PHYSICAL REVIEW C VOLUME 17, NUMBER 1 JANUARY 1978

# Multiphonon $K^\pi = 0^+$ states in even-even deformed nuclei. II. Calculation of matrix elements of a general Hamiltonian

B. Silvestre-Brac and R. Piepenbring
*Institut des Sciences Nucléaires, B. P. 257, 38044 Grenoble-Cédex, France*
(Received 16 June 1977)

Matrix elements of a general Hamiltonian $H$ in a subspace spanned by collective $K^\pi = 0^+$ deformed phonons are derived with the help of recursion formulas. Various approximations are discussed both in the fermion space and in the boson space. Careful comparisons are made in the framework of a simple solvable model.

[NUCLEAR STRUCTURE Multiphonon $K^\pi = 0^+$ states in deformed nuclei. Exact and approximate relations for matrix elements of a general Hamiltonian. Application to a solvable model.]

## I. INTRODUCTION

In many theories of nuclear collective motion, the concept of the phonon is adopted in order to describe the lowest excitation energies of an even-even nucleus.

In spherical vibrational nuclei the first $2^+$ state is generally assumed to be a one-quadrupole-phonon state and the members of the triplet $0^+$, $2^+$, $4^+$ are two-phonon states. Nevertheless, anharmonic effects are observed and lead to more complex structures of these levels. A lot of work has been devoted to the study of such anharmonicities.

One of the most promising ways to tackle this problem is the boson expansion method. With these techniques Kishimoto and Tamura[1] explained very nicely on equal footing the vibrational spherical nuclei, transitional nuclei, the rotational excitation, and the one-phonon vibrational states of deformed nuclei. But so far very little has been done to study multiphonon intrinsic states of axially deformed nuclei, where the quadrupole phonon is split into two different phonons: One with $K^\pi = 0^+$ often called $\beta$ vibration and one with $K^\pi = 2^+$ ($\gamma$ vibration), degenerate with the $K^\pi = -2^+$ vibration. In some deformed nuclei where one-phonon intrinsic states appear well below the pairing gap there is some experimental evidence[2] for two-phonon intrinsic levels, showing also anharmonic effects.

This paper is an attempt to study in a microscopic way some of these effects. In the case of a deformed basis where the single-particle levels are only pairwise degenerate, boson expansions are expected to be poorly converging.[3] To avoid these difficulties, it has been proposed[4] to remain in the fermion space and to diagonalize the Hamiltonian in the collective space spanned by $(Q^\dagger)^n|0\rangle$ where $Q^\dagger$ is a phonon operator of collective type and $n = 1, 2, \ldots, N$. The Pauli principle is then correctly fulfilled but the calculation of the norms of these states and the matrix elements of $H$ between them is quite tedious. Holzwarth, Janssen, and Jolos[4] proposed an approximation to solve such a problem and more recently Iwasaki, Sakata, and Takada[5] proposed an exact recursion formula for the norms of multiphonon states described in a spherical basis. It seems, however, that the application of this relation to a realistic case is not very easy.

In the case of a deformed basis the coupling to a good angular momentum is not needed and the expressions are simpler. In a recent paper[6] the authors derived an exact recursion formula for the norms of multiphonons deformed collective states. They gave also approximations for these calculations and pointed out the appearance of a cutoff factor $N_c$ beyond which these approximations fail.

In this article we are concerned with the dynamical aspect of that question. Using the same techniques as in Ref. 4 we derive, in Sec. II, exact and approximate recursion formulas for the matrix elements of $H$. In the exact expressions the Pauli principle is properly taken into account but the coupling between collective and noncollective degrees of freedom is neglected. In Sec. III, we apply the formalism to the simple model of $2m$ particles interacting by pure pairing forces in $2m$ equidistant levels. Such a model allows an exact numerical treatment and a careful analysis of the validity of the various approximations with respect to the collectivity of the basic phonon and to the cutoff of the basis used in the diagonalization of the Hamiltonian.

## II. THEORY

### A. Situation of the problem

We start with an orthonormal basis of quasiparticles; they may describe the particle-hole excitations or the more general Bogolyubov-Valatin type of excitations. The only requirement is the well-known anticommutation rules:

$$\{\alpha_\mu, \alpha_\nu\} = 0 = \{\alpha_\mu^\dagger, \alpha_\nu^\dagger\},$$
$$\{\alpha_\mu, \alpha_\nu^\dagger\} = \delta_{\mu\nu}. \tag{1}$$

In terms of those basic operators, the Hamiltonian of a system of identical fermions interacting through a two body force is expressed by

$$H = U + H_{11} + H_{40} + H_{31} + H_{22} \tag{2}$$

with

$$\begin{aligned} H_{11} &= \sum_\nu E_\nu \alpha_\nu^\dagger \alpha_\nu, \\ H_{40} &= \sum_{\alpha\beta\gamma\delta} P_{\alpha\beta\gamma\delta}(\alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma^\dagger \alpha_\delta^\dagger + \alpha_\delta \alpha_\gamma \alpha_\beta \alpha_\alpha), \\ H_{31} &= \sum_{\alpha\beta\gamma\delta} R_{\alpha\beta\gamma\delta}(\alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma^\dagger \alpha_\delta + \alpha_\delta^\dagger \alpha_\gamma \alpha_\beta \alpha_\alpha), \\ H_{22} &= \sum_{\alpha\beta\gamma\delta} S_{\alpha\beta\delta\gamma} \alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma \alpha_\delta \quad (S_{\alpha\beta\delta\gamma} = S_{\delta\gamma\alpha\beta}). \end{aligned} \tag{3}$$

The $P, R, S$ coefficients are assumed to be real, but this is, for what follows, of no importance. The diagonalization of the total Hamiltonian in the space generated by all the quasiparticle states is of course numerically impossible in most cases; moreover, the eigenvalues refer to nuclei differing by the number of particles. When dealing with even nuclei, one generally does the diagonalization in the two-quasiparticle (2 qp) space; this constitutes the Tamm-Dancoff approximation (TDA). It appears that among all the states obtained, one is collective in the sense that it is composed with a large number of 2 qp states. So let us introduce the TDA operators

$$Q_K^\dagger(i) = \frac{1}{2} \sum_{\mu\nu} X_{\mu\nu}^K(i) \alpha_\mu^\dagger \alpha_\nu^\dagger. \tag{4}$$

$K$ stands for the projection of the intrinsic angular momentum on the axis of symmetry and $i$ for all other quantum numbers.

