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**MULTIPHONON THEORY : GENERALIZED WICK'S THEOREM  
AND RECURSION FORMULAS**

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MULTIPHONON THEORY : GENERALIZED WICK'S THEOREM

AND RECURSION FORMULAS.

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**Abstract** . Overlaps and matrix elements of one and two-body operators are calculated in a space spanned by multiphonons of different types taking properly the Pauli principle 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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Recursion formulas for calculation of overlaps and matrix elements of one and two-body operators. Illustrative examples.

## I. INTRODUCTION.

In atomic nuclei, many excited states show a vibrational nature. To explain the properties of these states phenomenological bosons or "microscopic" quasi-bosons 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, leading 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 quickly inapplicable. To keep advantage of the collective nature of the vibrational states it appears better to introduce new entities: the phonons  $Q_i^\dagger$ , which are defined as a superposition of two quasiparticles

$$Q_i^\dagger = \frac{1}{2} \sum_{\mu\nu} \langle Z_i \rangle_{\mu\nu} \alpha_\mu^\dagger \alpha_\nu^\dagger \quad (1.1)$$

where  $\langle Z_i \rangle_{\mu\nu} = -\langle Z_i \rangle_{\nu\mu}$  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

$$[Q_1, Q_2^\dagger] = -\frac{1}{2} \text{Tr} (Z_1 Z_2) + \sum_{\mu,\nu} \langle Z_1 Z_2 \rangle_{\mu\nu} \alpha_\nu^\dagger \alpha_\mu \quad (1.2)$$

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

a) The boson expansion (BE) technique<sup>1)</sup> aims to come back 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 approximately taken into account and some spurious states may appear (see ref.<sup>3</sup>)).

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

The aim of the present 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

$$\begin{aligned} [\alpha_\nu \alpha_\mu, Q^\dagger] &= z_{\nu\mu} + \sum_\lambda (z_{\nu\lambda} \alpha_\lambda^\dagger \alpha_\mu - z_{\mu\lambda} \alpha_\lambda^\dagger \alpha_\nu) \\ [\alpha_\mu^\dagger \alpha_\nu, Q^\dagger] &= \sum_\lambda z_{\nu\lambda} \alpha_\mu^\dagger \alpha_\lambda^\dagger \end{aligned} \quad (2.1)$$

From these relations one deduces the double commutator

$$[[Q_1, Q_2^\dagger], Q_4^\dagger] = \sum_{\mu, \nu} (Z_4 Z_1 Z_2)_{\mu\nu} \alpha_\mu^\dagger \alpha_\nu^\dagger$$

According to the antisymmetry of the Z matrices one has

$$(Z_4 Z_1 Z_2)_{\mu\nu} = - (Z_2 Z_1 Z_4)_{\nu\mu}$$

which allows us to write

$$[[Q_1, Q_2^\dagger], Q_4^\dagger] = \frac{1}{2} \sum_{\mu, \nu} (Z_2 Z_1 Z_4 + Z_4 Z_1 Z_2)_{\mu\nu} \alpha_\mu^\dagger \alpha_\nu^\dagger \quad (2.2)$$

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

$$\tilde{Z}_{1;2,4} = Z_2 Z_1 Z_4 + Z_4 Z_1 Z_2 \quad (2.3)$$

(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  $| >$  is also the phonon vacuum.

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

$$\langle Q_1 Q_2^\dagger \rangle = \langle [Q_1, Q_2^\dagger] \rangle = -\frac{1}{2} \text{Tr}(Z_1 Z_2) \quad (2.4)$$

We define a "contraction of two operators"

$$\overline{Q_1 Q_2^\dagger} = \langle Q_1 Q_2^\dagger \rangle \quad (2.5)$$

For two phonons, we obtain explicitly

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

and using (2.2,5) we get :

$$\langle Q_3 Q_1 Q_2^\dagger Q_4^\dagger \rangle = \overline{Q_3 Q_2^\dagger} \overline{Q_1 Q_4^\dagger} + \overline{Q_3 Q_4^\dagger} \overline{Q_1 Q_2^\dagger} + \overline{Q_3 \tilde{Q}_{1;2,4}^\dagger}$$

If we define a "contraction of four operators"

$$\overline{Q_3 Q_1 Q_2^\dagger Q_4^\dagger} = \overline{Q_3 \tilde{Q}_{1;2,4}^\dagger} \quad (2.6)$$

we obtain

$$\langle Q_3 Q_1 Q_2^\dagger Q_4^\dagger \rangle = \sum \overline{QQ^\dagger} \overline{QQ^\dagger} + \overline{Q_3 Q_1 Q_2^\dagger Q_4^\dagger} \quad (2.7)$$

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

$$\begin{aligned} \langle Q_5 Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger} \rangle = & \langle Q_5 Q_3 Q_2^{\dagger} Q_4^{\dagger} [Q_1, Q_6^{\dagger}] \rangle + \langle Q_5 Q_3 Q_2^{\dagger} Q_6^{\dagger} [Q_1, Q_4^{\dagger}] \rangle \\ & + \langle Q_5 Q_3 Q_4^{\dagger} Q_6^{\dagger} [Q_1, Q_2^{\dagger}] \rangle + \langle Q_5 Q_3 Q_2^{\dagger} [[Q_1, Q_4^{\dagger}], Q_6^{\dagger}] \rangle \\ & + \langle Q_5 Q_3 Q_4^{\dagger} [[Q_1, Q_2^{\dagger}], Q_6^{\dagger}] \rangle + \langle Q_5 Q_3 Q_6^{\dagger} [[Q_1, Q_2^{\dagger}], Q_4^{\dagger}] \rangle \end{aligned} \quad (2.8)$$

Using relations (2.2-7) and setting

$$\overbrace{Q_5 Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} = \sum_{i \leq j} \overbrace{Q_5 Q_3 Q_{2k}^{\dagger} Q_{1;2i,2j}^{\dagger}} \quad (2.9)$$

for the "contraction of six operators", we get :

