tfrac{1}{2}\sum_{\mu\nu}(Z_2Z_1Z_4+Z_4Z_1Z_2)_{\mu\nu}\alpha_\mu^\dagger\alpha_\nu^\dagger\ . \tag{2.2}$$

This double commutator behaves like a new phonon (1.1), labeled $\tilde{Q}^\dagger_{1;2,4}$ of which the antisymmetric matrix $\tilde{Z}$ is given by

$$\tilde{Z}_{1;2,4}=Z_2Z_1Z_4+Z_4Z_1Z_2\ . \tag{2.3}$$

(Note that for further convenience we have put even indices to creation operators and odd ones to annihilation operators.) With the choice (1.1) the quasiparticle vacuum $|\ \rangle$ is also the phonon vacuum.

We now calculate explicitly the overlaps for states with one, two, and three phonons. For one phonon we have

$$\langle Q_1Q_2^\dagger\rangle=\langle[Q_1,Q_2^\dagger]\rangle=-\tfrac{1}{2}\mathrm{tr}(Z_1Z_2)\ . \tag{2.4}$$

We define a "contraction of two operators"

$$C[Q_1Q_2^\dagger]=\langle Q_1Q_2^\dagger\rangle\ . \tag{2.5}$$

For two phonons, we obtain explicitly

$$\begin{aligned}\langle Q_3Q_1Q_2^\dagger Q_4^\dagger\rangle=&\ \langle Q_3Q_2^\dagger[Q_1,Q_4^\dagger]\rangle\\ &+\langle Q_3Q_4^\dagger[Q_1,Q_2^\dagger]\rangle\\ &+\langle Q_3[[Q_1,Q_2^\dagger],Q_4^\dagger]\rangle\end{aligned}$$

and using (2.2) and (2.5) we get

$$\begin{aligned}\langle Q_3Q_1Q_2^\dagger Q_4^\dagger\rangle=&\ C[Q_3Q_2^\dagger]C[Q_1Q_4^\dagger]\\ &+C[Q_3Q_4^\dagger]C[Q_1Q_2^\dagger]\\ &+C[Q_3\tilde{Q}^\dagger_{1;2,4}]\ .\end{aligned}$$

If we define a "contraction of four operators"

$$C[Q_3Q_1Q_2^\dagger Q_4^\dagger]=C[Q_3\tilde{Q}^\dagger_{1;2,4}] \tag{2.6}$$

we obtain

$$\begin{aligned}\langle Q_3Q_1Q_2^\dagger Q_4^\dagger\rangle=&\sum C[QQ^\dagger]C[QQ^\dagger]\\ &+C[Q_3Q_1Q_2^\dagger Q_4^\dagger]\ ,\end{aligned} \tag{2.7}$$

where the summation runs over all different possible products of contractions of two operators.

For three phonons the successive commutations of Q_1 with all creation operators lead to

$$\begin{aligned}\langle Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger\rangle=&\ \langle Q_5Q_3Q_2^\dagger Q_4^\dagger[Q_1,Q_6^\dagger]\rangle+\langle Q_5Q_3Q_2^\dagger Q_6^\dagger[Q_1,Q_4^\dagger]\rangle+\langle Q_5Q_3Q_4^\dagger Q_6^\dagger[Q_1,Q_2^\dagger]\rangle\\ &+\langle Q_5Q_3Q_2^\dagger[[Q_1,Q_4^\dagger],Q_6^\dagger]\rangle+\langle Q_5Q_3Q_4^\dagger[[Q_1,Q_2^\dagger],Q_6^\dagger]\rangle\\ &+\langle Q_5Q_3Q_6^\dagger[[Q_1,Q_2^\dagger],Q_4^\dagger]\rangle\ .\end{aligned} \tag{2.8}$$

Using relations (2.2)–(2.7) and setting

$$C[Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger]=\sum_{i<j}C[Q_5Q_3Q_{2k}^\dagger\tilde{Q}^\dagger_{1;2i,2j}] \tag{2.9}$$

for the "contraction of six operators," we get

$$\begin{aligned}\langle Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger\rangle=&\ C[Q_1Q_2^\dagger]C[Q_3Q_4^\dagger]C[Q_5Q_6^\dagger]+C[Q_1Q_2^\dagger]C[Q_3Q_6^\dagger]C[Q_5Q_4^\dagger]\\ &+C[Q_1Q_4^\dagger]C[Q_3Q_2^\dagger]C[Q_5Q_6^\dagger]+C[Q_1Q_4^\dagger]C[Q_3Q_6^\dagger]C[Q_5Q_2^\dagger]\\ &+C[Q_1Q_6^\dagger]C[Q_3Q_2^\dagger]C[Q_5Q_4^\dagger]+C[Q_1Q_6^\dagger]C[Q_3Q_4^\dagger]C[Q_5Q_2^\dagger]\\ &+C[Q_1Q_2^\dagger]C[Q_5Q_3Q_4^\dagger Q_6^\dagger]+C[Q_1Q_4^\dagger]C[Q_5Q_3Q_2^\dagger Q_6^\dagger]+C[Q_1Q_6^\dagger]C[Q_5Q_3Q_2^\dagger Q_4^\dagger]\\ &+C[Q_3Q_2^\dagger]C[Q_5Q_1Q_4^\dagger Q_6^\dagger]+C[Q_3Q_4^\dagger]C[Q_5Q_1Q_2^\dagger Q_6^\dagger]+C[Q_3Q_6^\dagger]C[Q_5Q_1Q_2^\dagger Q_4^\dagger]\\ &+C[Q_5Q_2^\dagger]C[Q_3Q_1Q_4^\dagger Q_6^\dagger]+C[Q_5Q_4^\dagger]C[Q_3Q_1Q_2^\dagger Q_6^\dagger]+C[Q_5Q_6^\dagger]C[Q_3Q_1Q_2^\dagger Q_4^\dagger]\\ &+C[Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger]\ .\end{aligned} \tag{2.10}$$

This relation can be summarized by

$$\langle Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger\rangle=\sum C[QQ^\dagger]C[QQ^\dagger]C[QQ^\dagger]+\sum C[QQ^\dagger]C[QQQ^\dagger Q^\dagger]+C[Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger]\ , \tag{2.11}$$

where the summations still run over all different possible products of contractions.

Equations (2.5), (2.7), and (2.11) give the explicit form of a generalized Wick's theorem for 1, 2, and 3 phonons. The "new contractions of 2, 4, and 6 operators" are defined, respectively, by (2.5), (2.6), and (2.9).

We note that if the Q's would have been boson operators only the first term of Eqs. (2.5), (2.7), and (2.11) would have appeared. All the other terms are due to the fact that the Pauli principle is properly taken into account in considering phonons of the type (1.1).

The generalized Wick's theorem for phonons can now be formulated in the following way: The overlap of a state built on p different creation operators

$$|Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger\rangle$$

with a state built on p different annihilation operators

$$\langle Q_1Q_3\cdots Q_{2p-1}|$$

is the sum of all *different* products of possible contractions; the contraction of $2p$ operators being defined from the contractions of $(2p-2)$ operators by

$$C[Q_{2p-1}Q_{2p-3}\cdots Q_3Q_1Q_2^\dagger\cdots Q_{2p}^\dagger]=\sum_{i<j}C[Q_{2p-1}Q_{2p-3}\cdots Q_3Q^\dagger\cdots Q^\dagger\tilde{Q}^\dagger_{1;2i,2j}]\ , \tag{2.12}$$

where $Q^\dagger\cdots Q^\dagger$ is a sequence of $(p-2)$ operators $Q^\dagger$ where $Q_{2i}^\dagger$ and $Q_{2j}^\dagger$ are missing.

Equations (2.5), (2.7), and (2.11) show that the theorem is true for 1, 2, and 3 phonons. The proof of the generalized theorem will be made by induction. But first, it is necessary to know how to calculate the involved contractions.

Let us look for the first contractions. From Eqs. (2.4) and (2.5) one has

$$C[Q_1Q_2^\dagger]=-\tfrac{1}{2}\mathrm{tr}(Z_1Z_2)\ .$$

Further, from Eqs. (2.3), (2.5), and (2.6) we get

$$\begin{aligned}C[Q_3Q_1Q_2^\dagger Q_4^\dagger]&=C[Q_3\tilde{Q}^\dagger_{1;2,4}]\\&=-\tfrac{1}{2}[\mathrm{tr}(Z_1Z_2Z_3Z_4)+\mathrm{tr}(Z_1Z_4Z_3Z_2)]\ ,\end{aligned} \tag{2.13}$$

where we have used the property that under a trace one can perform a cyclic permutation.