Now we shall focus our interest only to $K^\pi = 0^+$ collective states and omit indices $i$ and $K$ henceforth. [The restriction to $K^\pi = 0^+$ states is introduced in order to simplify the formalism developed in Sec. II. We note that multiphonon states with $K = 0$ can be built up with couples of $Q_L^\dagger Q_{-L}^\dagger$ with $L \neq 0$. We do not consider those states in this paper.] The $X$ matrix is assumed to be real and antisymmetric and this is the reason of the $\frac{1}{2}$ factor in relation (4). The states $(Q^\dagger)^n|0\rangle$ contain $2n$ quasiparticles but they are expected to appear much lower in energy than other $2n$ qp levels. The two-phonon states $(Q^\dagger)^2|0\rangle$ present peculiar interest since they may lie below the gap and hence below the 2 qp spectrum. To avoid the tremendous eigenvalue problem in the qp space we treat here the diagonalization of $H$ in the "collective subspace $\mathcal{F}_c$" spanned by the set $(Q^\dagger)^n|0\rangle$, $\{n = 0, 1, \ldots, N\}$. We introduce normalized multiphonon states $|n\rangle = N_n (Q^\dagger)^n |0\rangle$. Due to the Pauli principle the calculation of the norm $N_n$ and of the matrix elements $\langle n|H|m\rangle$ is not easy. One convenient way to get them is to look for recursion formulas. This was done in Ref. 6 for the norm $N_n$; in this paper we repeat the same kind of techniques for the more complicated case of matrix elements $\langle n|H|m\rangle$. Before going further it is necessary to define two important quantities:

1. the successive powers of the $X$ matrix defined in the usual way and which contain most of the physical pieces of information

$$(X^k)_{\mu\nu} = \sum_{\{\rho_i\}} X_{\mu\rho_1} X_{\rho_1\rho_2} \cdots X_{\rho_{k-1}\nu}; \tag{5}$$

2. the "reduced norm" $\mathfrak{N}_n$ which measures the deviation of the fermion state $|n\rangle$ from a pure boson state $|n) = N_n^B (B^\dagger)^n |0)$

$$\mathfrak{N}_n = \frac{(N_n^B)^4}{(N_n)^2} = (n! N_n)^{-2}. \tag{6}$$

### B. Recursion formulas in fermion space

In Ref. 6 it was shown that the recursion formula for the norm in terms of $\mathfrak{N}_n$ is very simple:

$$n\mathfrak{N}_n = \mathfrak{N}_{n-1} - \frac{1}{2} \sum_{l=1}^{n-1} \mathrm{Tr}(X^{2l+2}) \mathfrak{N}_{n-l-1}; \tag{7}$$

the summation of the right-hand side is the exchange term due to the Pauli principle which makes that $Q^\dagger$ is not a pure boson.

It is possible to repeat exactly the same arguments for the $H_{11}$ part of the Hamiltonian. Defining formally an $E$ matrix by $(E)_{\mu\nu} = E_\nu \delta_{\mu\nu}$ where $E_\nu$ is the quasiparticle energy, we get

$$\mathfrak{N}_n \langle n|H_{11}|n\rangle = -\sum_{l=1}^{n} \mathrm{Tr}(EX^{2l}) \mathfrak{N}_{n-l}. \tag{8}$$

Once again the introduction of the reduced norm leads to a very simple relation.

We shall prove later that this is a very general feature; the $\mathfrak{N}_n$ are "the best tools" for our recursion formulas.

In the same way as approximations for $\mathfrak{N}_n$ were deduced in Ref. 6 it is possible to build approximations of order $p$ to the matrix elements of $H_{11}$.

They give the exact values of the quantity $\langle n|H_{11}|n\rangle$ up to $n=p$ and their expression is the following:

$$\mathfrak{N}_n\langle n|H_{11}|n\rangle^{(p)} = -\sum_{l=1}^{p-1}\mathrm{Tr}(EX^{2l})\mathfrak{N}_{n-l} - (n-p+1) \times \mathrm{Tr}(EX^{2p})\mathfrak{N}_{n-p+1}. \tag{9}$$

Let us now derive the calculation of the matrix elements for the two body part of the Hamiltonian. As an example of the method the $H_{40}$ term is treated in detail. It is obvious that the only non-vanishing elements are

$$\langle n+2|H_{40}|n\rangle = \langle n|H_{40}|n+2\rangle .$$

Consequently we study

$$\langle n+2|\alpha_\alpha^\dagger\alpha_\beta^\dagger\alpha_\gamma^\dagger\alpha_\delta^\dagger|n\rangle .$$

We define $R_n$ operators by induction

$$R_1 = \alpha_\alpha^\dagger\alpha_\beta^\dagger\alpha_\gamma^\dagger\alpha_\delta^\dagger,$$

$$R_{2p} = \Big[Q,\Big[Q,\Big[Q,[Q,R_{2p-1}]\Big]\Big]\Big], \tag{10}$$

$$R_{2p+1} = \Big[\Big[\Big[[R_{2p},Q^\dagger],Q^\dagger\Big],Q^\dagger\Big],Q^\dagger\Big]$$

and intermediate operators $R_n^{(i)}$ $(i=1,2,3)$ by

$$R_{2p}^{(i)} = \Big[\ldots\Big[[R_{2p},Q^\dagger],Q^\dagger\Big]\ldots,Q^\dagger\Big],$$

and (11)

$$R_{2p+1}^{(i)} = \Big[Q,\ldots,[Q,R_{2p+1}]\ldots\Big],$$

where there are $i$ operators $Q^\dagger$ and $i$ operators $Q$. It is only a matter of lengthy algebra to check the following properties

$$R_{2p} = (4!)^{2p-1}\sum_{\lambda\mu\sigma\rho}\alpha_\rho\alpha_\sigma\alpha_\mu\alpha_\lambda(X^{2p-1})_{\alpha\rho}(X^{2p-1})_{\beta\sigma}(X^{2p-1})_{\gamma\mu}(X^{2p-1})_{\delta\lambda}, \tag{12}$$

$$R_{2p+1} = (4!)^{2p}\sum_{\lambda\mu\sigma\rho}\alpha_\lambda^\dagger\alpha_\mu^\dagger\alpha_\sigma^\dagger\alpha_\rho^\dagger(X^{2p})_{\alpha\lambda}(X^{2p})_{\beta\mu}(X^{2p})_{\gamma\sigma}(X^{2p})_{\delta\rho},$$

$$\langle 0|R_{2p+1}T|0\rangle = 0 = \langle 0|R_{2p+1}^{(1)}T|0\rangle = \langle 0|TR_{2p}|0\rangle = \langle 0|TR_{2p}^{(1)}|0\rangle$$

for any operator $T$,

$$[R_{2p+1},Q^\dagger] = 0 = [Q,R_{2p}],$$

$$\langle 0|QR_{2p+1}^{(1)}|0\rangle = 2(4!)^{2p}\{(X^{4p+1})_{\alpha\beta}(X^{4p+1})_{\gamma\delta} + (X^{4p+1})_{\alpha\delta}(X^{4p+1})_{\beta\gamma} - (X^{4p+1})_{\alpha\gamma}(X^{4p+1})_{\beta\delta}\},$$

$$\langle 0|R_{2p}^{(1)}Q^\dagger|0\rangle = 2(4!)^{2p-1}\{(X^{4p-1})_{\alpha\beta}(X^{4p-1})_{\gamma\delta} + (X^{4p-1})_{\alpha\delta}(X^{4p-1})_{\beta\gamma} - (X^{4p-1})_{\alpha\gamma}(X^{4p-1})_{\beta\delta}\}.$$

In the course of the demonstration it is convenient, in order to avoid heavy expressions, to define the new quantities:

$$\begin{aligned} A_{2p}(n) &= \langle 0|Q^{n-4p+2}R_{2p}(Q^\dagger)^{n+4-4p}|0\rangle, \\ A_{2p+1}(n) &= \langle 0|Q^{n-4p+2}R_{2p+1}(Q^\dagger)^{n-4p}|0\rangle, \\ L_i^{(k)}(2p+1,n) &= \langle 0|Q^iR_{2p+1}^{(k)}Q^{n-4p+2-k-i}(Q^\dagger)^{n-4p}|0\rangle, \\ L_i^{(k)}(2p,n) &= \langle 0|Q^{n-4p+2}(Q^\dagger)^{n+4-4p-k-i}R_{2p}^{(k)}(Q^\dagger)^i|0\rangle \end{aligned} \tag{13}$$

with $k=1,2,3$. An interesting property connecting the $L_i^{(k)}$ may be proved (when no risk of misunderstanding arises we omit the arguments of the quantities $L_i^{(k)}$):

$$L_i^{(k)}(2p+1,n) = \langle 0|Q^{i-1}[Q,R_{2p+1}^{(k)}]Q^{n-4p+2-k-i}(Q^\dagger)^{n-4p}|0\rangle + \langle 0|Q^{i-1}R_{2p+1}^{(k)}Q^{n-4p+3-k-i}(Q^\dagger)^{n-4p}|0\rangle .$$

Since $[Q,R_{2p+1}^{(k)}] = R_{2p+1}^{(k+1)}$ by definition (11) it becomes

$$L_i^{(k)}(2p+1,n) = L_{i-1}^{(k+1)}(2p+1,n) + L_{i-1}^{(k)}(2p+1,n). \tag{14}$$

The same relation holds for the $L_i^{(k)}(2p,n)$.