$$\begin{aligned} \langle Q_5 Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger} \rangle = & \overbrace{Q_1^{\dagger} Q_2^{\dagger} Q_3^{\dagger} Q_4^{\dagger} Q_5^{\dagger} Q_6^{\dagger}} + \overbrace{Q_1^{\dagger} Q_2^{\dagger} Q_3^{\dagger} Q_6^{\dagger} Q_5^{\dagger} Q_4^{\dagger}} \\ & + \overbrace{Q_1^{\dagger} Q_4^{\dagger} Q_3^{\dagger} Q_2^{\dagger} Q_5^{\dagger} Q_6^{\dagger}} + \overbrace{Q_1^{\dagger} Q_4^{\dagger} Q_3^{\dagger} Q_6^{\dagger} Q_5^{\dagger} Q_2^{\dagger}} \\ & + \overbrace{Q_1^{\dagger} Q_6^{\dagger} Q_3^{\dagger} Q_2^{\dagger} Q_5^{\dagger} Q_4^{\dagger}} + \overbrace{Q_1^{\dagger} Q_6^{\dagger} Q_3^{\dagger} Q_4^{\dagger} Q_5^{\dagger} Q_2^{\dagger}} \\ & + \overbrace{Q_1^{\dagger} Q_2^{\dagger} Q_5^{\dagger} Q_3^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} + \overbrace{Q_1^{\dagger} Q_4^{\dagger} Q_5^{\dagger} Q_3^{\dagger} Q_2^{\dagger} Q_6^{\dagger}} \\ & + \overbrace{Q_1^{\dagger} Q_6^{\dagger} Q_5^{\dagger} Q_3^{\dagger} Q_2^{\dagger} Q_4^{\dagger}} + \overbrace{Q_3^{\dagger} Q_2^{\dagger} Q_5^{\dagger} Q_1^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} \\ & + \overbrace{Q_3^{\dagger} Q_4^{\dagger} Q_5^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_6^{\dagger}} + \overbrace{Q_3^{\dagger} Q_6^{\dagger} Q_5^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_4^{\dagger}} \\ & + \overbrace{Q_5^{\dagger} Q_2^{\dagger} Q_3^{\dagger} Q_1^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} + \overbrace{Q_5^{\dagger} Q_4^{\dagger} Q_3^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_6^{\dagger}} \\ & + \overbrace{Q_5^{\dagger} Q_6^{\dagger} Q_3^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_4^{\dagger}} + \overbrace{Q_5^{\dagger} Q_3^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} \end{aligned} \quad (2.10)$$

This relation can be summarized by

$$\begin{aligned} \langle Q_5 Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger} \rangle = & \sum \overbrace{Q_5^{\dagger} Q_3^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} \\ & + \sum \overbrace{Q_5^{\dagger} Q_3^{\dagger} Q_1^{\dagger} Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} \end{aligned} \quad (2.11)$$

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

Equations (2.5,7 and 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, 6 and 9).

We note that if the Q would have been boson operators only the first term of eqs. (2.5,7 and 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  $|Q_2^\dagger Q_4^\dagger \dots Q_{2p}^\dagger\rangle$  with a state built on p different annihilation operators  $\langle Q_1 Q_3 \dots Q_{2p-1}|$  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

$$\overline{Q_{2p-1} Q_{2p-3} \dots Q_3 Q_1 Q_2^\dagger \dots Q_{2p}^\dagger} = \sum_{i < j} Q_{2p-1} Q_{2p-3} \dots Q_3 \overline{Q_i^\dagger \dots Q_j^\dagger} \tilde{Q}_{1;2i,2j}^\dagger \quad (2.12)$$

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

Eqs.(2.5,7 and 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 before, it is necessary to know how to calculate the involved contractions.

Let us look for the first contractions. From eqs.(2.4-5) one has

$$\overline{Q_1 Q_2^\dagger} = -\frac{1}{2} \text{Tr} (Z_1 Z_2)$$

Further, from eqs(2.3,5-6)we get

$$\begin{aligned} \overline{Q_3 Q_1 Q_2^\dagger Q_4^\dagger} &= Q_3 \overline{Q_1^\dagger Q_2^\dagger} = Q_3 \tilde{Q}_{1;2,4}^\dagger \\ &= -\frac{1}{2} [\text{Tr} (Z_1 Z_2 Z_3 Z_4) + \text{Tr} (Z_1 Z_4 Z_3 Z_2)] \end{aligned} \quad (2.13)$$

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

In a similar way eqs.(2.3,9,13) lead to

$$\begin{aligned}
\overbrace{Q_5 Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} Q_6^{\dagger}} &= -\frac{1}{2} \{ \text{Tr} (Z_1 Z_2 Z_3 Z_4 Z_5 Z_6) + \text{Tr} (Z_1 Z_2 Z_3 Z_6 Z_5 Z_4) \\
&+ \text{Tr} (Z_1 Z_4 Z_3 Z_6 Z_5 Z_2) + \text{Tr} (Z_1 Z_4 Z_3 Z_2 Z_5 Z_6) \\
&+ \text{Tr} (Z_1 Z_6 Z_3 Z_2 Z_5 Z_4) + \text{Tr} (Z_1 Z_6 Z_3 Z_4 Z_5 Z_2) \\
&+ \text{Tr} (Z_1 Z_6 Z_5 Z_4 Z_3 Z_2) + \text{Tr} (Z_1 Z_4 Z_5 Z_6 Z_3 Z_2) \\
&+ \text{Tr} (Z_1 Z_2 Z_5 Z_6 Z_3 Z_4) + \text{Tr} (Z_1 Z_6 Z_5 Z_2 Z_3 Z_4) \\
&+ \text{Tr} (Z_1 Z_4 Z_5 Z_2 Z_3 Z_6) + \text{Tr} (Z_1 Z_2 Z_5 Z_4 Z_3 Z_6) \} \quad (2.14)
\end{aligned}$$

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

$$C_{2p} = \overbrace{Q_{2p-1} \dots Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger}} = -\frac{1}{2} \sum_{P, R_1} \text{Tr} (Z_1 Z_{P(2)} Z_{R_1(3)} Z_{P(4)} \dots Z_{R_1(2p-1)} Z_{P(2p)}) \quad (2.15)$$

Eqs. (2.4, 13 and 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  $1, 3, \dots, 2p-1$  and consider

$$S = \sum_{P, R} \text{Tr} (Z_{R(1)} Z_{P(2)} Z_{R(3)} \dots Z_{R(2p-1)} Z_{P(2p)}) \quad (2.16)$$

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

$$S = p \sum_{P, R_1} \text{Tr} (Z_1 Z_{P(2)} Z_{R_1(3)} \dots Z_{R_1(2p-1)} Z_{P(2p)})$$

Hence the contraction of  $2p$  operators writes also

$$\overbrace{Q_{2p-1} \dots Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger}} = -\frac{1}{2p} \sum_{P, R} \text{Tr} (Z_{R(1)} Z_{P(2)} Z_{R(3)} Z_{R(2p-1)} Z_{P(2p)}) \quad (2.17)$$



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

$$C_{2p+2} = \overbrace{Q_{2p+1} Q_{2p-1} \dots Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger} Q_{2p+2}^{\dagger}}^{(2.18)}$$

$$= \sum_{i < j} \underbrace{Q_{2p+1} Q_{2p-1} \dots Q_3 Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger} Q_{2p+2}^{\dagger}}_{\text{sequence of } Q^{\dagger} \text{ where } Q_{2i}^{\dagger} \text{ and } Q_{2j}^{\dagger} \text{ are missing.}} \tilde{Q}_{1;2i,2j}^{\dagger}$$