In a similar way Eqs. (2.3), (2.9), and (2.13) lead to

$$\begin{aligned}C[Q_5Q_3Q_1Q_2^\dagger Q_4^\dagger Q_6^\dagger]=-\tfrac{1}{2}\{&\mathrm{tr}(Z_1Z_2Z_3Z_4Z_5Z_6)+\mathrm{tr}(Z_1Z_2Z_3Z_6Z_5Z_4)+\mathrm{tr}(Z_1Z_4Z_3Z_6Z_5Z_2)\\&+\mathrm{tr}(Z_1Z_4Z_3Z_2Z_5Z_6)+\mathrm{tr}(Z_1Z_6Z_3Z_2Z_5Z_4)+\mathrm{tr}(Z_1Z_6Z_3Z_4Z_5Z_2)\\&+\mathrm{tr}(Z_1Z_6Z_5Z_4Z_3Z_2)+\mathrm{tr}(Z_1Z_4Z_5Z_6Z_3Z_2)+\mathrm{tr}(Z_1Z_2Z_5Z_6Z_3Z_4)\\&+\mathrm{tr}(Z_1Z_6Z_5Z_2Z_3Z_4)+\mathrm{tr}(Z_1Z_4Z_5Z_2Z_3Z_6)+\mathrm{tr}(Z_1Z_2Z_5Z_4Z_3Z_6)\}\ .\end{aligned} \tag{2.14}$$

If P is one of the $p!$ permutations of the even indices $2,4,6,\ldots,2p$ and R_1 is one of the $(p-1)!$ permutations of the odd indices $3,5,\ldots,2p-1$, we can give the recipe to calculate *explicitly* the contraction of $2p$ operators *defined in recursion formula* (2.12)

$$\begin{aligned}C_{2p}&=C[Q_{2p-1}\cdots Q_3Q_1Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger]\\&=-\tfrac{1}{2}\sum_{P,R_1}\mathrm{tr}(Z_1Z_{P(2)}Z_{R_1(3)}Z_{P(4)}\cdots Z_{R_1(2p-1)}Z_{P(2p)})\ .\end{aligned} \tag{2.15}$$

Equations (2.4), (2.13), and (2.14) show that this recipe works for $p=1$, 2, and 3. Let us prove it by induction.

In relation (2.15), the index 1 plays a peculiar role and we prefer to write this equation in a way where all odd indices are treated on an equal footing. Therefore, we introduce the $p!$ permutations R of the odd indices $1,3,\ldots, 2p-1$ and consider

$$S=\sum_{P,R} \mathrm{tr}(Z_{R(1)}Z_{P(2)}Z_{R(3)}\cdots Z_{R(2p-1)}Z_{P(2p)}) \; . \tag{2.16}$$

Using the property that under a trace one can always perform a cyclic permutation one can for each permutation R bring the matrix $Z_1=Z_{R(2i-1)}$ in front of the product. Since there are p odd indices, it is then easy to see that

$$S=p\sum_{P,R_1} \mathrm{tr}(Z_1Z_{P(2)}Z_{R_1(3)}\cdots Z_{R_1(2p-1)}Z_{P(2p)}) \; .$$

Hence the contraction of $2p$ operators also writes

$$C[Q_{2p-1}\cdots Q_3Q_1Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger]=-\frac{1}{2p}\sum_{P,R} \mathrm{tr}(Z_{R(1)}Z_{P(2)}Z_{R(3)}\cdots Z_{R(2p-1)}Z_{P(2p)}) \; . \tag{2.17}$$

From (2.17) we see that one can choose any of the Z_i to play the particular role attributed previously to Z_1. The proof of the recipe is now made by induction.

By definition, we have

$$\begin{aligned} C_{2p+2}&=C[Q_{2p+1}Q_{2p-1}\cdots Q_3Q_1Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger Q_{2p+2}^\dagger] \\ &=\sum_{i<j} C[Q_{2p+1}Q_{2p-1}\cdots Q_3Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger Q_{2p+2}^\dagger \widetilde{Q}^\dagger_{1;2i,2j}] \; . \end{aligned} \tag{2.18}$$

In the term being summed, $Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger Q_{2p+2}^\dagger$ is a sequence of $Q^\dagger$ where $Q_{2i}^\dagger$ and $Q_{2j}^\dagger$ are missing. We apply the recipe for $2p$ contractions, bearing in mind that the matrix related to $\widetilde{Q}^\dagger_{1;2i,2j}$ is

$$\widetilde{Z}_{1;2i,2j}=Z_{2i}Z_1Z_{2j}+Z_{2j}Z_1Z_{2i}$$

and yield successively

$$C_{2p+2}=-\tfrac{1}{2}\sum_{i<j}\sum_{P,R_1} \mathrm{tr}(Z_{R_1(3)}Z_{P(2)}Z_{R_1(5)}\cdots Z_{P(2p+2)}Z_{R_1(2p+1)}\widetilde{Z}_{1;2i,2j}) \tag{2.19}$$

$$\begin{aligned} &=-\tfrac{1}{2}\sum_{i<j}\sum_{P_{ij}R_1} \{\mathrm{tr}(Z_1Z_{2i}Z_{R_1(3)}Z_{P_{ij}(2)}\cdots Z_{P_{ij}(2p+2)}Z_{R_1(2p+1)}Z_{2j}) \\ &\qquad\qquad +\mathrm{tr}(Z_1Z_{2j}Z_{R_1(3)}Z_{P_{ij}(2)}\cdots Z_{P_{ij}(2p+2)}Z_{R_1(2p+1)}Z_{2i})\} \end{aligned} \tag{2.20}$$

$$=-\tfrac{1}{2}\sum_{R_1}\sum_{ij}\sum_{P_{ij}} \mathrm{tr}(Z_1Z_{2j}Z_{R_1(3)}Z_{P_{ij}(2)}\cdots Z_{P_{ij}(2p+2)}Z_{R_1(2p+1)}Z_{2i}) \; , \tag{2.21}$$

where R_1 now labels one of the $p!$ permutations of the odd indices $3,5,\ldots,2p+1$ and P_{ij} one of the $(p-1)!$ permutations of the even indices $2,4,\ldots,2p+2$ where $2i$ and $2j$ are missing. In Eq. (2.19) we have applied the recipe for a contraction of $2p$ operators where $\widetilde{Z}$ plays the predominant role, in Eq. (2.20) we have brought Z_1 in front of the products, and in Eq. (2.21) we have suppressed the restriction $i<j$. Finally, we note that $\sum_{i,j}\sum_{P_{ij}}$ represents simply the summation over all permutations P of the even indices $2,4,\ldots,2p+2$ so that the searched contraction C_{2p+2} writes

$$C_{2p+2}=-\tfrac{1}{2}\sum_{R_1}\sum_{P} \mathrm{tr}(Z_1Z_{P(2)}Z_{R_1(3)}\cdots Z_{R_1(2p+1)}Z_{P(2p+2)}) \; , \tag{2.22}$$

which achieves the proof of the recipe.

We would like to add here the following comments:

The summation in (2.15) contains $p!(p-1)!$ terms. This number can be reduced by a factor of 2 since, according to the antisymmetry properties of matrices Z, one has

$$\mathrm{tr}(Z_1Z_2\cdots Z_{2p-1}Z_{2p})=\mathrm{tr}(Z_{2p}Z_{2p-1}\cdots Z_2Z_1) \; .$$

Despite this reduction one sees that this number increases quite rapidly with p, which leads to an obvious limitation of practical applications of the generalized Wick's theorem. We emphasize, however, the fact that this limitation is far beyond that one had had by direct use of the Wick's theorem for fermions.

We also emphasize the fact that Eq. (2.17) simply translates the commutation properties of the products of the creation or annihilation operators of phonons, namely

$$C[Q_{R(2p-1)}\cdots Q_{R(3)}Q_{R(1)}Q^{\dagger}_{P(2)}Q^{\dagger}_{P(4)}\cdots Q^{\dagger}_{P(2p)}]=C[Q_{2p-1}\cdots Q_3Q_1Q^{\dagger}_2Q^{\dagger}_4\cdots Q^{\dagger}_{2p}]$$

for every P and R, which were not at all evident from the original definition (2.12).