After these definitions, we start the calculation of

$$\begin{aligned} A_1(n) &= \langle Q^{n+2}\alpha_\alpha^\dagger\alpha_\beta^\dagger\alpha_\gamma^\dagger\alpha_\delta^\dagger(Q^\dagger)^n\rangle \\ &= \langle Q^{n+2}R_1(Q^\dagger)^n\rangle \\ &= \langle Q^{n+1}[Q,R_1](Q^\dagger)^n\rangle + \langle Q^{n+1}R_1Q(Q^\dagger)^n\rangle \\ &= \langle Q^{n+1}R_1^{(1)}(Q^\dagger)^n\rangle + \langle Q^nR_1^{(1)}Q(Q^\dagger)^n\rangle \\ &\quad + \langle Q^nR_1Q^2(Q^\dagger)^n\rangle . \end{aligned}$$

Carrying on this process till $R_1$ acts directly on the vacuum one gets $A_1(n) = \sum_{i=0}^{n+1}L_i^{(1)}(1,n)$.

Introducing $S_l^{(k)} = \sum_{j=0}^{l}L_j^{(k)}$, noting that $L_0^{(1)} = 0$ because of relation (12) and using Eq. (14), one gets

$$A_1(n) = S_{n+1}^{(1)} = S_n^{(1)} + S_n^{(2)}. \tag{15}$$

Elimination of $S_n^{(1)}$ from this recursion formula leads to

$$S_{n+1}^{(1)} = \sum_{i=1}^{n}S_i^{(2)}. \tag{16}$$

Repeating exactly the same algebraic manipulations one gets

$$S_i^{(2)} = C_{i+1}^1 L_0^{(2)}(1,n) + \sum_{l=0}^{i-1} S_l^{(3)} \tag{17}$$

and

$$S_i^{(3)} = C_{i+1}^1 L_0^{(3)}(1,n) + C_{i+1}^2 A_2(n) \tag{18}$$

where the $C_n^p$ are the usual binomial coefficients. Removing the $S_j$ expressions from relations (18), (17), (16), and (15) and making use of identity

$$\sum_{i=0}^{k} C_{i+1}^p = C_{k+2}^{p+1}$$

the result for $A_1(n)$ is

$$A_1(n) = C_{n+2}^2 L_0^{(2)}(1,n) + C_{n+2}^3 L_0^{(3)}(1,n) + C_{n+2}^4 A_2(n) . \tag{19}$$

By the same techniques it is possible to show the more general relation

$$A_p(n) = C_{n+4-2p}^2 L_0^{(2)}(p,n) + C_{n+4-2p}^3 L_0^{(3)}(p,n) + C_{n+4-2p}^4 A_{p+1}(n) . \tag{20}$$

The procedure ends at the following $A_p(n)$:

$$A_{n/2+1}(n) = L_0^{(2)}(n/2+1, n)$$

if $n$ is even,

and

$$A_{(n+1)/2}(n) = 3 L_0^{(2)}[(n+1)/2, n] + L_0^{(3)}[(n+1)/2, n]$$

if $n$ is odd. (21)

The recursion formula (20) with the "boundary" condition (21) is sufficient to determine $A_1(n)$ once the $L_0^{(2)}$ and $L_0^{(3)}$ quantities are known. $L_0^{(2)}$ is directly deduced from its definition; the calculation of $L_0^{(3)}$ is more involved: It uses the following lemma (analogous to the recursion formulation[6] for the norm)

$$\langle Q^{n-1} \alpha_\mu \alpha_\lambda (Q^\dagger)^n \rangle = \langle Q^n \alpha_\lambda^\dagger \alpha_\mu^\dagger (Q^\dagger)^{n-1} \rangle = n!\,(n-1)! \sum_{l=0}^{n-1} (X^{2l+1})_{\lambda\mu} \mathfrak{N}_{n-l-1} . \tag{22}$$

The result for $L_0^{(2)}$ and $L_0^{(3)}$ is

$$L_0^{(2)}(p,n) = 2(4!)^{p-1} \{ (X^{2p-1})_{\alpha\beta} (X^{2p-1})_{\gamma\delta} + (X^{2p-1})_{\alpha\delta} (X^{2p-1})_{\beta\gamma} - (X^{2p-1})_{\alpha\gamma} (X^{2p-1})_{\beta\delta} \} N_{n+2-2p}^{-2} ,$$

$$L_0^{(3)}(p,n) = 6(4!)^{p-1} (n+2-2p)!\,(n+1-2p)!$$

$$\times \sum_{l=0}^{n+1-2p} \mathfrak{N}_{n+1-2p-l} \{ (X^{2p+1+2l})_{\alpha\beta} (X^{2p-1})_{\gamma\delta} + (X^{2p-1})_{\alpha\beta} (X^{2p+1+2l})_{\gamma\delta} + (X^{2p+1+2l})_{\alpha\delta} (X^{2p-1})_{\beta\gamma} + (X^{2p-1})_{\alpha\delta} (X^{2p+1+2l})_{\beta\gamma} - (X^{2p+1+2l})_{\alpha\gamma} (X^{2p-1})_{\beta\delta} - (X^{2p-1})_{\alpha\gamma} (X^{2p+1+2l})_{\beta\delta} \} . \tag{23}$$

At this stage the problem of the determination of $A_1(n)$ is wholly solved but the equations are not very tempting. One can do a little bit more by elimination of the $A_p(n)$ quantities from the recursion formula. After some simplification one gets the final result:

$$(\mathfrak{N}_{n+2}\mathfrak{N}_n)^{1/2} \langle n+2 \,|\, \alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma^\dagger \alpha_\delta^\dagger \,|\, n \rangle = \sum_{l=0}^{[n/2]} \mathfrak{N}_{n-2l} \{ (X^{2l+1})_{\alpha\beta} (X^{2l+1})_{\gamma\delta} + (X^{2l+1})_{\alpha\delta} (X^{2l+1})_{\beta\gamma} - (X^{2l+1})_{\alpha\gamma} (X^{2l+1})_{\beta\delta} \}$$

$$+ \sum_{l=0}^{[(n-1)/2]} \sum_{k=0}^{n-1-2l} \mathfrak{N}_{n-1-2l-k} \{ (X^{2l+3+2k})_{\alpha\beta} (X^{2l+1})_{\gamma\delta} + (X^{2l+1})_{\alpha\beta} (X^{2l+3+2k})_{\gamma\delta} + (X^{2l+3+2k})_{\alpha\delta} (X^{2l+1})_{\beta\gamma} + (X^{2l+1})_{\alpha\delta} (X^{2l+3+2k})_{\beta\gamma} - (X^{2l+3+2k})_{\alpha\gamma} (X^{2l+1})_{\beta\delta} - (X^{2l+1})_{\alpha\gamma} (X^{2l+3+2k})_{\beta\delta} \} . \tag{24}$$

In the upper bound of the summation the symbol $[x]$ stands for integer $m$ such that $m \leq x < m+1$. It is easy to check that all symmetry properties of $\alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma^\dagger \alpha_\delta^\dagger$ are fulfilled in the explicit expression of the matrix elements (24). One sees again that the reduced norms play an important role.