We apply the recipe for  $2p$  contractions, bearing in mind that the matrix related to  $\tilde{Q}_{1;2i,2j}^{\dagger}$  is

$$\tilde{Z}_{1;2i,2j}^{\dagger} = Z_{2i} Z_1 Z_{2j} + Z_{2j} Z_1 Z_{2i}$$

and yield successively

$$C_{2p+2} = -\frac{1}{2} \sum_{i < j} \sum_{P, R_1} \text{Tr} ( Z_{R_1(3)} Z_{P(2)} Z_{R_1(5)} \dots Z_{P(2p+2)} Z_{R_1(2p+1)} \tilde{Z}_{1;2i,2j}^{\dagger} ) \quad (2.19)$$

$$= -\frac{1}{2} \sum_{i < j} \sum_{P_{ij} R_1} \left\{ \text{Tr} ( Z_1 Z_{2i} Z_{R_1(3)} Z_{P_{ij}(2)} \dots Z_{P_{ij}(2p+2)} Z_{R_1(2p+1)} Z_{2j} ) \right. \quad (2.20)$$

$$\left. + \text{Tr} ( Z_1 Z_{2j} Z_{R_1(3)} Z_{P_{ij}(2)} Z_{P_{ij}(2p+2)} Z_{R_1(2p+1)} Z_{2i} ) \right\}$$

$$= -\frac{1}{2} \sum_{R_1} \sum_{ij} \sum_{P_{ij}} \text{Tr} ( Z_1 Z_{2j} Z_{R_1(3)} Z_{P_{ij}(2)} \dots Z_{P_{ij}(2p+2)} Z_{R_1(2p+1)} Z_{2i} ) \quad (2.21)$$

where  $R_1$  labels now one of the  $p!$  permutations of the odd indices  $3, 5, \dots, 2p+1$  and  $P_{ij}$  one of the  $(p-1)!$  permutations of the even indices  $2, 4, \dots, 2p+2$  where  $2i$  and  $2j$  are missing. In eq. (2.19) we have applied the recipe for a contraction of  $2p$  operators where  $\tilde{Z}$  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  $2, 4, \dots, 2p+2$  so that the searched contraction  $C_{2p+2}$  writes

$$C_{2p+2} = -\frac{1}{2} \sum_{R_1} \sum_P \text{Tr}(Z_{1(2)} Z_{P(2)} Z_{R_1(3)} \dots Z_{R_1(2p+1)} Z_{P(2p+2)}) \quad (2.22)$$

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 2 since, according to the antisymmetry properties of matrices  $Z$ , one has

$$\text{Tr}(Z_1 Z_2 \dots Z_{2p-1} Z_{2p}) = \text{Tr}(Z_{2p} Z_{2p-1} \dots Z_2 Z_1)$$

Despite this reduction one sees that this number increases quite rapidly with  $p$ , leading 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

$$= \frac{Q_{R(2p-1)} \dots Q_{R(3)} Q_{R(1)} Q_{P(2)}^\dagger Q_{P(4)}^\dagger \dots Q_{P(2p)}^\dagger}{Q_{2p-1} \dots Q_3 Q_1 Q_2^\dagger Q_4^\dagger \dots Q_{2p}^\dagger} \quad \text{for every } P \text{ and } R,$$

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

$\{p_1, p_2, \dots, p_k\}$  of the integer  $p$  so that

$$p = p_1 + p_2 + \dots + p_k$$

where  $p_1 \leq p_2 \leq p_3 \leq \dots \leq p_k$

The Wick's theorem for  $p$  can be written

$$\begin{aligned}
& \langle Q_{2p-1} \dots Q_3 Q_1 Q_2^\dagger Q_4^\dagger \dots Q_{2p}^\dagger \rangle \quad (2.23) \\
& = \sum_{\{P_1, P_2, \dots, P_k\}} \sum_{P, R} \overbrace{Q_{R(2P_1-1)} \dots Q_{R(3)} Q_{R(1)} Q_{P(2)}^\dagger \dots Q_{P(2P_1)}^\dagger} \\
& \quad \overbrace{Q_{R(2P_1+2P_2-1)} \dots Q_{R(2P_1+1)} Q_{P(2P_1+2)}^\dagger \dots Q_{P(2P_1+2P_2)}^\dagger} \\
& \quad \dots \overbrace{Q_{R(2P-1)} \dots Q_{R(2P-2P_k+1)} Q_{P(2P-2P_k+2)}^\dagger \dots Q_{P(2P)}^\dagger}
\end{aligned}$$

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)

$$\begin{aligned}
& \langle Q_{2p+1} \dots Q_3 Q_1 Q_2^\dagger \dots Q_{2p+2}^\dagger \rangle \\
& = \sum_{i=1}^{p+1} \overbrace{Q_1 Q_{2i}^\dagger} \langle Q_{2p+1} \dots Q_3 Q_2^\dagger \dots Q_{2p+2}^\dagger \rangle \quad (2.24) \\
& \quad \text{product of } Q^\dagger \text{ where } Q_{2i}^\dagger \text{ is missing} \\
& + \sum_{i < j} \langle Q_{2p+1} \dots Q_3 \overbrace{Q_{1; 2i, 2j}^\dagger} Q_2^\dagger \dots Q_{2p+2}^\dagger \rangle \\
& \quad \text{product of } Q^\dagger \text{ where } Q_{2i}^\dagger \text{ and } Q_{2j}^\dagger \text{ are} \\
& \quad \text{missing.}
\end{aligned}$$

In these two terms, respectively referred to, as A and B, arise overlaps of p operators 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 terms A contain necessarily a product of at least two contractions it is obvious that the total contraction  $C_{2p+2}$  arise necessarily from part B, with total contraction of the 2p operators involved.

$$C_{2p+2} = \overbrace{Q_{2p+1} \dots Q_3 Q_1 Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p+2}^{\dagger}}$$

$$= \sum_{i < j} \overbrace{Q_{2p+1} \dots Q_3 Q_{1;2i,2j}^{\dagger} Q_2^{\dagger} \dots Q_{2p+2}^{\dagger}}$$

sequence where  $Q_{2i}^{\dagger}$  and  $Q_{2j}^{\dagger}$  are missing

which is coherent with our definition (2.12).

We showed that way that  $C_{2p+2}$  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  $\overline{Q_1 Q_{2\ell}^{\dagger}}$  and those where  $Q_1$  does not appear in such a contraction. Products of contractions containing the factor  $\overline{Q_1 Q_{2i}^{\dagger}}$  cannot arise from B terms, since according to the presence of index 1 in  $\overline{Q_{1;2i,2j}^{\dagger}}$  the lowest possible contraction is  $\overline{Q_{2k+1} Q_{1;2i,2j}^{\dagger}} = \overline{Q_{2k+1} Q_1 Q_2^{\dagger} Q_{2j}^{\dagger}}$ . We consider a general product of contractions containing a factor  $\overline{Q_1 Q_{2\ell}^{\dagger}}$ , e.g.

$$\overline{Q_1 Q_{2\ell}^{\dagger}} \overline{Q \dots Q^{\dagger}} \overline{Q \dots Q^{\dagger}} \dots \overline{Q \dots Q^{\dagger}} \quad (2.25)$$

The product of contractions in the factor of  $\overline{Q_1 Q_{2\ell}^{\dagger}}$  appear in a given partition of integer  $p$ . It is evident that the term (2.25) appears in part A of (2.24) for  $i = \ell$ :

$$\overline{Q_1 Q_{2\ell}^{\dagger}} < \overbrace{Q_{2p+1} \dots Q_3 Q_2^{\dagger} \dots Q_{2p+2}^{\dagger}} > \quad (2.26)$$

product where  $Q_{2\ell}^{\dagger}$  is missing

Furthermore, its unicity is ensured since a given product of contractions in a given partition of  $(p-1)$  appears once and only once in the product of contractions obtained by applying the Wick's theorem for  $p$  phonons in the factor of  $\overline{Q_1 Q_{2\ell}^{\dagger}}$  in eq.(2.26). With the terms of type (2.5) we exhaust the part A of (2.24).