Let us now come back to the proof of the generalized Wick's theorem. Here too, we proceed by induction. We first reformulate the theorem for $2p$ operators in a more mathematical way. We introduce the partitions

$$\{p_1,p_2,\ldots,p_k\}$$

of the integer p so that

$$p=p_1+p_2+\cdots+p_k\ ,$$

where

$$p_1\le p_2\le p_3\le\cdots p_k\ .$$

The Wick's theorem for p can be written

$$\begin{aligned}\langle Q_{2p-1}\cdots Q_3Q_1Q^{\dagger}_2Q^{\dagger}_4\cdots Q^{\dagger}_{2p}\rangle=&\sum_{\{p_1,p_2,\ldots,p_k\}}\sum_{P,R}C[Q_{R(2p_1-1)}\cdots Q_{R(3)}Q_{R(1)}Q^{\dagger}_{P(2)}\cdots Q_{P(2p_1)}]\\ &\times C[Q_{R(2p_1+2p_2-1)}\cdots Q_{R(2p_1+1)}Q^{\dagger}_{P(2p_1+2)}\cdots Q^{\dagger}_{P(2p_1+2p_2)}]\\ &\times\cdots C[Q_{R(2p-1)}\cdots Q_{R(2p-2p_k+1)}Q_{P(2p-2p_k+2)}\cdots Q^{\dagger}_{P(2p)}]\ ,\end{aligned}\tag{2.23}$$

where the sum over the permutations P of even and R of odd indices runs over *all formally different contractions.*

We assume that the theorem is true for p and calculate (as we have done for the first values of p)

$$\begin{aligned}\langle Q_{2p+1}\cdots Q_3Q_1Q^{\dagger}_2\cdots Q^{\dagger}_{2p+2}\rangle=&\sum_{i=1}^{p+1}C[Q_1Q^{\dagger}_{2i}]\langle Q_{2p+1}\cdots Q_3Q^{\dagger}_2\cdots Q^{\dagger}_{2p+2}\rangle\\ &+\sum_{i<j}\langle Q_{2p+1}\cdots Q_3\tilde{Q}^{\dagger}_{1;2i,2j}Q^{\dagger}_2\cdots Q^{\dagger}_{2p+2}\rangle\ .\end{aligned}\tag{2.24}$$

In the first sum, $Q^{\dagger}_2\cdots Q^{\dagger}_{2p+2}$ is a product of $Q^{\dagger}$ where $Q^{\dagger}_{2i}$ is missing and, in the second sum, where $Q^{\dagger}_{2i}$ and $Q^{\dagger}_{2j}$ are missing.

In these two terms, respectively referred to as A and B, overlaps of p operators arise for which one can apply the Wick's theorem. We shall show that any product of contractions corresponding to a given partition of $(p+1)$ will appear once, and only once, in terms either A or B.

Since term A necessarily contains a product of at least two contractions it is obvious that the total contraction C_{2p+2} arises necessarily from part B, with total contraction of the $2p$ operators involved.

$$\begin{aligned}C_{2p+2}&=C[Q_{2p+1}\cdots Q_3Q_1Q^{\dagger}_2Q^{\dagger}_4\cdots Q^{\dagger}_{2p+2}]\\ &=\sum_{i<j}C[Q_{2p+1}\cdots Q_3\tilde{Q}^{\dagger}_{1;2i,2j}Q^{\dagger}_2\cdots Q^{\dagger}_{2p+2}]\ .\end{aligned}$$

Here, $Q^{\dagger}_2\cdots Q^{\dagger}_{2p+2}$ is a sequence where $Q^{\dagger}_{2i}$ and $Q^{\dagger}_{2j}$ are missing which is coherent with our definition (2.12). That way showed C_{2p+2} arises once, and only once, in (2.24).

Let us now consider the partitions of $p+1$ where $p_1=1$. Among these there are those where Q_1 appears in a contraction of two operators $C[Q_1Q_{2l}^\dagger]$ and those where Q_1 does not appear in such a contraction. Products of contractions containing the factor $C[Q_1Q_{2i}^\dagger]$ cannot arise from B terms, since according to the presence of index 1 in $\widetilde{Q}_{1;2i,2j}^\dagger$ the lowest possible contraction is

$$C[Q_{2k+1}\widetilde{Q}_{1;2i,2j}^\dagger]=C[Q_{2k+1}Q_1Q_{2i}^\dagger Q_{2j}^\dagger]\ .$$

We consider a general product of contractions containing a factor $Q_1Q_{2l}^\dagger$, e.g.,

$$C[Q_1Q_{2l}^\dagger]C[Q\cdots Q^\dagger] \\ C[Q\cdots Q^\dagger]\cdots C[Q\cdots Q^\dagger]\ . \quad (2.25)$$

The product of contractions in the factor of $C[Q_1Q_{2l}^\dagger]$ appears in a given partition of integer p. It is evident that the term (2.25) appears in part A of (2.24) for $i=l$

$$C[Q_1Q_{2l}^\dagger]\langle Q_{2p+1}\cdots Q_3Q_2^\dagger\cdots Q_{2p+2}^\dagger\rangle\ . \quad (2.26)$$

$Q_2^\dagger\cdots Q_{2p+2}^\dagger$ is a product where $Q_{2l}^\dagger$ is missing. Furthermore, its unicity is ensured since a given product of contractions in a given partition of p appears once, and only once, in the product of contractions obtained by applying the Wick's theorem for p phonons in the factor of $C[Q_1Q_{2l}^\dagger]$ in Eq. (2.26). With the terms of type (2.25) we exhaust part A of (2.24).

Let us now look for a product of contractions corresponding to a given partition of $(p+1)$ where Q_1 does not appear in a contraction of two operators, but in contraction C of, say, $2p_l$ operators, which we can always relabel with indices

$$\begin{aligned} &P(2),P(4)\cdots P(2p_l);\\ &R(1)=1,R(3)\cdots R(2p_l-1)\ . \end{aligned} \quad (2.27)$$

The factor F of this contraction corresponds to a given partition of $(p+1-p_l)$ where the operators are labeled by the "complementary" indices, i.e., all indices different from those involved in (2.27).

Let us look for such a term among the contribution of sum B, where we apply the Wick's theorem for p and the definition (2.12), thereby ensuring the existence and the unicity of each product of contractions corresponding to each partition.

The sought contraction C, involving Q_1, will appear once and only once in the set of all different contractions of $2p_l-2$ operators where one of the $Q^\dagger$ has been replaced by $\widetilde{Q}_{1;2i,2j}^\dagger$, where the odd indices are $R(3),R(5),\ldots,R(2p_l-1)$, and where the even ones are

$$P(2),P(4),\ldots,\\ P(2m)=i,\ldots,P(2n)=j,\ldots,P(2p_l)$$

with $m<n\le p_l$. Its factor F, will appear too, and only once, among the products of contractions involving the partitions of $(p+1-p_l)$ and the complementary indices, thereby proving the theorem. At this point, we would like to emphasize that in the application of (2.23) one must first formally write all terms of the sum considering all phonons as different and do the regroupings and simplifications due to the appearance of identical and/or orthogonal phonons afterwards. (This procedure is, in fact, similar to that used in the application of the usual Wick's theorem for fermions.)

We need now to show that this Wick's theorem also allows us to calculate in a rather easy way the matrix elements of any operator T containing one and two body parts. As usual we express T in terms of normal ordered quasiparticles.

$$T=T_{00}+T_{11}+T_{20}+T_{40}+T_{31}+T_{22}\ ,$$

where the indices ij of T_{ij} indicate the number of creation and annihilation quasiparticle operators. The part T_{00} leads simply to an overlap matrix. The contribution of

$$T_{11}=\sum_{\mu\nu}(t_{11})_{\mu\nu}\alpha_\mu^\dagger\alpha_\nu$$

can be brought to the application of the new Wick's theorem after one commutation. Indeed

$$\langle Q_{2p-1}\cdots Q_3Q_1T_{11}Q_2^\dagger Q_4^\dagger\cdots Q_{2p}^\dagger\rangle=\sum_{i=1}^{p}\langle Q_{2p-1}\cdots Q_3Q_1[T_{11},Q_{2i}^\dagger]Q_2^\dagger\cdots Q_{2p}^\dagger\rangle\ ,$$

where in the product $Q_2^\dagger\cdots Q_{2p}^\dagger,Q_{2i}^\dagger$ is missing. We note that

$$[T_{11},Q_{2i}^\dagger]$$

behaves like a new phonon

$$\widetilde{Q}_{2i}^\dagger=\tfrac{1}{2}\sum(\widetilde{Z}_i)_{\mu\nu}\alpha_\mu^\dagger\alpha_\nu^\dagger\ ,$$

where

$$(\widetilde{Z}_i)_{\mu\nu}=(tZ_i-Z_it)_{\mu\nu}\ .$$

It is evident that the T_{20} and T_{40} can be treated directly, while T_{31} needs one commutation similarly to T_{11}. Finally T_{22} needs, as can be seen from Eq. (2.1), two commutations.