It is always possible to choose the $P_{\alpha\beta\gamma\delta}$ coefficient of the $H_{40}$ part of the Hamiltonian (3) in such a way that it verifies all the symmetry properties of $\alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma^\dagger \alpha_\delta^\dagger$; for instance,

$$P_{\alpha\beta\gamma\delta} = P_{\alpha\gamma\delta\beta} = -P_{\alpha\gamma\beta\delta} = P_{\gamma\delta\alpha\beta} = \cdots .$$

We assume that this choice is done once for all with the unique aim to simplify the writing of formulas. In that case we need only one physical quantity for $H_{40}$, namely,

$$\mathcal{P}(l,m) = \sum_{\alpha\beta\gamma\delta} P_{\alpha\beta\gamma\delta} (X^l)_{\alpha\beta} (X^m)_{\gamma\delta} . \tag{25}$$

Then

$$\frac{(\mathcal{N}_{n+2}\mathcal{N}_n)^{1/2}}{3}\langle n+2|H_{40}|n\rangle = \sum_{l=0}^{[n/2]} \mathcal{P}(2l+1,2l+1)\mathcal{N}_{n-2l} + 2\sum_{l=0}^{[(n-1)/2]}\sum_{k=0}^{n-1-2l}\mathcal{P}(2l+3+2k,2l+1)\,\mathcal{N}_{n-1-2l-k} \tag{26}$$

As was already mentioned in Ref. 6 for the calculation of the norm and as is obvious from (25) what is numerically time consuming is the evaluation of the power $X^l$ with large $l$. One way to avoid those lengthy computations would be to assume that the operator $R_p$ scatters only in collective states. Within that approximation the boundary condition (21) is replaced by

$$A_p(n) = N_2^{\,2}\langle R_p^{(2)}\rangle / N_{n+4-2p}^{\,2} = N_2^{\,2}N_{n+2-2p}^{\,2}L_0^{(2)}(p,n)/N_{n+4-2p}^{\,2}. \tag{27}$$

The matrix element $\langle n|H_{40}|n-2\rangle$ is still exactly given up to $n=2p$. The approximation (27) is therefore called of order $2p$ and replaces Eq. (26) by

$$\frac{(\mathcal{N}_{n+2}\mathcal{N}_n)^{1/2}}{3}\langle n+2|H_{40}|n\rangle^{(2p)} = \sum_{l=0}^{p-2}\mathcal{P}(2l+1,2l+1)\mathcal{N}_{n-2l} + 2\sum_{l=0}^{p-2}\sum_{k=0}^{n-1-2l}\mathcal{P}(2l+3+2k,2l+1)\mathcal{N}_{n-1-2l-k} + C^2_{n+4-2p}\mathcal{N}_{n+4-2p}\mathcal{N}_2^{-1}\mathcal{P}(2p+1,2p+1). \tag{28}$$

To be self-consistent in this relation, it is necessary to take the $(2p-1)$th approximation for the norm defined in Ref. 6. Comparison between (28) and (26) shows that the terms neglected in the summations of (26) are partially taken into account through an extra term in (28). The violation of the Pauli principle is caused by that replacement.

Actually in the double summation of Eq. (26) the largest power $X^l$ to be calculated is $X^{2n+1}$ ($l=0$, $k=n-1$); the same power $X^{2n+1}$ occurs in the $2p$th approximation. So we see that the amount of difficulties is quite analogous in the approximative expression and in the exact one; therefore the $2p$th approximations are of little interest in practice. There is, however, an important exception, namely the second approximation; in the case, the double summation is absent and one is left only with the extra term whose maximum power of $X$ is $X^3$. This approximation just corresponds to that described in detail by Holzwarth *et al.*[4]

The treatment of the collective matrix elements of $H_{40}$ has been done in great detail. We do not insist upon the derivation of those of $H_{31}$ and $H_{22}$ which is quite similar. The results are listed below rather briefly. The only nonvanishing elements for $H_{31}$ are $\langle n+1|H_{31}|n\rangle = \langle n|H|n+1\rangle$. Assuming again that the $R_{\alpha\beta\gamma\delta}$ have the good properties of symmetry $R_{\alpha\beta\gamma\delta} = R_{\gamma\alpha\beta\delta} = -R_{\alpha\gamma\beta\delta} = \ldots$ and defining the dynamical quantity

$$\mathcal{R}(l,m) = \sum_{\alpha\beta\gamma\delta} R_{\alpha\beta\gamma\delta}(X^l)_{\alpha\beta}(X^m)_{\gamma\delta}, \tag{29}$$

the matrix element of $H_{31}$ looks like

$$\frac{(\mathcal{N}_{n+1}\mathcal{N}_n)^{1/2}}{3}\langle n+1|H_{31}|n\rangle = -\sum_{l=1}^{[(n+1)/2]}\mathcal{R}(2l-1,2l)\mathcal{N}_{n+1-2l} - \sum_{l=1}^{[n/2]}\sum_{k=0}^{n-2l}\mathcal{N}_{n-2l-k}\{\mathcal{R}(2l+1+2k,2l)+\mathcal{R}(2l-1,2l+2+2k)\}. \tag{30}$$

In that case the $2p$th approximation give the exact matrix element up to $\langle 2p|H_{31}|2p-1\rangle$ and its explicit expression is

$$\frac{(\mathcal{N}_{n+1}\mathcal{N}_n)^{1/2}}{3}\langle n+1|H_{31}|n\rangle^{(2p)} = -\sum_{l=1}^{p-1}\mathcal{R}(2l-1,2l)\mathcal{N}_{n+1-2l} - \sum_{l=1}^{p-1}\sum_{k=0}^{n-2l}\mathcal{N}_{n-2l-k}\{\mathcal{R}(2l+1+2k,2l)+\mathcal{R}(2l-1,2l+2+2k)\} - C^2_{n+3-2p}\mathcal{N}_{n+3-2p}\mathcal{N}_2^{-1}\mathcal{R}(2p-1,2p). \tag{31}$$

Here again only the second approximation is of practical interest.

For the determination of $\langle n|H_{22}|n\rangle$ two different dynamical quantities are needed:

$$\mathcal{S}_{\mathrm{I}}(p,q) = \sum_{\alpha\beta\gamma\delta} S_{\alpha\beta\delta\gamma}(X^p)_{\alpha\beta}(X^q)_{\gamma\delta}, \qquad \mathcal{S}_{\mathrm{II}}(p,q) = \sum_{\alpha\beta\gamma\delta} S_{\alpha\beta\delta\gamma}(X^p)_{\alpha\gamma}(X^q)_{\beta\delta}. \tag{32}$$

Then

$$\mathfrak{N}_n\langle n|H_{22}|n\rangle = -\sum_{l=0}^{n-1} \mathcal{S}_{\mathrm{I}}(2l+1,1)\mathfrak{N}_{n-l-1} - \sum_{l=1}^{[n/2]} \mathfrak{N}_{n-2l}\{\mathcal{S}_{\mathrm{I}}(2l-1,2l+1)+2\mathcal{S}_{\mathrm{II}}(2l,2l)\}$$

$$-\sum_{l=1}^{[(n-1)/2]}\sum_{k=0}^{n-2l-1} \mathfrak{N}_{n-2l-1-k}\{\mathcal{S}_{\mathrm{I}}(2l+1+2k,2l+1)+\mathcal{S}_{\mathrm{I}}(2l-1,2l+3+2k)+4\mathcal{S}_{\mathrm{II}}(2l+2+2k,2l)\}. \quad (33)$$