Let us now seek 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,  $2p_{\ell}$  operators, which we can always relabel with indices

$$P(2), P(4) \dots P(2\ell); R(1) = 1, R(3) \dots R(2\ell-1) \quad (2.27)$$

The factor  $F$  of this contraction corresponds to a given partition of  $(p-p_\ell)$  where the operators are labelled 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), ensuring thereby 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  $2p_\ell - 2$  operators where one of the  $Q^\dagger$  has been replaced by  $\tilde{Q}_1^\dagger; 2i, 2j$ , where the odd indices are  $R(3), R(5), \dots, R(2p_\ell - 1)$  and where the even ones are  $P(2), P(4), \dots, P(2m) = i, \dots, P(2n) = j, \dots, P(2\ell)$  with  $m < n \leq \ell$ . Its factor  $F$ , will appear too, and only once, among the products of contractions involving the partitions of  $(p-p_\ell)$  and the complementary indices, proving thereby the theorem. At this point, we would like to emphasize that in the application of (2.23) one must first write formally 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 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

$$\begin{aligned} & \langle Q_{2p-1} \dots Q_3 Q_1 T_{11} Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger} \rangle = \\ & \sum_{i=1}^p \langle Q_{2p-1} \dots Q_3 Q_1 [T_{11}, Q_{2i}^{\dagger}] \underbrace{Q_2^{\dagger} Q_{2p}^{\dagger}}_{\text{product of } Q^{\dagger} \text{ where } Q_{2i}^{\dagger} \text{ is missing}} \rangle \end{aligned}$$

We note that

$$[T_{11}, Q_{2i}^{\dagger}] \text{ behaves like a new phonon}$$

$$\tilde{Q}_{2i}^{\dagger} = \frac{1}{2} \sum_{\mu\nu} (\tilde{Z}_{2i})_{\mu\nu} \alpha_{\mu}^{\dagger} \alpha_{\nu}$$

where

$$(\tilde{Z}_{2i})_{\mu\nu} = (tZ_i - Z_i t)_{\mu\nu}$$

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.

### 3. RECURSION FORMULAS

In this section we analyze the previous problem in a completely different way. First of all, we rewrite the basic states  $Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger} | \rangle$  by grouping together all phonons of the same kind; this is specially 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  $\langle | Q_{2p-1} \dots Q_3 Q_1$ . There are  $r$  different types of phonons appearing in both  $Q_2^{\dagger} Q_4^{\dagger} \dots Q_{2p}^{\dagger}$  and  $Q_{2p-1} \dots Q_3 Q_1$ . They are denoted

once for all, after a relabelling of the indices,  $Q_1^\dagger, Q_2^\dagger, \dots, Q_r^\dagger$ . Thus, the previous problem is now fully equivalent to the calculation of the quantity

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

$$\text{with } k_1' + k_2' + \dots + k_r' = k_1 + k_2 + \dots + k_r = p$$

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

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

is needed.

The index (20) means that it appears in the calculation of matrix elements of  $T_2$ .

The indices  $\mu, \nu$  refer to the quasiparticle excitation  $\alpha_{\mu}^\dagger, \alpha_{\nu}^\dagger$  and parameters  $k_1, k_2, \dots, k_r$  (and  $k_1', k_2', \dots, k_r'$ ) stand for the number of phonons  $Q_1^\dagger, Q_2^\dagger, \dots, Q_r^\dagger$  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

$$A_{\mu\nu}^{(20)}(k_1', k_2', \dots, k_r'; k_1, k_2, \dots, k_r) = 0 \quad \text{if} \quad k_1' + k_2' + \dots + k_r' \neq k_1 + k_2 + \dots + k_r + 1 \quad (3.3)$$

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

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

$$N(k_n'; k_n) = \frac{1}{2} \sum_{\mu, \nu} \langle z_n \rangle_{\mu\nu} A_{\mu\nu}^{(20)}(k_n'; k_n - 1) \quad \text{for every } n \quad (3.4)$$

In the following, it will be convenient to consider  $A_{\mu\nu}$  as the matrix

elements of a matrix A. Hence equation (3.4) can be written in a more compact form

$$N(k'_n; k_n) = -\frac{1}{2} \text{Tr} \left[ Z_n \Lambda^{(20)} (k'_n; k_{n-1}) \right] \text{ for every } n \quad (3.5)$$

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  $\langle | \alpha_\mu^\dagger \alpha_\nu^\dagger$  which vanishes.

$$\text{Thus} \quad A_{\mu\nu} = \sum_{n=1}^r \sum_{i=0}^{k'_n-1} J_{\mu\nu}^{ni} \quad (3.6)$$

$$\text{with } J_{\mu\nu}^{ni} = \langle Q_r^{k'_r} \dots Q_{n+1}^{k'_{n+1}} Q_n^i [Q_n, \alpha_\mu^\dagger \alpha_\nu^\dagger] Q_n^{k'_n-i-1} \dots Q_1^{k'_1} Q_1^{\dagger k'_1} \dots Q_r^{\dagger k'_r} \rangle \quad (3.7)$$

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

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

$$\text{with } K_{\mu\nu}^{nn} = \langle [Q_n, [Q_n, \alpha_\mu^\dagger \alpha_\nu^\dagger]] Q_r^{k'_r} \dots Q_n^{k'_n-2} \dots Q_1^{k'_1} Q_1^{\dagger k'_1} \dots Q_r^{\dagger k'_r} \rangle \quad (3.9)$$

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 to the bra  $\langle |$ . Hence,  $K_{\mu\nu}^{nn}$  is independent of  $i$ . From equation (3.8)  $J_{\mu\nu}^{ni}$  can easily be calculated

$$J_{\mu\nu}^{ni} = \binom{i}{0} J_{\mu\nu}^{n0} + \binom{i}{1} K_{\mu\nu}^{nn} \quad (3.10)$$

where  $\binom{i}{p}$  are the usual binomial coefficients. Performing the summation over  $i$  (in 3.6) and using relations (3.10) and  $\sum_{i=p}^k \binom{i}{p} = \binom{k+1}{p+1}$  one finds

$$A_{\mu\nu} = \sum_{n=1}^r \left[ \binom{k'_n}{1} J_{\mu\nu}^{n0} + \binom{k'_n}{2} K_{\mu\nu}^{nn} \right] \quad (3.11)$$

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



$$J_{\mu\nu}^{n0} = \sum_{n'=n+1}^r \sum_{i=0}^{k'_i-1} K_{\mu\nu}^{nn'} + L_{\mu\nu}^n \quad (3.12)$$

with

$$K_{\mu\nu}^{nn'} = \langle 0 | [Q_n, [Q_n, \alpha_\mu^\dagger \alpha_\nu^\dagger]] Q_r^{k'_r} \dots Q_n^{k'_n-1} \dots Q_n^{k'_n-1} \dots Q_1^{k'_1} Q_1^{k'_1} \dots Q_r^{k'_r} | 0 \rangle$$

$$L_{\mu\nu}^n = \langle 0 | [Q_n, \alpha_\mu^\dagger \alpha_\nu^\dagger] Q_r^{k'_r} \dots Q_n^{k'_n-1} \dots Q_1^{k'_1} \dots Q_r^{k'_r} | 0 \rangle \quad (3.13)$$

Inserting (3.12) in (3.11) one gets

$$A_{\mu\nu} = \sum_{n=1}^r \binom{k'_n}{1} L_{\mu\nu}^n + \sum_{n=1}^r \binom{k'_n}{2} K_{\mu\nu}^{nn} + \sum_{n=1}^r \sum_{n'=n+1}^r \binom{k'_n}{1} \binom{k'_{n'}}{1} K_{\mu\nu}^{nn'} \quad (3.14)$$

It remains to calculate the quantities K and L.