III. RECURSION FORMULAS

In this section we analyze the previous problem in a completely different way. First of all, we rewrite the basic states

$$Q_2^\dagger Q_4^\dagger \cdots Q_{2p}^\dagger \mid \rangle$$

by grouping together all phonons of the same kind; this is especially suited when the phonons are of some collective nature as will be assumed hereafter. This is always possible since

$$[Q_i^\dagger, Q_j^\dagger]=0 .$$

The same thing is made for the bra vector

$$\langle \mid Q_{2p-1} \cdots Q_3 Q_1 .$$

There are r different types of phonons appearing in both $Q_2^\dagger Q_4^\dagger \cdots Q_{2p}^\dagger$ and $Q_{2p-1} \cdots Q_3 Q_1$. They are denoted once for all, after a relabeling of the indices, $Q_1^\dagger, Q_2^\dagger, \ldots, Q_r^\dagger$. Thus, the previous problem is now fully equivalent to the calculation of the quantity

$$N(k_1',k_2',\ldots,k_r';k_1,k_2,\ldots,k_r)=\langle Q_r^{k_r'} \cdots Q_2^{k_2'} Q_1^{k_1'} Q_1^{\dagger^{k_1}} Q_2^{\dagger^{k_2}} \cdots Q_r^{\dagger^{k_r}} \rangle \tag{3.1}$$

with

$$k_1+k_2+\cdots+k_r=k_1'+k_2'+\cdots k_r'=p .$$

Some of the k_i (or k_i') may be zero if the i phonon is absent from the ket (or bra) state but present in the bra (or ket) state.

To calculate (3.1) another quantity

$$A_{\mu\nu}^{(20)}(k_1',k_2',\ldots,k_r';k_1,k_2,\ldots,k_r)=\langle Q_r^{k_r'} \cdots Q_2^{k_2'} Q_1^{k_1'} \alpha_\mu^\dagger \alpha_\nu^\dagger Q_1^{\dagger^{k_1}} Q_2^{\dagger^{k_2}} \cdots Q_r^{\dagger^{k_r}} \rangle \tag{3.2}$$

is needed. The index (20) means that it appears in the calculation of matrix elements of T_{20}.

The indices μ,ν refer to the quasiparticle excitations $\alpha_\mu^\dagger \alpha_\nu^\dagger$ and parameters $k_1,k_2,\ldots,k_r$ (and $k_1',k_2',\ldots,k_r'$) stand for the number of phonons $Q_1^\dagger,Q_2^\dagger,\ldots,Q_r^\dagger$ in the ket (bra) vector. In order to clear up the formulas as much as possible the index (20) and the parameters k_i are omitted hereafter except when some confusion may arise. In particular, in writing the equations, we indicate only the parameters k_i submitted to some changes. Since the phonons are made of two quasiparticle excitations it is obvious from (3.2) that

$$A_{\mu\nu}^{(20)}(k_1'k_2',\ldots,k_r';k_1,k_2,\ldots,k_r)=0$$

if

$$k_1'+k_2'+\cdots+k_r' \neq k_1+k_2+\cdots+k_r+1 , \tag{3.3}$$

$$A_{\mu\nu}^{(20)}=-A_{\nu\mu}^{(20)} .$$

The quantity N is related to the quantity $A_{\mu\nu}^{(20)}$ by means of the phonon definition.

$$N(k_n';k_n)=\frac{1}{2}\sum_{\mu\nu}(Z_n)_{\mu\nu}A_{\mu\nu}^{(20)}(k_n';k_n-1) \tag{3.4}$$

for every n. In the following, it will be convenient to consider $A_{\mu\nu}$ as the matrix elements of a matrix A. Hence Eq. (3.4) can be written in a more compact form

$$N(k_n';k_n)=-\frac{1}{2}\mathrm{tr}[Z_n A^{(20)}(k_n';k_n-1)] \tag{3.5}$$

for every n.

Starting from (3.2) we move $\alpha_\mu^\dagger \alpha_\nu^\dagger$ to the left by introducing the commutator $[Q_i,\alpha_\mu^\dagger \alpha_\nu^\dagger]$ with each type of phonon; finally the last term contains the bra $\langle \mid \alpha_\mu^\dagger \alpha_\nu^\dagger$ which vanishes.

Thus

$$A_{\mu\nu}=\sum_{n=1}^{r}\sum_{i=0}^{k_n'-1} J_{\mu\nu}^{ni} \tag{3.6}$$

with

$$J_{\mu\nu}^{ni}=\langle Q_r^{k_r'} \cdots Q_{n+1}^{k_{n+1}'} Q_n^i [Q_n,\alpha_\mu^\dagger \alpha_\nu^\dagger] Q_n^{k_n'-i-1} \cdots Q_1^{k_1'} Q_1^{\dagger^{k_1}} \cdots Q_r^{\dagger^{k_r}} \rangle . \tag{3.7}$$

A recursion formula for $J_{\mu\nu}^{ni}$ is obtained by commuting $[Q_n,\alpha_\mu^\dagger \alpha_\nu^\dagger]$ with Q_n

$$J_{\mu\nu}^{ni}=J_{\mu\nu}^{n(i-1)}+K_{\mu\nu}^{nn} \tag{3.8}$$

and with

$$K_{\mu\nu}^{nn}=\langle [Q_n,[Q_n,\alpha_\mu^\dagger\alpha_\nu^\dagger]]Q_r^{k_r'}\cdots Q_n^{k_n'-2}\cdots Q_1^{k_1'}Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}\rangle , \tag{3.9}$$

where

$$[Q_n,[Q_n,\alpha_\mu^\dagger\alpha_\nu^\dagger]] ,$$

which commutes with all Q_j, has been moved to the left to act directly on the bra $\langle\ |$. Hence, $K_{\mu\nu}^{nn}$ is independent of i. From Eq. (3.8) $J_{\mu\nu}^{ni}$ can easily be calculated

$$J_{\mu\nu}^{ni}=\begin{bmatrix} i \\ 0 \end{bmatrix} J_{\mu\nu}^{n0}+\begin{bmatrix} i \\ 1 \end{bmatrix} K_{\mu\nu}^{nn} , \tag{3.10}$$

where

$$\begin{bmatrix} i \\ p \end{bmatrix}$$

are the usual binomial coefficients. Performing the summation over i [in (3.6)] and using relations (3.10) and

$$\sum_{i=p}^{k}\begin{bmatrix} i \\ p \end{bmatrix}=\begin{bmatrix} k+1 \\ p+1 \end{bmatrix}$$

one finds

$$A_{\mu\nu}=\sum_{n=1}^{r}\left[\begin{bmatrix} k_n' \\ 1 \end{bmatrix} J_{\mu\nu}^{n0}+\begin{bmatrix} k_n' \\ 2 \end{bmatrix} K_{\mu\nu}^{nn}\right] . \tag{3.11}$$

Moving the operator $[Q_n,\alpha_\mu^\dagger\alpha_\nu^\dagger]$ in the definition of $J_{\mu\nu}^{n0}$ to the left until it acts on the bra $\langle\ |$ leads to

$$J_{\mu\nu}^{n0}=\sum_{n'=n+1}^{r}\sum_{i=0}^{k_{n'}'-1}K_{\mu\nu}^{nn'}+L_{\mu\nu}^{n} \tag{3.12}$$

with

$$\begin{aligned} K_{\mu\nu}^{nn'} &=\langle 0|[Q_{n'},[Q_n,\alpha_\mu^\dagger\alpha_\nu^\dagger]]Q_r^{k_r'}\cdots Q_{n'}^{k_{n'}'-1}\cdots Q_n^{k_n'-1}\cdots Q_1^{k_1'}Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}|0\rangle , \\ L_{\mu\nu}^{n} &=\langle 0|[Q_n,\alpha_\mu^\dagger\alpha_\nu^\dagger]Q_r^{k_r'}\cdots Q_n^{k_n'-1}\cdots Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}|0\rangle . \end{aligned} \tag{3.13}$$

Inserting (3.12) in (3.11) one gets

$$A_{\mu\nu}=\sum_{n=1}^{r}\begin{bmatrix} k_n' \\ 1 \end{bmatrix} L_{\mu\nu}^{n}+\sum_{n=1}^{r}\begin{bmatrix} k_n' \\ 2 \end{bmatrix} K_{\mu\nu}^{nn}+\sum_{n=1}^{r}\sum_{n'=n+1}^{r}\begin{bmatrix} k_n' \\ 1 \end{bmatrix}\begin{bmatrix} k_{n'}' \\ 1 \end{bmatrix} K_{\mu\nu}^{nn'} . \tag{3.14}$$

It remains to calculate the quantities K and L.