The $2p$th approximation gives the exact result up to $\langle 2p|H_{22}|2p\rangle$ and has the following expression:

$$\mathfrak{N}_n\langle n|H_{22}|n\rangle^{(2p)} = -\sum_{l=0}^{2p-2} \mathcal{S}_{\mathrm{I}}(2l+1,1)\mathfrak{N}_{n-l-1} - \sum_{l=0}^{p-1} \mathfrak{N}_{n-2l}\{\mathcal{S}_{\mathrm{I}}(2l-1,2l+1)+2\mathcal{S}_{\mathrm{II}}(2l,2l)\}$$

$$-\sum_{l=1}^{p-1}\sum_{k=0}^{n-2l-1} \mathfrak{N}_{n-2l-1-k}\{\mathcal{S}_{\mathrm{I}}(2l+1+2k,2l+1)+\mathcal{S}_{\mathrm{I}}(2l-1,2l+3+2k)+4\mathcal{S}_{\mathrm{II}}(2l+2+2k,2l)\}$$

$$-C^1_{n+1-2p}\mathfrak{N}_{n+1-2p}\mathcal{S}_{\mathrm{I}}(4p-1,1) - C^2_{n+2-2p}\mathfrak{N}_{n+2-2p}\mathfrak{N}_2^{-1}\{\mathcal{S}_{\mathrm{I}}(2p-1,2p+1)+2\mathcal{S}_{\mathrm{II}}(2p,2p)\}. \quad (34)$$

The relations (8), (26), (30), and (33) allow an exact diagonalization of $H$ in the subspace of the collective subspace $\mathfrak{F}_C$.

### C. Recursion formulas in boson space

In $\mathfrak{F}_C$, the exact treatment in a realistic case is limited by the numerical evaluation of the powers of the matrix $X$. We have shown that the $2p$th approximations, which are introduced naturally in the theory, are of no practical help except the second approximation.

In order to avoid this difficulty it is possible to deal with the boson representation of the Hamiltonian through the modified Marumori's expansion intially studied by Kleber[7] and analyzed in more detail by Lie and Holzwarth.[8] The aim of the method is to establish a one to one correspondence between the fermion states $|n\rangle$ in $\mathfrak{F}_C$ and the boson states $|n)$ in $\mathfrak{B}_C$.

The mapping operator is $U = \sum_n |n\rangle(n|$ and the boson Hamiltonian

$$H^B_{\mathrm{col}} = \sum_{n,n'=0}^{\infty} \langle n|H|n'\rangle [n!n'!]^{-1/2}(B^\dagger)^n|0)(0|B^{n'}$$
$$= U^\dagger H_{\mathrm{col}} U .$$

Expressing the collective part of $|0)(0|$ by its value

$$|0)(0| = :\exp -B^\dagger B: = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!}(B^\dagger)^k B^k$$

we get

$$H^B_{\mathrm{col}} = \sum_{n,n',k=0}^{\infty} \langle n|H|n'\rangle [n!n'!]^{-1/2}\frac{(-1)^k}{k!}(B^\dagger)^{n+k}B^{n'+k}. \quad (35)$$

Equation (35) is exact in the sense that $\langle n|H|m\rangle = (n|H^B_{\mathrm{col}}|m)$ for all $|n\rangle$ and $|m\rangle$. Nevertheless, it is of no practical use because its application necessitates the computation of the matrix elements $\langle n|H|n'\rangle$ for all $|n\rangle$ and $|n'\rangle$ and hence the problem is as difficult as in the fermion state.

One way to simplify the treatment was suggested by Holzwarth *et al.*[4]: It consists in the truncation of the summation in relation (35) to low values of $n$ and $n'$ so that $n+n' < N_{\max}$ and consequently to the truncation of $k$ in a self-consistent manner. It is possible in the boson space $\mathfrak{B}_C$ to define a $2p$th approximation in a very similar way as in the fermion space by requiring the matrix elements to be exact up to $\langle 2p|H|p'\rangle$ $(2p \geq p')$.

Explicitly the $2p$th approximation of the boson Hamiltonian is

$$H^{B(2p)}_{\mathrm{col}} = \sum_{n=0}^{2p}\frac{\langle n|H|n\rangle}{n!}\sum_{k=0}^{2p-n}\frac{(-1)^k}{k!}(B^\dagger)^{n+k}B^{n+k} + \sum_{n=0}^{2p-1}\frac{\langle n+1|H|n\rangle}{[n!(n+1)!]^{1/2}}\sum_{k=0}^{2p-1-n}\frac{(-1)^k}{k!}[(B^\dagger)^{n+1+k}B^{n+k}+(B^\dagger)^{n+k}B^{n+1+k}]$$

$$+\sum_{n=0}^{2p-2}\frac{\langle n+2|H|n\rangle}{[n!(n+2)!]^{1/2}}\sum_{k=0}^{2p-2-n}\frac{(-1)^k}{k!}[(B^\dagger)^{n+2+k}B^{n+k}+(B^\dagger)^{n+k}B^{n+2+k}]. \quad (36)$$

The advantage of this approximation with respect to the corresponding one in the fermion space is that it is a recursion formula on the matrix elements of the Hamiltonian (and not on the norms) and the numerical difficulty already mentioned for the fermion matrix elements disappear in the present case. One can also define odd order approximations but they are not useful for comparison with the fermion case.

### D. Summary

In the preceding subsections, general theoretical expressions were given for the matrix elements of the Hamiltonian in the subspace $\mathfrak{F}_C$. They completely fulfill the Pauli requirements. However, in realistic situations, the numerical computation is more and more time consuming when increasing the number of phonons and hence an approximate treatment becomes necessary. If one works in the fermion subspace $\mathfrak{F}_C$, it was shown that only the second approximation presents some simplification to the problem. Higher order approximations can be obtained easily only in the boson space $\mathfrak{B}_C$. In that case to get $(n|H^B_{\text{coll}}|m)$ for $n \gg 2p$ one needs exact values of $\langle k|H|l\rangle$ in fermion space up to $l \leq k \leq 2p$ and geometrical factors such as $(n|B^{\dagger p}B^q|m)$. So the computation of $(n|H^B_{\text{col}}|m)$ is always tractable even if $n \gg 2p$. The discussion and comparison of those different approximations in a numerically solvable case is the subject of the next section.

## III. APPLICATION AND DISCUSSION

### A. Choice of the model

The general formalism developed in the preceding section is applied to a simple model which allows an exact numerical treatment and is realistic enough to exhibit some systematic features. We consider $2m$ particles filling $2m$ equidistant pairwise degenerate levels; the distance between two consecutive ones is $2D$ and all levels are assumed to have different projection $\Omega$ of $j$ on the axis of symmetry. The particles interact via a pure constant monopole pairing force $G$. We do not want to solve the exact physical problem but our main interest is the comparison of various approximations within the same model space. So we perform a Bogolyubov-Valatin transformation which keeps the average value for the number of particles equal to $2m$ and our model space is spanned by those quasiparticle operators. We have in mind that spurious solutions appear in the treatment and hence do not try to compare our results to exact physical ones. What we aim to point out is the quality of different approaches to the same problem as a function of the collectivity of the basic phonon.

Within this schematic model the dispersion equation for the TDA solutions splits into two different equations:

A first one whose lowest level (solution I) may be considered as collective and which has the symmetry property $X_{2m+1-i,-(2m+1-i)} = X_{i,-i}$ $(i = 1, \ldots, m)$.