Using equation (2.1) one deduces

$$[Q_n, [Q_n, \alpha_\mu^\dagger \alpha_\nu^\dagger]] = \sum_{\mu', \nu'} \left[ (Z_n)_{\mu\nu'} (Z_n)_{\nu\mu'} + (Z_n)_{\nu\nu'} (Z_n)_{\mu\mu'} \right] \alpha_{\nu'} \alpha_{\mu'} \quad (3.15)$$

and then

$$L_{\mu\nu}^n = (Z_n)_{\mu\nu} N(k'_n - 1; k_n)$$

$$K_{\mu\nu}^{nn'} = \sum_{\mu', \nu'} \left[ (Z_n)_{\mu\nu'} (Z_n)_{\nu\mu'} + (Z_n)_{\mu\mu'} (Z_n)_{\nu\nu'} \right] A_{\mu'\nu'}(k; k'_n - 1, k'_n - 1) \quad (3.16)$$

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

$$A^{(20)}(k'_n, k'_n; k_n, k_n) = \sum_{n=1}^r \binom{k'_n}{1} N(k'_n - 1; k_n) Z_n$$

$$+ \sum_{n=1}^r Z_n \binom{k'_n}{2} Z_n A^{(20)}(k_n; k'_n - 2) Z_n + \quad (3.17)$$

$$\sum_{n=1}^r \sum_{n'=n+1}^r \binom{k'_n}{1} \binom{k'_{n'}}{1} \left[ Z_n A^{(20)}(k_n, k_n; k'_n - 1, k'_{n'} - 1) Z_n + \right.$$

$$\left. Z_n A^{(20)}(k_n, k_n; k'_n - 1, k'_{n'} - 1) Z_n \right]$$

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  $k_1! k_2! \dots k_r! k'_1! k'_2! \dots k'_r!$  Furthermore we gather the two last

terms of (3.17) in one. Then equations (3.4) and (3.17) become

$$k_n \mathcal{N}(k'_n; k_n) = -\frac{1}{2} \text{Tr} \left[ Z_n \mathcal{A}^{(20)}(k'_n; k_n - 1) \right] \quad \text{for every } n \quad (3.18)$$

$$\begin{aligned} \mathcal{A}^{(20)}(k'_n, k'_n; k_n, k_n) &= \sum_{n=1}^r \mathcal{N}(k'_n - 1; k_n) Z_n \quad (3.19) \\ &+ \frac{1}{2!} \sum_{n, n'} \left[ Z_n \mathcal{A}^{(20)}(k_n, k_n; k'_n - 1, k'_n - 1) Z_{n'} + Z_{n'} \mathcal{A}^{(20)}(k_n, k_n; k'_n - 1, k'_n - 1) \right] \end{aligned} \quad (3.19)$$

The second term in (3.19) reflects the effect of the Pauli principle; if  $n=n'$  then  $\mathcal{A}^{(20)}(k_n, k_n; k'_n - 1, k'_n - 1)$  must be understood as  $\mathcal{A}^{(20)}(k_n, k'_n - 2)$ .

Basically the two previous equations are coupled recursion relations: the recursion acts on the total number  $p+p'$  of phonons; they are coupled since  $\mathcal{A}^{(20)}$  is a function of  $\mathcal{N}$  and  $\mathcal{N}$  is a function of  $\mathcal{A}^{(20)}$ . Once the matrix  $\mathcal{A}^{(20)}$  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  $\mathcal{A}^{(11)}$ :

$$\mathcal{A}_{\text{IV}}^{(11)}(k'_1, k'_2, \dots, k'_r; k_1, k_2, \dots, k_r) = \langle Q_r^\dagger \dots Q_2^\dagger Q_1^\dagger \alpha_\mu^\dagger \alpha_\nu Q_1^\dagger Q_2^\dagger \dots Q_r^\dagger \rangle \quad (3.20)$$

and using equation (2.1) one gets

$$\mathcal{A}^{(11)}(k'_n; k_n) = - \sum_{n=1}^r \binom{k_n}{1} \left[ \mathcal{A}^{(20)}(k'_n; k_n - 1) Z_n \right] \quad (3.21)$$

introducing again the reduced quantity  $\mathcal{A}^{(11)}$  by dividing  $\mathcal{A}^{(11)}$  by the product of all the factorials  $k_i, k'_i$  it comes

$$\mathcal{A}^{(11)}(k'_n; k_n) = - \sum_{n=1}^r \left[ \mathcal{A}^{(20)}(k'_n; k_n - 1) Z_n \right] \quad (3.22)$$

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

$$\mathcal{A}^{(11)}(k'_n; k_n) = - \sum_{n=1}^r \left[ Z_n \mathcal{A}^{(20)}(k_n; k'_n - 1) \right] \quad (3.23)$$

The formalism concerning matrix elements for one body operators and

for overlap matrices has been developed in details. The same philosophy is followed and the same technics 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

$$A_{\mu\nu\rho\sigma}^{(40)}(k_1', \dots, k_r'; k_1, \dots, k_r) = \frac{\langle Q_r^{k_r} \dots Q_1^{k_1} \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\rho^\dagger \alpha_\sigma^\dagger Q_1^{k_1} \dots Q_r^{k_r} \rangle}{k_1! \dots k_r! k_1! \dots k_r!} \quad (3.24)$$

It vanishes if  $k_1' + \dots + k_r' \neq k_1 + \dots + k_r + 2$ . If  $\mathcal{P}_{\mu\nu\rho\sigma}$  is any permutation on the indices  $\mu, \nu, \rho, \sigma$  the symmetry properties of  $\alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\rho^\dagger \alpha_\sigma^\dagger$  hold also for  $A_{\mu\nu\rho\sigma}^{(40)}$ . More precisely one has

$$\mathcal{P}_{\mu\nu\rho\sigma} A_{\mu\nu\rho\sigma}^{(40)} = (-1)^{\mathcal{P}} A_{\mu\nu\rho\sigma}^{(40)} \quad (3.25)$$

where  $(-1)^{\mathcal{P}}$  is the signature of the permutation. To evaluate  $A_{\mu\nu\rho\sigma}^{(40)}$  we need the following commutators :

$$a) \left[ Q_{n_2}, \left[ Q_{n_1}, \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\rho^\dagger \alpha_\sigma^\dagger \right] \right] = E_{\mu\nu\rho\sigma}^{(n_1, n_2)} + \text{terms } \alpha^\dagger \alpha + \text{terms } \alpha^\dagger \alpha^\dagger \alpha \alpha \quad (3.26)$$

with  $E_{\mu\nu\rho\sigma}^{(n_1, n_2)} = \frac{1}{4} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} \mathcal{P}_{\mu\nu\rho\sigma} \left[ (Z_{n_1})_{\mu\nu} (Z_{n_2})_{\rho\sigma} \right] \quad (3.27)$