Using Eq. (2.1) one deduces

$$[Q_{n'},[Q_n,\alpha_\mu^\dagger\alpha_\nu^\dagger]]=\sum_{\mu',\nu'}[(Z_{n'})_{\mu\nu'}(Z_n)_{\nu\mu'}+(Z_{n'})_{\nu\nu'}(Z_n)_{\mu'\mu}]\alpha_{\nu'}\alpha_{\mu'} \tag{3.15}$$

and then

$$\begin{aligned} L_{\mu\nu}^{n} &=(Z_n)_{\mu\nu}N(k_n'-1;k_n) , \\ K_{\mu\nu}^{nn'} &=\sum_{\mu',\nu'}[(Z_{n'})_{\mu\nu'}(Z_n)_{\nu\mu'}+(Z_n)_{\mu\mu'}(Z_{n'})_{\nu'\nu}]A_{\mu'\nu'}(k;k_n'-1,k_{n'}'-1) . \end{aligned} \tag{3.16}$$

Thus $A_{\mu\nu}$ can be written in matrix notation

$$\begin{aligned} A^{(20)}(k_n',k_{n'}';k_n,k_{n'})= &\sum_{n=1}^{r}\begin{bmatrix} k_n' \\ 1 \end{bmatrix} N(k_n'-1;k_n)Z_n+\sum_{n=1}^{r}2\begin{bmatrix} k_n' \\ 2 \end{bmatrix} Z_nA^{(20)}(k_n;k_n'-2)Z_n \\ &+\sum_{n=1}^{r}\sum_{n'=n+1}^{r}\begin{bmatrix} k_n' \\ 1 \end{bmatrix}\begin{bmatrix} k_{n'}' \\ 1 \end{bmatrix}[Z_nA^{(20)}(k_n,k_{n'};k_n'-1,k_{n'}'-1)Z_{n'} \\ &+Z_{n'}A^{(20)}(k_n,k_{n'};k_n'-1,k_{n'}'-1)Z_n] . \end{aligned} \tag{3.17}$$

In order to simplify the formulas we define reduced quantities $\mathcal{N}$ and $\mathcal{A}^{(20)}$ by dividing the quantities N and $A^{(20)}$ defined in (3.1) and (3.2) by

$k_1!k_2! \cdots k_r!k_1'k_2'! \cdots k_r'!$.

Furthermore, we gather the two last terms of (3.17) in one. Then Eqs. (3.4) and (3.17) become

$$k_n\mathcal{N}(k_n';k_n) = -\tfrac{1}{2}\,\mathrm{tr}[Z_n\mathscr{A}^{(20)}(k_n';k_n-1)] \tag{3.18}$$

for every n.

$$\mathscr{A}^{(20)}(k_n',k_{n'}';k_n,k_{n'}) = \sum_{n=1}^{r}\mathcal{N}(k_n'-1;k_n)Z_n + \frac{1}{2!}\sum_{n,n'}[Z_n\mathscr{A}^{(20)}(k_n,k_{n'};k_n'-1,k_{n'}'-1)Z_{n'} + Z_{n'}\mathscr{A}^{(20)}(k_n,k_{n'};k_n'-1,k_{n'}'-1)Z_n] \; . \tag{3.19}$$

The second term in (3.19) reflects the effect of the Pauli principle; if $n = n'$ then

$$\mathscr{A}^{(20)}(k_n,k_{n'};k_n'-1,k_{n'}'-1)$$

must be understood as

$$\mathscr{A}^{(20)}(k_n;k_n'-2) \; .$$

Basically the two previous equations are coupled recursion relations: The recursion acts on the total number $p+p'$ of phonons; they are coupled since $\mathscr{A}^{(20)}$ is a function of $\mathcal{N}$ and $\mathcal{N}$ is a function of $\mathscr{A}^{(20)}$. Once the matrix $\mathscr{A}^{(20)}$ is calculated, the matrix elements of the T_{11} part of any operator T are easily determined. Defining in a similar way as in (3.2) the matrix $A^{(11)}$:

$$A_{\mu\nu}^{(11)}(k_1',k_2',\ldots,k_r';k_1,k_2,\ldots,k_r) = \langle Q_r^{k_r'} \cdots Q_2^{k_2'}Q_1^{k_1'}\alpha_\mu^\dagger\alpha_\nu Q_1^{\dagger k_1}Q_2^{\dagger k_2} \cdots Q_r^{\dagger k_r}\rangle \tag{3.20}$$

and using Eq. (2.1) one gets

$$A^{(11)}(k_n';k_n) = -\sum_{n=1}^{r}\begin{bmatrix}k_n\\1\end{bmatrix}[A^{(20)}(k_n';k_n-1)Z_n] \; . \tag{3.21}$$

Introducing again the reduced quantity $\mathscr{A}^{(11)}$ by dividing $A^{(11)}$ by the product of all the factorials k_i,k_i' yields

$$\mathscr{A}^{(11)}(k_n';k_n) = -\sum_{n=1}^{r}[\mathscr{A}^{(20)}(k_n';k_n-1)Z_n] \; . \tag{3.22}$$

If, instead of using $[\alpha^\dagger\alpha,Q^\dagger]$ we use $[Q,\alpha^\dagger\alpha]$, we get an equivalent formulation

$$\mathscr{A}^{(11)}(k_n';k_n) = -\sum_{n=1}^{r}[Z_n\mathscr{A}^{(20)}(k_n;k_n'-1)] \; . \tag{3.23}$$

The formalism concerning matrix elements for one body operators and for overlap matrices has been developed in detail. The same philosophy is followed and the same techniques are used for the computation of matrix elements for two body operators T_{40}, T_{31}, and T_{22}. The derivation is much more involved since in that case we need to commute four phonon operators Q with $\alpha^\dagger\alpha^\dagger\alpha^\dagger\alpha^\dagger$ to get something which commutes with Q. Nevertheless, the demonstration is straightforward, although lengthy; here only the basic relations are quoted.

Let us define the quantity

$$\mathscr{A}_{\mu\nu\rho\sigma}^{(40)}(k_1',\ldots,k_r';k_1,\ldots,k_r) = \frac{\langle Q_r^{k_r'} \cdots Q_1^{k_1'}\alpha_\mu^\dagger\alpha_\nu^\dagger\alpha_\rho^\dagger\alpha_\sigma^\dagger Q_1^{\dagger k_1} \cdots Q_r^{\dagger k_r}\rangle}{k_1'! \cdots k_r'!k_1! \cdots k_r!} \; . \tag{3.24}$$

It vanishes if

$$k_1' + \cdots + k_r' \neq k_1 + \cdots k_r + 2 \; .$$

If $\mathscr{P}_{\mu\nu\rho\sigma}$ is any permutation on the indices μ,ν,ρ,σ, the symmetry properties of $\alpha_\mu^\dagger\alpha_\nu^\dagger\alpha_\rho^\dagger\alpha_\sigma^\dagger$ hold also for $\mathscr{A}_{\mu\nu\rho\sigma}^{(40)}$. More precisely one has

$$\mathscr{P}_{\mu\nu\rho\sigma}\mathscr{A}^{(40)}_{\mu\nu\rho\sigma}=(-1)^{\mathscr{P}}\mathscr{A}^{(40)}_{\mu\nu\rho\sigma}\,, \tag{3.25}$$

where $(-1)^{\mathscr{P}}$ is the signature of the permutation. To evaluate $\mathscr{A}^{(40)}$ we need the following commutators:

$$[Q_{n_2},[Q_{n_1},\alpha^\dagger_\mu\alpha^\dagger_\nu\alpha^\dagger_\rho\alpha^\dagger_\sigma]]=E^{(n_1n_2)}_{\mu\nu\rho\sigma}+\text{terms }\alpha^\dagger\alpha+\text{terms }\alpha^\dagger\alpha^\dagger\alpha\alpha\,, \tag{3.26}$$

with

$$E^{(n_1n_2)}_{\mu\nu\rho\sigma}=\tfrac{1}{4}\sum_{\mathscr{P}}(-1)^{\mathscr{P}}\mathscr{P}_{\mu\nu\rho\sigma}[(Z_{n_1})_{\mu\nu}(Z_{n_2})_{\rho\sigma}]\,, \tag{3.27}$$

as the first commutator.