A second one whose lowest level (solution II) lies in the vicinity of the gap $2\Delta$ and which has the symmetry property $X_{2m+1-i,-(2m+1-i)} = -X_{i,-i}$.

Solution II being never collective, we use solution I in the rest of the paper.

The parameter varying the collectivity is $D/G$ or equivalently $D/\Delta$. The smaller the ratio $D/\Delta$ the stronger the collectivity. Because we consider $0^+$ states and because all levels are characterized by different values of $\Omega$ the $X$ matrix only has "diagonal" elements $X_{\nu,-\nu}$ so that

$$Q^\dagger = \sum_{\nu>0} X_{\nu,-\nu} \alpha^\dagger_\nu \alpha^\dagger_{-\nu} .$$

In more realistic situations the diagonal elements $X_{\nu,-\nu}$ are known to be predominant and hence the choice of our model is not unreasonable. The simplicity of the matrix $X$ makes the calculations of the various quantities extremely fast and allows an exact treatment.

### B. Discussion of the cutoff factor $N_c$

In Ref. 6 different approximations for the norm $\mathfrak{N}_n$ are discussed and it is shown that there exists a critical value of $n$ noted $N_c$ such that all approximations, irrespective of their order of accuracy, fails for $n > N_c$. The $N_c$ values, and consequently the validity of the approximations, increase with the collectivity of the phonon $Q^\dagger$. In practice it is important to have an idea of $N_c$ and it was suggested[6] that a good criterion for this is the ratio

$$\eta = \left| \frac{\mathrm{Tr}(X^4)}{\mathrm{Tr}(X^2)} \right| = \frac{|\mathrm{Tr}(X^4)|}{2} .$$

When the TDA solution is a pure two-quasiparticle state, one $X_{\nu-\nu}$ equals $1/\sqrt{2}$ and all others vanish, leading to $\eta = \frac{1}{2}$. When the solution presents a maximum of collectivity all the $X_{\nu-\nu}$ are equal and the value for $\eta$ is $1/(2m)$. We have studied for

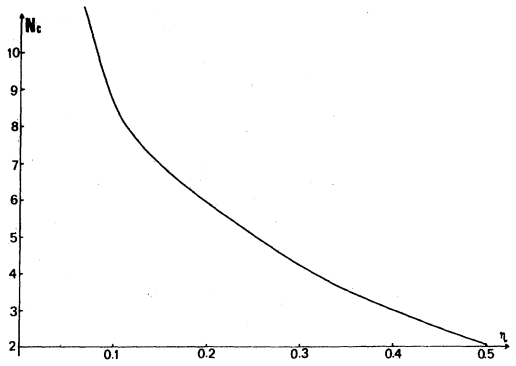


FIG. 1. The critical cutoff factor $N_c$ is plotted as a function of the parameter $\eta$ defined in Sec. III B.

different choices of $m$ and $D/\Delta$ the relationship between $N_c$ and $\eta$. It appears that this is a bijection, in the sense that two situations with the same $\eta$ give roughly the same $N_c$. Figure 1 illustrates the correspondence between $\eta$ and $N_c$. In more realistic treatments the same kind of conclusion ought to be valid: The parameter $\eta$ is a good indication for the determination of $N_c$.

### C. Matrix elements in $\mathfrak{F}_c$

Let us now come to the calculation of the fermion matrix elements $\langle n|H|m\rangle$ and their $2p$th approximation $\langle n|H|m\rangle^{(2p)}$. Table I summarizes the results in the case of 10 single particle levels ($2m = 10$) for a typical value 0.2 of $D/\Delta$. For these parameters $N_c$ equals 6 and the table may be divided into two parts, one with $n < N_c$ and one with $n \geq N_c$. We write the matrix elements for $H_{11}$, $H_{22}$, $H_{\mathrm{TDA}} = H_{11} + H_{22}$ and $H_{40}$. The symmetry properties of the phonon considered here make $\langle n|H_{31}|n-1\rangle$ vanish identically. Concerning the $2p$th approximations ($p = 1, 2, 3$) we apply the formulas given in the preceding section with the $(2p-1)$th approximation $\mathfrak{N}_n^{(2p-1)}$ for the norm. Within this approximation $\mathfrak{N}_n^{(2p-1)}$ can be found negative for some values of $n \geq N_c$ and hence the factor $(\mathfrak{N}_n\mathfrak{N}_{n-2})^{1/2}$ appearing in the matrix element $\langle n|H_{40}|n-2\rangle^{(2p)}$ is meaningless; the corresponding cases in Table I are marked with an asterisk. The comparison between the exact results and the various approximations shows that the accuracy is rather good for matrix elements with $n < N_c$; for $n \geq N_c$ all approximations are equally wrong. The existence of a critical number $N_c$ which was deduced[6] from the examination of the norms $\mathfrak{N}_n^{(p)}$ is stiffened greatly from the dynamical point of view; in fact, the two aspects are related because the norms are ingredients of the recursion formulas for the matrix elements of $H$. However, there is a notable exception: although $\langle n|H_{11}|n\rangle^{(2)}$ and $\langle n|H_{22}|n\rangle^{(2)}$ are separately false for $n > N_c$, their sum $\langle n|H_{\mathrm{TDA}}|n\rangle^{(2)}$ is remarkably good for all $n$. This is true only for the second approximation. We have no definite explanation for such a phenomenon; it is probably due to the symmetry properties of our problem. In general, for $n < N_c$, the accuracy increases when the phonon $Q^\dagger$ is very collective (low values of $D/\Delta$) and when the order of the approximation increases.

Another important point of discussion is the results of the diagonalization of $H$ in $\mathfrak{F}_C$. Figure 2 deals with the resulting spectrum when increasing the number of basic states of $\mathfrak{F}_C$. The lower the excited state is, the faster the stability is reached. At once, let us point out an important feature which does not appear in the figure. When the dimension of the basis is greater than $N_c$, "dangerous" states appear in the fourth and sixth approximations; by dangerous we mean that those states are low in energy (even they may be the "ground state") but composed predominantly with a great number of phonons. To be fair we must add that in order to carry out the diagonalization it was necessary to fix a determined value to the "impossible" $\langle n|H_{40}|n-2\rangle^{(2p)}$ (the boxes with * in

TABLE I. Matrix elements $\langle n|H_i|m\rangle$ in MeV of different parts of the Hamiltonian in the collective subspace $\mathfrak{F}_C$. Exact values and approximate ones ($2p = 2, 4, 6$) are listed. The parameters used are $2m = 10$, $D = 0.2$ MeV, and $\Delta = 1$ MeV and lead to $N_c = 6$. For $n \leq 2p$ one has $\langle n|H|m\rangle^{(2p)} = \langle n|H|m\rangle$ and consequently the corresponding values are not written in the table. As quoted in Sec. III C, the asterisk represents quantities impossible to calculate because the argument of $(\mathfrak{N}_{n+2}^{(2p)}\mathfrak{N}_n^{(2p)})^{1/2}$ is negative.