In fact, the summation in (3.27) contains only six different terms (due 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 equation (3.27) one can check that

$$\begin{aligned} \mathcal{P}_{\mu\nu\rho\sigma} E_{\mu\nu\rho\sigma}^{(n_1, n_2)} &= (-1)^{\mathcal{P}} E_{\mu\nu\rho\sigma}^{(n_1, n_2)} \\ \mathcal{P}_{n_1 n_2} E_{\mu\nu\rho\sigma}^{(n_1, n_2)} &= E_{\mu\nu\rho\sigma}^{(n_1, n_2)} \end{aligned} \quad (3.28)$$

$$b) \left[ Q_{n_3}, \left[ Q_{n_2}, \left[ Q_{n_1}, \left[ \alpha_\mu^+ \alpha_\nu^+ \alpha_\rho^+ \alpha_\sigma^+ \right] \right] \right] \right] = \sum_{\mu', \nu'} F_{\mu\nu\rho\sigma, \mu' \nu'}^{(n_1 n_2 n_3)} \alpha_\nu \alpha_{\mu'} + \text{terms } \alpha^+ \alpha \alpha \quad (3.2)$$

with

$$F_{\mu\nu\rho\sigma, \mu' \nu'}^{(n_1 n_2 n_3)} = -\frac{1}{4} \sum_{\mathcal{P}} \sum_{\mathcal{Q}} (-1)^{\mathcal{Q}} \mathcal{P}_{n_1 n_2 n_3}^{\mathcal{Q}} F_{\mu\nu\rho\sigma} \left[ (Z_{n_1})_{\mu\mu'}, (Z_{n_2})_{\nu\nu'}, (Z_{n_3})_{\rho\rho'} \right] \quad (3.30)$$

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  $(n_1 n_2) (\nu\nu') (\mu'\nu')$  give the same result. One can also check that

$$\begin{aligned} \mathcal{P}_{\mu\nu\rho\sigma}^{(n_1 n_2 n_3)} F_{\mu\nu\rho\sigma, \mu' \nu'} &= (-1)^{\mathcal{Q}} F_{\mu\nu\rho\sigma, \mu' \nu'}^{(n_1 n_2 n_3)} \\ \mathcal{Q}_{n_1 n_2 n_3}^{(n_1 n_2 n_3)} F_{\mu\nu\rho\sigma, \mu' \nu'} &= F_{\mu\nu\rho\sigma, \mu' \nu'}^{(n_1 n_2 n_3)} \end{aligned} \quad (3.31)$$

$$c) \left[ Q_{n_4}, \left[ Q_{n_3}, \left[ Q_{n_2}, \left[ Q_{n_1}, \left[ \alpha_\mu^+ \alpha_\nu^+ \alpha_\rho^+ \alpha_\sigma^+ \right] \right] \right] \right] \right] = \sum_{\mu', \nu', \rho', \sigma'} G_{\mu\nu\rho\sigma, \mu' \nu' \rho' \sigma'}^{(n_1 n_2 n_3 n_4)} \alpha_\sigma \alpha_{\rho'} \alpha_{\nu'} \alpha_{\mu'}$$

with

(3.32)

$$\begin{aligned} G_{\mu\nu\rho\sigma, \mu' \nu' \rho' \sigma'}^{(n_1 n_2 n_3 n_4)} &= \sum_{\mathcal{Q}} (-1)^{\mathcal{Q}} \mathcal{Q}_{\mu\nu\rho\sigma} \left[ (Z_{n_1})_{\mu\mu'}, (Z_{n_2})_{\nu\nu'}, (Z_{n_3})_{\rho\rho'}, (Z_{n_4})_{\sigma\sigma'} \right] \\ &= \sum_{\mathcal{Q}} \mathcal{Q}_{n_1 n_2 n_3 n_4} \left[ (Z_{n_1})_{\mu\mu'}, (Z_{n_2})_{\nu\nu'}, (Z_{n_3})_{\rho\rho'}, (Z_{n_4})_{\sigma\sigma'} \right] \end{aligned} \quad (3.33)$$

which has the following properties

$$\begin{aligned} \mathcal{Q}_{\mu\nu\rho\sigma}^{(n_1 n_2 n_3 n_4)} G_{\mu\nu\rho\sigma, \mu' \nu' \rho' \sigma'} &= (-1)^{\mathcal{Q}} G_{\mu\nu\rho\sigma, \mu' \nu' \rho' \sigma'}^{(n_1 n_2 n_3 n_4)} \\ \mathcal{Q}_{n_1 n_2 n_3 n_4}^{(n_1 n_2 n_3 n_4)} G_{\mu\nu\rho\sigma, \mu' \nu' \rho' \sigma'} &= G_{\mu\nu\rho\sigma, \mu' \nu' \rho' \sigma'}^{(n_1 n_2 n_3 n_4)} \end{aligned} \quad (3.34)$$

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

$$\begin{aligned}
 & A^{(20)}(k'_1, \dots, k'_n; k_1, \dots, k_n) = \\
 & \frac{1}{n!} \sum_{\mu\nu\sigma\zeta} \mathcal{N}(k'_1, \dots, k'_n; k'_1, \dots, k'_n; k'_1, \dots, k'_n; k'_1, \dots, k'_n) E_{\mu\nu\sigma\zeta}^{(m_1 n_2)} \\
 & + \frac{1}{4!} \sum_{n_1 n_2 n_3} \sum_{\mu' \nu' \sigma' \zeta'} F_{\mu' \nu' \sigma' \zeta'}^{(n_1 n_2 n_3)} A_{\mu' \nu' \sigma' \zeta'}^{(20)}(k'_1, \dots, k'_n; k'_1, \dots, k'_n; k'_1, \dots, k'_n; k'_1, \dots, k'_n) \\
 & \frac{1}{4!} \sum_{n_1 n_2 n_3 n_4} \sum_{\mu' \nu' \sigma' \zeta'} G_{\mu' \nu' \sigma' \zeta'}^{(n_1 n_2 n_3 n_4)} A_{\mu' \nu' \sigma' \zeta'}^{(40)}(k'_1, \dots, k'_n; k'_1, \dots, k'_n; k'_1, \dots, k'_n; k'_1, \dots, k'_n)
 \end{aligned} \quad (3.35)$$