In fact, the summation in (3.27) contains only six different terms [owing to the antisymmetry for the Z matrices, to each permutation there corresponds 2!2! permutations coming from a transposition in the indices of (Z_{n_1}) and (Z_{n_2}) which give the same result; this remark explains the $\frac{1}{4}$ factor in (3.27)].

Directly from Eq. (3.27) one can check that

$$\begin{aligned}&\mathscr{P}_{\mu\nu\rho\sigma}E^{(n_1n_2)}_{\mu\nu\rho\sigma}=(-1)^{\mathscr{P}}E^{(n_1n_2)}_{\mu\nu\rho\sigma}\,,\\&\mathscr{P}_{n_1n_2}E^{(n_1n_2)}_{\mu\nu\rho\sigma}=E^{(n_1n_2)}_{\mu\nu\rho\sigma}\,.\end{aligned} \tag{3.28}$$

The second commutator

$$[Q_{n_3},[Q_{n_2},[Q_{n_1},\alpha^\dagger_\mu\alpha^\dagger_\nu\alpha^\dagger_\rho\alpha^\dagger_\sigma]]]=\sum_{\mu'\nu'}F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}\alpha_{\nu'}\alpha_{\mu'}+\text{terms }\alpha^\dagger\alpha\alpha\alpha \tag{3.29}$$

with

$$F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}=-\tfrac{1}{4}\sum_{\mathscr{P}'_{n_1n_2n_3}}\sum_{\mathscr{P}_{\mu\nu\rho\sigma}}(-1)^{\mathscr{P}}\mathscr{P}'_{n_1n_2n_3}\mathscr{P}_{\mu\nu\rho\sigma}[(Z_{n_1})_{\mu\mu'}(Z_{n_2})_{\nu\nu'}(Z_{n_3})_{\rho\sigma}]\,. \tag{3.30}$$

The summation in (3.30) contains only 36 different terms due to the fact that the transposition $\rho\sigma$ in (Z_{n_3}) and the triple transposition $(n_1n_2)(\mu\nu)(\mu'\nu')$ give the same result. One can also check that

$$\begin{aligned}&\mathscr{P}_{\mu\nu\rho\sigma}F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}=(-1)^{\mathscr{P}}F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}\,,\\&\mathscr{P}'_{n_1n_2n_3}F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}=F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}\,.\end{aligned} \tag{3.31}$$

The third commutator

$$[Q_{n_4},[Q_{n_3},[Q_{n_2},[Q_{n_1},\alpha^\dagger_\mu\alpha^\dagger_\nu\alpha^\dagger_\rho\alpha^\dagger_\sigma]]]]=\sum_{\mu'\nu'\rho'\sigma'}G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma,\mu'\nu'\rho'\sigma'}\alpha_{\sigma'}\alpha_{\rho'}\alpha_{\nu'}\alpha_{\mu'} \tag{3.32}$$

with

$$\begin{aligned}G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma;\mu'\nu'\rho'\sigma'}&=\sum(-1)^{\mathscr{P}}\mathscr{P}_{\mu\nu\rho\sigma}[(Z_{n_1})_{\mu\mu'}(Z_{n_2})_{\nu\nu'}(Z_{n_3})_{\rho\rho'}(Z_{n_4})_{\sigma\sigma'}]\\&=\sum\mathscr{P}_{n_1n_2n_3n_4}[(Z_{n_1})_{\mu\mu'}(Z_{n_2})_{\nu\nu'}(Z_{n_3})_{\rho\rho'}(Z_{n_4})_{\sigma\sigma'}]\,,\end{aligned} \tag{3.33}$$

which has the following properties:

$$\begin{aligned}&\mathscr{P}_{\mu\nu\rho\sigma}G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma,\mu'\nu'\rho'\sigma'}=(-1)^{\mathscr{P}}G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma,\mu'\nu'\rho'\sigma'}\,,\\&\mathscr{P}_{n_1n_2n_3n_4}G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma,\mu'\nu'\rho'\sigma'}=G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma,\mu'\nu'\rho'\sigma'}\,.\end{aligned} \tag{3.34}$$

The recursion formula for $\mathscr{A}^{(40)}$ now reads

$$\mathscr{A}^{(40)}_{\mu\nu\rho\sigma}(k'_1,\ldots,k'_r;k_1,\ldots,k_r)=\frac{1}{2!}\sum_{n_1n_2}\mathscr{N}(k_1,\ldots,k_r;k'_1,\ldots,k'_{n_1}-1,\ldots,k'_{n_2}-1,\ldots,k'_r)E^{(n_1n_2)}_{\mu\nu\rho\sigma}$$

$$+\frac{1}{3!}\sum_{n_1n_2n_3}\sum_{\mu'\nu'}F^{(n_1n_2n_3)}_{\mu\nu\rho\sigma,\mu'\nu'}\mathscr{A}^{(20)}_{\mu'\nu'}(k_1,\ldots,k_r;k'_1,\ldots,k'_{n_1}-1,\ldots,k'_{n_2}-1,\ldots,k'_{n_3}-1,\ldots,k'_r)$$
$$+\frac{1}{4!}\sum_{n_1n_2n_3n_4}\sum_{\mu'\nu'\rho'\sigma'}G^{(n_1n_2n_3n_4)}_{\mu\nu\rho\sigma,\mu'\nu'\rho'\sigma'}$$
$$\times\mathscr{A}^{(40)}_{\mu'\nu'\rho'\sigma'}(k_1,\ldots,k_r;k'_1,\ldots,k'_{n_1}-1,\ldots,k'_{n_2}-1,\ldots,k'_{n_3}-1,\ldots,k'_{n_4}-1,\ldots,k'_r)\,. \tag{3.35}$$

In this relation, as in the equivalent one (3.19), if l ($l=1,\ldots,4$) phonons n_i are identical the parameters $k'_{n_i}-1$ must be understood as $k'_{n_i}-l$. To calculate the elements $\mathscr{A}^{(40)}_{\mu\nu\rho\sigma}$ for a total number $p+p'$ phonons, one needs the overlap matrix $\mathscr{N}$ for $p+p'-2$, the one body matrix $\mathscr{A}^{(20)}_{\mu\nu}$ for $p+p'-3$, and $\mathscr{A}^{(40)}_{\mu\nu\rho\sigma}$ itself for $p+p'-4$.

The matrix elements of T_{31} and T_{22} of the two body operator are obtained from $\mathscr{A}^{(40)}$ by the following equations:

$$\mathscr{A}^{(31)}_{\mu\nu\rho\sigma}(k'_1,\ldots,k'_r;k_1,\ldots,k_r)=\frac{\langle Q_r^{k'_r}\cdots Q_1^{k'_1}\alpha^\dagger_\mu\alpha^\dagger_\nu\alpha^\dagger_\rho\alpha_\sigma Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}\rangle}{k'_1!\cdots k'_r!k_1!\cdots k_r!}$$
$$=\sum_n\sum_{\sigma'}(Z_n)_{\sigma\sigma'}\mathscr{A}^{(40)}_{\mu\nu\rho\sigma'}(k'_1,\ldots,k'_r;k_1,\ldots,k_n-1,\ldots,k_r)\,, \tag{3.36}$$

$$\mathscr{A}^{(22)}_{\mu\nu\rho\sigma}(k'_1,\ldots,k'_r;k_1,\ldots,k_r)=\frac{\langle Q_r^{k'_r}\cdots Q_1^{k'_1}\alpha^\dagger_\mu\alpha^\dagger_\nu\alpha_\rho\alpha_\sigma Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}\rangle}{k'_1!\cdots k'_r!k_1!\cdots k_r!}$$
$$=\sum_n(Z_n)_{\sigma\rho}\mathscr{A}^{(20)}_{\mu\nu}(k'_1,\ldots,k'_r;k_1,\ldots,k_n-1,\ldots,k_r)$$
$$+\tfrac{1}{2}\sum_{n_1n_2}\sum_{\rho'\sigma'}[(Z_{n_1})_{\sigma\sigma'}(Z_{n_2})_{\rho\rho'}+(Z_{n_1})_{\rho\rho'}(Z_{n_2})_{\sigma\sigma'}]$$
$$\times\mathscr{A}^{(40)}_{\mu\nu\rho'\sigma'}(k'_1,\ldots,k'_r;k_1,\ldots,k_{n_1}-1,\ldots,k_{n_2}-1,\ldots,k_r)\,, \tag{3.37}$$

with the same convention on the parameters as in (3.19) in the case of identical phonons.