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| $\langle n\|H_{11}\|n\rangle$ | 2.390 | 4.873 | 7.471 | 10.198 | 13.066 | 16.080 | 19.241 | 22.540 | 25.971 | 29.519 |
| $\langle n\|H_{11}\|n\rangle^{(2)}$ | | | 7.526 | 10.530 | 14.469 | 22.879 | −29.512 | 8.608 | 14.121 | 17.544 |
| $\langle n\|H_{11}\|n\rangle^{(4)}$ | | | | | 13.446 | 6.637 | 15.048 | 18.591 | 15.207 | 21.329 |
| $\langle n\|H_{11}\|n\rangle^{(6)}$ | | | | | | | 11.796 | 16.736 | 19.504 | 22.408 |
| $\langle n\|H_{22}\|n\rangle$ | −1.145 | −2.065 | −2.771 | −3.267 | −3.560 | −3.649 | −3.536 | −3.222 | −2.707 | −2.001 |
| $\langle n\|H_{22}\|n\rangle^{(2)}$ | | | −2.836 | −3.639 | −5.059 | −10.630 | 44.918 | 10.273 | 8.553 | 9.243 |
| $\langle n\|H_{22}\|n\rangle^{(4)}$ | | | | | −3.277 | −11.521 | −6.835 | −3.936 | −29.535 | −12.816 |
| $\langle n\|H_{22}\|n\rangle^{(6)}$ | | | | | | | −10.241 | −8.604 | −8.833 | −8.913 |
| $\langle n\|H_{\mathrm{TDA}}\|n\rangle$ | 1.245 | 2.808 | 4.700 | 6.931 | 9.507 | 12.431 | 15.704 | 19.318 | 23.264 | 27.518 |
| $\langle n\|H_{\mathrm{TDA}}\|n\rangle^{(2)}$ | | | 4.690 | 6.891 | 9.410 | 12.248 | 15.405 | 18.881 | 22.675 | 26.788 |
| $\langle n\|H_{\mathrm{TDA}}\|n\rangle^{(4)}$ | | | | | 10.169 | −4.883 | 8.212 | 14.655 | −14.328 | 8.513 |
| $\langle n\|H_{\mathrm{TDA}}\|n\rangle^{(6)}$ | | | | | | | 1.555 | 8.131 | 10.670 | 13.495 |
| $\langle n\|H_{\mathrm{TDA}}\|n-2\rangle$ | 0 | 0.807 | 1.253 | 1.568 | 1.762 | 1.836 | 1.788 | 1.614 | 1.309 | 0.858 |
| $\langle n\|H_{40}\|n-2\rangle^{(2)}$ | | | 1.131 | 1.221 | 1.084 | 0.708 | * | 0.403 | −1.498 | 2.730 |
| $\langle n\|H_{40}\|n-2\rangle^{(4)}$ | | | | | 1.914 | * | * | −5.166 | * | * |
| $\langle n\|H_{40}\|n-2\rangle^{(6)}$ | | | | | | | * | * | 0.035 | −1.295 |

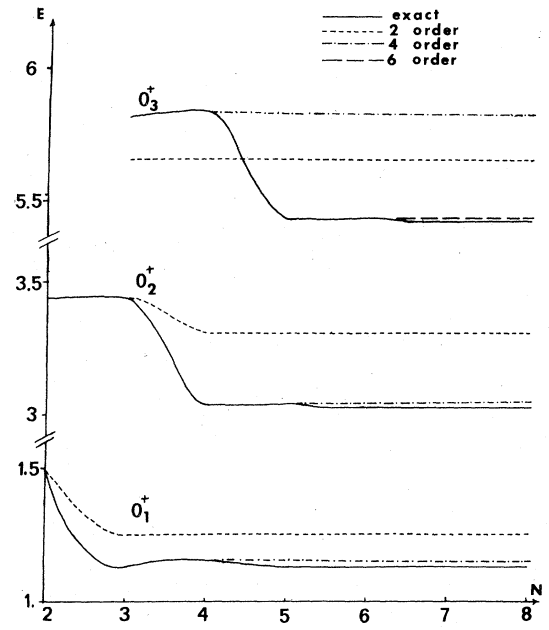


FIG. 2. Energy spectra for the three first excited states versus the dimension $N+1$ of the fermion collective subspace $\mathfrak{F}_C$. Exact treatment and 2nd, 4th, and 6th approximations are compared; as explained in Sec. III C the "dangerous" states have been omitted. The parameters are $2m=8$, $D=0.3$ MeV, and $\Delta=1$ MeV; $E$ is expressed in MeV. For the two first excited states the 6th approximation cannot be distinguished from the exact ones.

Table I). Arbitrarily we put them equal to zero and this may explain partly the above disagreement. Systematically those dangerous states have been skipped out in the plot of Fig. 2. Nevertheless, it seems that $N_c$ is another source of disagreement. The important thing is that those dangerous states do not appear at all in the second approximation, which again have some originality among all other ones (this fact may be related to the above mentioned behavior of $\langle n|H_{\mathrm{TDA}}|n\rangle^{(2)}$ for all $n$). The accuracy of the approximations (except the dangerous states) increases with their order $2p$ and with the collectivity of the basic phonon $Q^\dagger$; moreover, they are quite good for the first excited states. This is not surprising since these approximations are built to fulfill those conditions.

### D. Collective noncollective coupling

The collective subspace $\mathfrak{F}_C$ is introduced in order to take into account the major part of the physical information and to avoid a diagonalization beyond measure. This simplification obviously neglects the coupling between collective and noncollective degrees of freedom. Our aim now is to test the influence of this coupling. In our case, $\mathfrak{F}_C$, whose dimension is $2m+1$, is a part of the more general space $\mathfrak{F}_T$ spanned by the state of "zero seniority" $|\nu_1\nu_2\cdots\nu_k\rangle=\alpha^\dagger_{\nu_1}\alpha^\dagger_{-\nu_1}\alpha^\dagger_{\nu_2}\alpha^\dagger_{-\nu_2}\cdots\alpha^\dagger_{\nu_k}\alpha^\dagger_{-\nu_k}|0\rangle$ of dimension $2^m$.

We only retain in the complete spectrum the states whose overlap with the collective states $|n\rangle$ is near unity; the difference in energy between the two states measures the coupling with the noncollective phonons Table II summarizes this effect as well as the contribution of each part of the Hamiltonian in the two extreme cases a very collective one and a noncollective one. From examination of the spectrum in $\mathfrak{F}_T$, one sees that the influence of the $H_{40}$ term of the Hamiltonian is to lower the first excited state and to raise the others; this feature is *grosso modo* reinforced by addition of $H_{31}$. The perturbation due to $H_{40}$ is more important than that of $H_{31}$ for low values of $D/\Delta$ but it is of the same order of magnitude for larger values. Concerning the diagonalization in $\mathfrak{F}_C$, it was underlined above that fortuitously the contribution of the $H_{31}$ part vanishes. Hence the comparison with $\mathfrak{F}_T$ must be done only for $H_{\mathrm{TDA}}$ and $H_{\mathrm{RPA}}$. For $D/\Delta=0.1$ the truncation of the basis has practically no influence upon the collective states, the coupling with noncollective branches being less than $10^{-3}$. For not very collective TD phonons ($D/\Delta=0.5$) the diagonalization in the restricted space is nevertheless quite reasonable since the coupling is of order of a few percent in that case.