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

The matrix elements of  $T_{31}$  and  $T_{22}$  of the two body operator are obtained from  $A_{\mu\nu\sigma\zeta}^{(40)}$  by the following equations

$$\begin{aligned}
 A_{\mu\nu\sigma\zeta}^{(31)}(k_1, \dots, k'_2; k_1, \dots, k_1) &= \frac{\langle Q_\mu^{k'_2} \dots Q_\nu^{k'_1} \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\sigma^\dagger \alpha_\zeta^\dagger Q_\mu^{k_1} \dots Q_\nu^{k_1} \rangle}{k'_2! \dots k'_1! k_1! \dots k_1!} \\
 &= \sum_n \sum_{\sigma'} \sum_{\sigma''} A_{\mu\nu\sigma\zeta}^{(40)}(k_1, \dots, k'_2; k_1, \dots, k_n-1, \dots, k_1)
 \end{aligned} \quad (3.36)$$

$$A_{\mu\nu\sigma\zeta}^{(32)}(k'_1, \dots, k'_n; k_1, \dots, k_n) = \frac{\langle Q_\mu^{k'_1} \dots Q_\nu^{k'_n} \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\sigma^\dagger \alpha_\zeta^\dagger Q_\mu^{k_1} \dots Q_\nu^{k_n} \rangle}{k'_1! \dots k'_n! k_1! \dots k_n!}$$

$$= \sum_m (Z_m)_{\sigma\zeta} A_{\mu\nu}^{(20)}(k'_1, \dots, k'_n; k_1, \dots, k_n-1, \dots, k_n)$$

$$+ \frac{1}{2} \sum_{n_1 n_2} \sum_{\zeta' \zeta''} [(Z_{n_1})_{\sigma\zeta'} (Z_{n_2})_{\zeta''} + (Z_{n_2})_{\sigma\zeta'} (Z_{n_1})_{\zeta''}] A_{\mu\nu\sigma\zeta'}^{(40)}(k'_1, \dots, k'_n; k_1, \dots, k_n-1, \dots, k_n)$$

(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  $Q_1^{k_1} \dots Q_r^{k_r} |0\rangle$ , we use "reduced" states  $|k_1 \dots k_r\rangle = \frac{Q_1^{k_1} \dots Q_r^{k_r}}{k_1! \dots k_r!} | \rangle^*$ ; the reduced quantities are now the matrix elements in this "reduced" basis. Starting from  $\mathcal{M}(0,0,\dots,0;0,0,\dots,0)$  all the recursion formulas given above allow to calculate overlap matrices and matrix elements for one and two body operators concerning any general multiphonon state  $|k_1, \dots, k_r\rangle$

#### 4 . 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 arises now 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 contain few phonons, all of different types. On the contrary, the recursion formulas ought to be used if the basis contain several phonons of the same

\*Note that normalized boson states would write

$$\frac{B_1^{k_1} \dots B_r^{k_r} |0\rangle}{\sqrt{k_1! \dots k_r!}}$$

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 systems 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 needs 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  $\{ |k\rangle = \frac{Q^\dagger k}{k!} |0\rangle, k = 1, \dots, N \}$ . The overlap matrix is simply the norm matrix

$$\mathcal{N}_k = \mathcal{N}(k,k) = \langle k | k \rangle \quad (4.1)$$

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

$$k \mathcal{N}_k = -\frac{1}{2} \text{Tr} [z \mathcal{A}_k] \quad (4.2)$$

$$\mathcal{A}_k = z \mathcal{N}_{k-1} + z \mathcal{A}_{k-1} z \quad (4.3)$$

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

$$A_k = \sum_{l=1}^k \mathcal{N}_{k-l} [Z]^{2l-1} \quad (4.4)$$

$$k \mathcal{N}_k = -\frac{1}{2} \sum_{l=1}^k \mathcal{N}_{k-l} \text{Tr} [Z^{2l}] \quad (4.5)$$

Starting from  $\mathcal{N}_0 = 1$ , equation (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  $\text{Tr}(Z^{2m})$  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<sup>4)</sup> and in more realistic situations<sup>3)</sup>.

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 Wick's theorem. The phonons  $Q_0^\dagger$  and  $Q_1^\dagger$  are assumed to be orthonormalized thus

$$\begin{aligned} \overbrace{Q_0 Q_0^\dagger} &= -\frac{1}{2} \text{Tr}(Z_0^2) = 1 \\ \overbrace{Q_1 Q_1^\dagger} &= -\frac{1}{2} \text{Tr}(Z_1^2) = 1 \\ \overbrace{Q_0 Q_1^\dagger} &= \overbrace{Q_1 Q_0^\dagger} = -\frac{1}{2} \text{Tr}(Z_0 Z_1) = 0 \end{aligned} \quad (4.6)$$

Besides (4.6) we need the following contractions

$$\begin{aligned} \overbrace{Q_0 Q_0 Q_0^\dagger Q_0^\dagger} &= -\text{Tr}(Z_0^4) \\ \overbrace{Q_0 Q_0 Q_1^\dagger Q_1^\dagger} &= -\text{Tr}(Z_0 Z_1 Z_0 Z_1) \\ \overbrace{Q_1 Q_1 Q_1^\dagger Q_1^\dagger} &= -\text{Tr}(Z_1^4) \\ \overbrace{Q_1 Q_0 Q_0^\dagger Q_1^\dagger} &= -\text{Tr}(Z_0^2 Z_1^2) \\ \overbrace{Q_0 Q_0 Q_0 Q_0^\dagger Q_0^\dagger Q_0^\dagger} &= -6 \text{Tr}(Z_0^6) \end{aligned}$$



$$\overline{q_1 q_1 q_1 q_0^{\dagger} q_0^{\dagger} q_1^{\dagger}} = -6 \text{Tr} (z_1^3 z_0 z_1 z_0) \quad (4.7)$$

$$\overline{q_0 q_0 q_0 q_0^{\dagger} q_1^{\dagger} q_1^{\dagger}} = -6 \text{Tr} (z_0^3 z_1 z_0 z_1)$$

$$\overline{q_1 q_1 q_0 q_0^{\dagger} q_1^{\dagger} q_1^{\dagger}} = -2 \text{Tr} (z_0 z_1^2 z_0 z_1^2) - 4 \text{Tr} (z_0^2 z_1^4)$$

$$\overline{q_1 q_0 q_0 q_0^{\dagger} q_0^{\dagger} q_1^{\dagger}} = -2 \text{Tr} (z_0^2 z_1 z_0^2 z_1) - 4 \text{Tr} (z_0^4 z_1^2)$$

$$\overline{q_1 q_1 q_1 q_1^{\dagger} q_1^{\dagger} q_1^{\dagger}} = -6 \text{Tr} (z_1^6)$$