The introduction of reduced quantities is useful to write the various equations in a more compact and elegant way. It is equivalent to say that instead of working with basis states

$$Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}|0\rangle\,,$$

we use "reduced" states[5]

$$|k_1\cdots k_r\rangle=\frac{Q_1^{\dagger k_1}\cdots Q_r^{\dagger k_r}|\,\rangle}{k_1!\cdots k_r!}\,;$$

the reduced quantites are now the matrix elements in this reduced basis. Starting from

$$\mathscr{N}(0,0,\ldots,0;0,0,\ldots,0)=1$$

all the recursion formulas given above allow us to calculate overlap matrices and matrix elements for one and two body operators concerning any general multiphonon state $|k_1,\ldots,k_r\rangle$.

IV. ILLUSTRATIVE EXAMPLES

The two methods presented in the previous sections represent two different ways for computing matrix elements in a multiphonon basis. They both take care of the Pauli principle rigorously and give, of course, the same results if no approximation is made. The question now arises as to which one is more suited for a given problem. Even if some phonons are identical the generalized Wick's technique requires performing the treatment as if they were all different, grouping together all identical contractions afterwards. Furthermore, the number of contractions up to a given order increases more or less exponentially with the phonon number. These few remarks explain why, according to us, the Wick's theorem is useful in the case where the multiphonon basis contains *few* phonons, *all of different types.* On the contrary, the recursion formulas ought to be used if the basis contains *several* phonons of the *same* type. The case of a great number of different phonons is difficult independently of the adopted method. From a numerical viewpoint, there are also differences between the two methods. In the Wick's formalism, the algorithm necessary to code all the system of contractions is not very easy but each matrix element of a given order can be computed separately. On the other hand, the use of recursion formulas allows a more elegant numerical formulation but requires the computation of several matrix elements at the same time. In practical cases, one often checks the stability of the results when increasing the basis. The matrix elements of order $p-1$ are then necessary also when one goes to further order p. The recursion formulas ought to be very well suited for such practical problems. Furthermore, with the contraction technique, since each matrix element is calculated separately, the computing time should be rather long but storage considerations are of minor importance whereas the contrary holds for a treatment based on recursion formulas.

Let us now examine two examples which illustrate the use of both methods; in order to keep a maximum of simplicity we focus our attention on overlaps only.

In the first example, only one type of collective phonon is considered and is denoted by $Q^\dagger$. The multiphonon basis is thus the set of vectors

$$\left\{ |k\rangle = \frac{Q^{\dagger k}}{k!}|0\rangle, k=1,\ldots,N \right\} .$$

The overlap matrix is simply the norm matrix

$$\mathcal{N}_k = \mathcal{N}(k,k) = \langle k \mid k \rangle . \tag{4.1}$$

The recursion technique is used in that case and we write $\mathcal{A}_k$ instead of $\mathcal{A}(k,k-1)$. The basic equations (3.18) and (3.19) are expressed here by

$$k\mathcal{N}_k = -\tfrac{1}{2}\mathrm{tr}[Z\mathcal{A}_k] , \tag{4.2}$$

$$\mathcal{A}_k = Z\mathcal{N}_{k-1} + Z\mathcal{A}_{k-1}Z . \tag{4.3}$$

It is possible to "decouple" these equations and to express everything in terms of the reduced norm $\mathcal{N}$; more precisely

$$\mathcal{A}_k = \sum_{l=1}^{k} \mathcal{N}_{k-l}[Z]^{2l-1} , \tag{4.4}$$

$$k\mathcal{N}_k = -\tfrac{1}{2}\sum_{l=1}^{k} \mathcal{N}_{k-l}\mathrm{tr}[Z^{2l}] . \tag{4.5}$$

Starting from $\mathcal{N}_0 = 1$, Eq. (4.5) allows a very easy numerical evaluation of $\mathcal{N}_k$. On the other hand, the replacement in (4.5) of $\mathcal{N}_{k-l}$ by its developed form in terms of $\mathrm{tr}(Z^{2m})$ would give the final expression obtained by use of the Wick's theorem; this expression is not simple at all and one sees in this special case the power of the recursion formulas. Applications of this example were investigated in detail for quadrupole phonons both in an exactly solvable model[4] and in more realistic situations.[3]

The second example deals with the coupling of an octupole $K^\pi = 0^-$ phonon $Q_1^\dagger$ and a quadrupole $K^\pi = 0^+$ phonon $Q_0^\dagger$, a problem of basic importance in the actinide region where the first octupole state lies very low in energy. Here we give only the overlaps for both $K^\pi = 0^+$ and $K^\pi = 0^-$ states up to third phonons by using the Wick's theorem. The phonons $Q_0^\dagger$ and $Q_1^\dagger$ are assumed to be orthonormalized thus

$$\begin{aligned}
&C[Q_0Q_0^\dagger] = -\tfrac{1}{2}\mathrm{tr}(Z_0{}^2) = 1 , \\
&C[Q_1Q_1^\dagger] = -\tfrac{1}{2}\mathrm{tr}(Z_1{}^2) = 1 , \\
&C[Q_0Q_1^\dagger] = C[Q_1Q_0^\dagger] = -\tfrac{1}{2}\mathrm{tr}(Z_0Z_1) = 0 .
\end{aligned} \tag{4.6}$$

Besides (4.6) we need the following contractions:

$$\begin{aligned}
&C[Q_0Q_0Q_0^\dagger Q_0^\dagger] = -\mathrm{tr}(Z_0{}^4) , \\
&C[Q_0Q_0Q_1^\dagger Q_1^\dagger] = -\mathrm{tr}(Z_0Z_1Z_0Z_1) , \\
&C[Q_1Q_1Q_1^\dagger Q_1^\dagger] = -\mathrm{tr}(Z_1{}^4) , \\
&C[Q_1Q_0Q_0^\dagger Q_1^\dagger] = -\mathrm{tr}(Z_0{}^2Z_1{}^2) , \\
&C[Q_0Q_0Q_0Q_0^\dagger Q_0^\dagger Q_0^\dagger] = -6\,\mathrm{tr}(Z_0{}^6) , \\
&C[Q_1Q_1Q_1Q_0^\dagger Q_0^\dagger Q_1^\dagger] = -6\,\mathrm{tr}(Z_1{}^3Z_0Z_1Z_0) , \\
&C[Q_0Q_0Q_0Q_0^\dagger Q_1^\dagger Q_1^\dagger] = -6\,\mathrm{tr}(Z_0{}^3Z_1Z_0Z_1) , \\
&C[Q_1Q_1Q_0Q_0^\dagger Q_1^\dagger Q_1^\dagger] = -2\,\mathrm{tr}(Z_0Z_1{}^2Z_0Z_1{}^2) \\
&\qquad -4\,\mathrm{tr}(Z_0{}^2Z_1{}^4) ,
\end{aligned} \tag{4.7}$$

$$C[Q_1Q_0Q_0Q_0^\dagger Q_0^\dagger Q_1^\dagger]=-2\,\mathrm{tr}(Z_0{}^2Z_1Z_0{}^2Z_1)-4\,\mathrm{tr}(Z_0{}^4Z_1{}^2)\,,$$

$$C[Q_1Q_1Q_1Q_1^\dagger Q_1^\dagger Q_1^\dagger]=-6\,\mathrm{tr}(Z_1{}^6)\,.$$

Concerning $K^\pi=0^+$ states there are six basic states, namely $|\,\rangle$, $Q_0^\dagger|\,\rangle$, $Q_0^{\dagger 2}|\,\rangle$, $Q_1^{\dagger 2}|\,\rangle$, $Q_0^{\dagger 3}|\,\rangle$, and $Q_0^\dagger Q_1^{\dagger 2}|\,\rangle$. Application of the generalized Wick's theorem leads to

$$\begin{aligned}
&\langle\,|\,\rangle=1\,,\\
&\langle Q_0Q_0^\dagger\rangle=C[Q_0Q_0^\dagger]=1\,,\\
&\langle Q_0{}^2Q_0^{\dagger 2}\rangle=2C[Q_0Q_0^\dagger]^2+C[Q_0Q_0Q_0^\dagger Q_0^\dagger]=2-\mathrm{tr}(Z_0{}^4)\,,\\
&\langle Q_0{}^2Q_1^{\dagger 2}\rangle=2C[Q_0Q_1^\dagger]^2+C[Q_0Q_0Q_1^\dagger Q_1^\dagger]=-\mathrm{tr}(Z_0Z_1Z_0Z_1)\,,\\
&\langle Q_1{}^2Q_1^{\dagger 2}\rangle=2C[Q_1Q_1^\dagger]^2+C[Q_1Q_1Q_1^\dagger Q_1^\dagger]=2-\mathrm{tr}(Z_1{}^4)\,,\\
&\langle Q_0{}^3Q_0^{\dagger 3}\rangle=6C[Q_0Q_0^\dagger]^3+9C[Q_0Q_0^\dagger]C[Q_0Q_0Q_0^\dagger Q_0^\dagger]+C[Q_0Q_0Q_0Q_0^\dagger Q_0^\dagger Q_0^\dagger]\\
&\qquad=6-9\,\mathrm{tr}(Z_0{}^4)-6\,\mathrm{tr}(Z_0{}^6)\,,
\end{aligned}\tag{4.8}$$

$$\begin{aligned}
\langle Q_0{}^3Q_0^\dagger Q_1^{\dagger 2}\rangle=\;&6C[Q_0Q_0^\dagger]C[Q_0Q_1^\dagger]^2+3C[Q_0Q_0^\dagger]C[Q_0Q_0Q_1^\dagger Q_1^\dagger]\\
&+6C[Q_0Q_1^\dagger]C[Q_0Q_0Q_0^\dagger Q_1^\dagger]+C[Q_0Q_0Q_0Q_0^\dagger Q_1^\dagger Q_1^\dagger]\\
=\;&-3\,\mathrm{tr}(Z_0Z_1Z_0Z_1)-6\,\mathrm{tr}(Z_0{}^3Z_1Z_0Z_1)\,,
\end{aligned}$$

$$\begin{aligned}
\langle Q_1{}^2Q_0Q_0^\dagger Q_1^{\dagger 2}\rangle=\;&2C[Q_0Q_0^\dagger]C[Q_1Q_1^\dagger]^2+4C[Q_0Q_1^\dagger]C[Q_1Q_0^\dagger]C[Q_1Q_1^\dagger]+C[Q_0Q_0^\dagger]C[Q_1Q_1Q_1^\dagger Q_1^\dagger]\\
&+2C[Q_0Q_1^\dagger]C[Q_1Q_1Q_0^\dagger Q_1^\dagger]+2C[Q_1Q_0^\dagger]C[Q_1Q_0Q_1^\dagger Q_1^\dagger]\\
&+4C[Q_1Q_1^\dagger]C[Q_1Q_0Q_0^\dagger Q_1^\dagger]+C[Q_1Q_1Q_0Q_0^\dagger Q_1^\dagger Q_1^\dagger]\\
=\;&2-\mathrm{tr}(Z_1{}^4)-4\,\mathrm{tr}(Z_0{}^2Z_1{}^2)-2\,\mathrm{tr}(Z_0Z_1{}^2Z_0Z_1{}^2)-4\,\mathrm{tr}(Z_0{}^2Z_1{}^4)\,.
\end{aligned}$$

For the $K^\pi=0^-$ states there are four basis states, namely $Q_1^\dagger|\,\rangle$, $Q_0^\dagger Q_1^\dagger|\,\rangle$, $Q_0^{\dagger 2}Q_1^\dagger|\,\rangle$, $Q_1^{\dagger 3}|\,\rangle$, and

$$\begin{aligned}
&\langle Q_1Q_1^\dagger\rangle=C[Q_1Q_1^\dagger]=1\,,\\
&\langle Q_1Q_0Q_0^\dagger Q_1^\dagger\rangle=C[Q_0Q_0^\dagger]C[Q_1Q_1^\dagger]+C[Q_0Q_1^\dagger]C[Q_1Q_0^\dagger]+C[Q_1Q_0Q_0^\dagger Q_1^\dagger]\\
&\qquad=1-\mathrm{tr}(Z_0{}^2Z_1{}^2)\,,\\
&\langle Q_1Q_0{}^2Q_0^{\dagger 2}Q_1^\dagger\rangle=2C[Q_0Q_0^\dagger]^2C[Q_1Q_1^\dagger]+4C[Q_0Q_1^\dagger]C[Q_1Q_0^\dagger]C[Q_0Q_0^\dagger]+C[Q_1Q_1^\dagger]C[Q_0Q_0Q_0^\dagger Q_0^\dagger]\\
&\qquad+2C[Q_0Q_1^\dagger]C[Q_1Q_0Q_0^\dagger Q_0^\dagger]+2C[Q_1Q_0^\dagger]C[Q_0Q_0Q_0^\dagger Q_1^\dagger]\\
&\qquad+4C[Q_0Q_0^\dagger]C[Q_1Q_0Q_0^\dagger Q_1^\dagger]+C[Q_1Q_0Q_0Q_0^\dagger Q_0^\dagger Q_1^\dagger]\\
&\qquad=2-\mathrm{tr}(Z_0{}^4)-4\,\mathrm{tr}(Z_0{}^2Z_1{}^2)-2\,\mathrm{tr}(Z_0{}^2Z_1Z_0{}^2Z_1)-4\,\mathrm{tr}(Z_0{}^4Z_1{}^2)\,,\\
&\langle Q_1{}^3Q_0^{\dagger 2}Q_1^\dagger\rangle=6C[Q_1Q_1^\dagger]C[Q_1Q_0^\dagger]^2+3C[Q_1Q_1^\dagger]C[Q_1Q_1Q_0^\dagger Q_0^\dagger]\\
&\qquad+6C[Q_1Q_0^\dagger]C[Q_1Q_1Q_0^\dagger Q_1^\dagger]+C[Q_1Q_1Q_1Q_0^\dagger Q_0^\dagger Q_1^\dagger]\\
&\qquad=-3\,\mathrm{tr}(Z_0Z_1Z_0Z_1)-6\,\mathrm{tr}(Z_1{}^3Z_0Z_1Z_0)\,,\\
&\langle Q_1{}^3Q_1^{\dagger 3}\rangle=6C[Q_1Q_1^\dagger]^3+9C[Q_1Q_1^\dagger]C[Q_1Q_1Q_1^\dagger Q_1^\dagger]+C[Q_1Q_1Q_1Q_1^\dagger Q_1^\dagger Q_1^\dagger]\\
&\qquad=6-9\,\mathrm{tr}(Z_1{}^4)-6\,\mathrm{tr}(Z_1{}^6)\,.
\end{aligned}\tag{4.9}$$

It is worthwhile noting that some matrix elements for $K^{\pi}=0^{+}$ states are obtained from contractions of lower order involving $K=0^{-}$ states (and conversely). The study of the coupling between 0^{-} and 0^{+} bands is in progress and more detailed analysis is postponed until future publications.

V. CONCLUSIONS

To properly treat the problem of multiphonon states of different types we have developed two methods which allow us to properly take into account the Pauli principle, thereby being much better than the different available boson expansion techniques.

The first method appears to be a generalization of the Wick's theorem for phonons. It seems especially suited for studying matrix elements of multiphonons states with a few phonons of many different types.

The second one, which is a recursion formulation of the same problem, is more easily handled in the case of numerous phonons of the same type or when only a few types of phonons are involved.

These two methods are complementary, the first one is formally more compact and elegant, the second one more useful for realistic numerical calculations.

Several applications are possible within this formalism: coupling of different vibrational states in deformed nuclei, coupling between collective and noncollective excitations, elimination of the spurious states due to nonconservation of particle number, etc.

In difficult realistic cases where the limitations of these methods may be rapidly reached it is possible to combine the multiphonon method for matrix elements involving few phonons with boson expansion techniques as shown in Ref. 3.

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[5]Note that normalized boson states would be written

$$\frac{B_1^{\dagger k_1} \cdots B_r^{\dagger k_r} |0)}{(k_1! \cdots k_r!)^{1/2}} .$$