Concerning  $K^{\pi} = 0^+$  states there are six basic states namely

$| \rangle$ ,  $q_0^{\dagger} | \rangle$ ,  $q_0^{\dagger 2} | \rangle$ ,  $q_1^{\dagger 2} | \rangle$ ,  $q_0^{\dagger 3} | \rangle$ ,  $q_0^{\dagger} q_1^{\dagger 2} | \rangle$ . Application of the generalized Wick's theorem leads to

$$\langle | \rangle = 1$$

$$\langle q_0 q_0^{\dagger} \rangle = \overline{q_0 q_0^{\dagger}} = 1$$

$$\langle q_0^2 q_0^{\dagger 2} \rangle = 2 \overline{(q_0 q_0^{\dagger})^2} + \overline{q_0 q_0 q_0^{\dagger} q_0^{\dagger}} = 2 - \text{Tr} (z_0^4)$$

$$\langle q_0^2 q_1^{\dagger 2} \rangle = 2 \overline{(q_0 q_1^{\dagger})^2} + \overline{q_0 q_0 q_1^{\dagger} q_1^{\dagger}} = -\text{Tr} (z_0 z_1 z_0 z_1)$$

$$\langle q_1^2 q_1^{\dagger 2} \rangle = 2 \overline{(q_1 q_1^{\dagger})^2} + \overline{q_1 q_1 q_1^{\dagger} q_1^{\dagger}} = 2 - \text{Tr} (z_1^4) \quad (4.8)$$

$$\begin{aligned} \langle q_0^3 q_0^{\dagger 3} \rangle &= 6 \overline{(q_0 q_0^{\dagger})^3} + 9 \overline{q_0 q_0^{\dagger} q_0 q_0^{\dagger} q_0^{\dagger}} + \overline{q_0 q_0 q_0 q_0^{\dagger} q_0^{\dagger} q_0^{\dagger}} \\ &= 6 - 9 \text{Tr} (z_0^4) - 6 \text{Tr} (z_0^6) \end{aligned}$$

$$\begin{aligned} \langle q_0^3 q_0^{\dagger} q_1^{\dagger 2} \rangle &= 6 \overline{q_0 q_0^{\dagger} (q_0 q_1^{\dagger})^2} + 3 \overline{q_0 q_0^{\dagger} q_0 q_0 q_1^{\dagger} q_1^{\dagger}} \\ &\quad + 6 \overline{q_0 q_1^{\dagger} q_0 q_0 q_0^{\dagger} q_1^{\dagger}} + \overline{q_0 q_0 q_0 q_0^{\dagger} q_1^{\dagger} q_1^{\dagger}} \end{aligned}$$

$$= -3 \text{Tr} (z_0 z_1 z_0 z_1) - 6 \text{Tr} (z_0^3 z_1 z_0 z_1)$$

$$\begin{aligned} \langle q_1^2 q_0 q_0^{\dagger} q_1^{\dagger 2} \rangle &= 2 \overline{q_0 q_0^{\dagger} (q_1 q_1^{\dagger})^2} + 4 \overline{q_0 q_1^{\dagger} q_1 q_0^{\dagger} q_1 q_1^{\dagger}} + \overline{q_0 q_0^{\dagger} q_1 q_1 q_1^{\dagger} q_1^{\dagger}} \\ &\quad + 2 \overline{q_0 q_1^{\dagger} q_1 q_1 q_0^{\dagger} q_1^{\dagger}} + 2 \overline{q_1 q_0^{\dagger} q_1 q_0^{\dagger} q_1^{\dagger} q_1^{\dagger}} \\ &\quad + 4 \overline{q_1 q_1^{\dagger} q_1 q_1 q_0^{\dagger} q_1^{\dagger}} + \overline{q_1 q_1 q_0 q_0^{\dagger} q_1^{\dagger} q_1^{\dagger}} \\ &= 2 - \text{Tr} (z_1^4) - 4 \text{Tr} (z_0^2 z_1^2) - 2 \text{Tr} (z_0 z_1^2 z_0 z_1^2) - 4 \text{Tr} (z_0^2 z_1^4) \end{aligned}$$

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

$$\begin{aligned} \langle Q_1 Q_1^{\dagger} \rangle &= \overline{Q_1 Q_1^{\dagger}} = 1 \\ \langle Q_1 Q_0 Q_0^{\dagger} Q_1^{\dagger} \rangle &= \overline{Q_0 Q_0^{\dagger} Q_1 Q_1^{\dagger}} + \overline{Q_0 Q_1^{\dagger} Q_1 Q_0^{\dagger}} + \overline{Q_1 Q_0 Q_0^{\dagger} Q_1^{\dagger}} \\ &= 1 - \text{Tr} (z_0^2 z_1^2) \\ \langle Q_1 Q_0^2 Q_0^{\dagger 2} Q_1^{\dagger} \rangle &= 2 \overline{(Q_0 Q_0^{\dagger})^2 Q_1 Q_1^{\dagger}} + 4 \overline{Q_0 Q_1^{\dagger} Q_1 Q_0^{\dagger} Q_0 Q_0^{\dagger}} + \overline{Q_1 Q_1^{\dagger} Q_0 Q_0^{\dagger} Q_0 Q_0^{\dagger}} \\ &\quad + 2 \overline{Q_0 Q_1^{\dagger} Q_1 Q_0 Q_0^{\dagger} Q_1^{\dagger}} + 2 \overline{Q_1 Q_0^{\dagger} Q_0 Q_0 Q_0^{\dagger} Q_1^{\dagger}} \\ &\quad + 4 \overline{Q_0 Q_0^{\dagger} Q_1 Q_0 Q_0^{\dagger} Q_1^{\dagger}} + \overline{Q_1 Q_0 Q_0 Q_0^{\dagger} Q_0^{\dagger} Q_1^{\dagger}} \\ &= 2 - \text{Tr} (z_0^4) - 4 \text{Tr} (z_0^2 z_1^2) - 2 \text{Tr} (z_0^2 z_1 z_0^2 z_1) \\ &\quad - 4 \text{Tr} (z_0^4 z_1^2) \end{aligned} \tag{4.10}$$

$$\begin{aligned} \langle Q_1^3 Q_0^{\dagger 2} Q_1^{\dagger} \rangle &= 6 \overline{Q_1 Q_1^{\dagger} (Q_1 Q_0^{\dagger})^2} + 3 \overline{Q_1 Q_1^{\dagger} Q_1 Q_1 Q_0^{\dagger} Q_0^{\dagger}} \\ &\quad + 6 \overline{Q_1 Q_0^{\dagger} Q_1 Q_1 Q_0^{\dagger} Q_1^{\dagger}} + \overline{Q_1 Q_1 Q_1 Q_0^{\dagger} Q_0^{\dagger} Q_1^{\dagger}} \\ &= -3 \text{Tr} (z_0 z_1 z_0 z_1) - 6 \text{Tr} (z_1^3 z_0 z_1 z_0) \end{aligned}$$

$$\begin{aligned} \langle Q_1^{\dagger} Q_1^{\dagger 3} \rangle &= 6 \overline{(Q_1 Q_1^{\dagger})^3} + 9 \overline{Q_1 Q_1^{\dagger} Q_1 Q_1 Q_1^{\dagger} Q_1^{\dagger}} + \overline{Q_1 Q_1 Q_1 Q_1^{\dagger} Q_1^{\dagger} Q_1^{\dagger}} \\ &= 6 - 9 \text{Tr} (z_1^4) - 6 \text{Tr} (z_1^6) \end{aligned}$$

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 to future publications.

## 5. Conclusions

To treat properly the problem of multiphonon states of different types we have developed two methods which allow to take properly into account the Pauli principle, being thereby 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 specially 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 non collective excitations, elimination of the spurious states due to non conservation 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 technics as shown in ref.<sup>3</sup>).

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