The major part of the interaction is contained in $H_{\mathrm{TDA}}$ and this explains that the choice of a TDA phonon as the starting point is rather good. It is obvious from Table II that the spectrum is no longer harmonic since the Pauli principle is taken into account correctly in that treatment. It may be noted also that the energy of the two-phonon state is larger than twice the energy of the one-phonon level (at least in our model dealing with a pure monopole pairing force); this is generally not the situation in actual nuclei. This suggests that a correct description of realistic cases certainly need another type of force (i.e., quadrupole quadrupole, quadrupole pairing, etc...). The conclusion of this section is that the diagonalization in $\mathfrak{F}_C$ is in most cases justified. We emphasize again that the obtained spectrum must not be compared with the actual physical one because of the presence of spurious states (due to the nonconservation of the number of particles) whose removing is not the aim of this paper. This problem was carried out by projection techniques by Gunsteren and Allaart[9] and by elimination of the "spurious space" by Iwasaki *et al.*[10]

TABLE II. Energies (in MeV) of excited states in the complete $\mathfrak{F}_T$ and collective $\mathfrak{F}_C$ spaces for different parts of Hamiltonian $H_{\rm TDA} = H_{11} + H_{22}$, $H_{\rm RPA} = H_{\rm TDA} + H_{40}$, $H = H_{\rm RPA} + H_{31}$, and for two extreme values of $D/\Delta$. Comparison between $\mathfrak{F}_C$ and $\mathfrak{F}_T$ gives the influence of the collective noncollective coupling. For the diagonalization of the total Hamiltonian $H$ in $\mathfrak{F}_T$ in the case $D/\Delta = 0.5$ the mixing of states is rather large and the overlap with the corresponding collective state is sometimes not very decisive. We write here the most-probable candidates.

| | Collective space $\mathfrak{F}_C$ | | | Complete space $\mathfrak{F}_T$ | | |
|---|---|---|---|---|---|---|
| | $H_{\rm TDA}$ | $H_{\rm RPA}$ | $H$ | $H_{\rm TDA}$ | $H_{\rm RPA}$ | $H$ |
| | | | $D/\Delta = 0.1$ | | | |
| 1 phonon | 1.0497 | 0.955 | 0.955 | 1.0497 | 0.956 | 0.924 |
| 2 phonons | 2.4483 | 2.547 | 2.547 | 2.4478 | 2.549 | 2.521 |
| 3 phonons | 4.195 | 4.467 | 4.467 | 4.194 | 4.469 | 4.428 |
| 4 phonons | 6.289 | 6.674 | 6.674 | 6.288 | 6.677 | 6.718 |
| 5 phonons | 8.729 | 9.127 | 9.127 | 8.728 | 9.131 | 9.408 |
| 6 phonons | 11.512 | 11.796 | 11.796 | 11.512 | 11.800 | 12.470 |
| | | | $D/\Delta = 0.5$ | | | |
| 1 phonon | 1.3505 | 1.266 | 1.266 | 1.3505 | 1.317 | 1.085 |
| 2 phonons | 3.3515 | 3.503 | 3.503 | 3.281 | 3.561 | 2.981 |
| 3 phonons | 6.351 | 6.668 | 6.668 | 6.238 | 6.736 | 6.468 |
| 4 phonons | 10.086 | 10.503 | 10.503 | 9.636 | 10.206 | 10.377 |
| 5 phonons | 14.689 | 15.134 | 15.134 | 14.614 | 15.279 | 16.246 |
| 6 phonons | 19.842 | 20.177 | 20.177 | 19.842 | 20.434 | 22.232 |

### E. Matrix elements in $\mathfrak{B}_c$

It was shown in the preceding section that the $2p$th approximations for matrix elements, except the second one, are of no practical use because they need the same amount of computational difficulties as the exact treatment. One way to remove this disagreement is to work in the boson space. One must note that the $2p$th boson Hamiltonian (which give exactly $(n|H_B|m)$ up to $(2p|H_B|p')$ is of $4p$ order in the boson expansion, the greatest order term being $(B^\dagger)^{2p}B^{2p}$. In what follows we shall consider only $H_B^{(2)}$ and $H_B^{(4)}$.

Table III is analog to Table I for the matrix elements $(n|H_B|m)$ in the boson space $\mathfrak{B}_C$. The parameters are identical with those of Table I. The first point is that no discontinuity occurs for $n = N_c$. This does not prove that $N_c$ has no influence as we shall see later.

Furthermore, $(n|H^B_{\rm TDA}|n)^{(2)}$ is rigorously equal to $\langle n|H_{\rm TDA}|n\rangle^{(2)}$ for reasons which are up to now not very clear to us and as already mentioned above this is a good approximation. As is easily seen from Table III the fourth boson approximation is even a better one since $(n|H_B|n)^{(4)}$ are accurate by nearly $10^{-3}$ and $(n|H_B|n-2)^{(4)}$ by less than 0.2. In particular, the maximum of the exact value of $(n|H_B|n-2)$ at $n=6$ is very nicely reproduced in the fourth order calculation. This is not the case for the second approximation. In that sense the boson expansion is rapidly converging and is much more suited for calculations which

TABLE III. Matrix elements $(n|H^B_{\rm coll}|m)$ in MeV of $H_{\rm TDA}$ and $H_{40}$ in the boson collective space $\mathfrak{B}_C$. Comparison between exact and approximate $(2p = 2, 4)$ values. The parameters used are identical to those of Table I.

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| $(n\|H^B_{\rm TDA}\|n)$ | 1.245 | 2.808 | 4.700 | 6.931 | 9.507 | 12.431 | 15.704 | 19.318 | 23.264 | 27.518 |
| $(n\|H^B_{\rm TDA}\|n)^{(2)}$ | 1.245 | 2.808 | 4.691 | 6.891 | 9.410 | 12.248 | 15.405 | 18.881 | 22.675 | 26.788 |
| $(n\|H^B_{\rm TDA}\|n)^{(4)}$ | 1.245 | 2.808 | 4.700 | 6.931 | 9.506 | 12.431 | 15.711 | 19.347 | 23.339 | 27.686 |
| $(n\|H^B_{40}\|n-2)$ | 0 | 0.807 | 1.252 | 1.568 | 1.762 | 1.836 | 1.788 | 1.614 | 1.309 | 0.858 |
| $(n\|H^B_{40}\|n-2)^{(2)}$ | 0 | 0.807 | 1.397 | 1.976 | 2.551 | 3.124 | 3.697 | 4.269 | 4.841 | 5.412 |
| $(n\|H^B_{40}\|n-2^{(4)}$ | 0 | 0.807 | 1.252 | 1.568 | 1.764 | 1.814 | 1.804 | 1.652 | 1.387 | 1.010 |

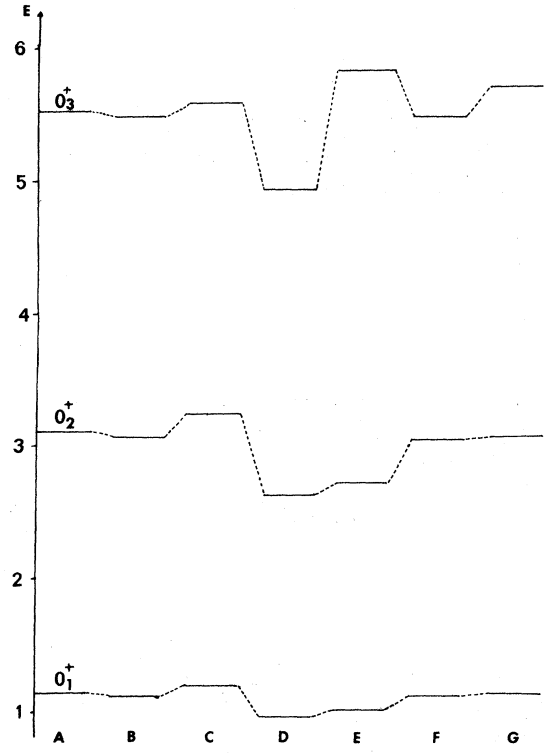


FIG. 3. Energy spectra of $H_{\mathrm{RPA}}$ for the three first excited states in different approximations: A, Diagonalization in the complete fermion space $\mathcal{F}_T$; B, Exact diagonalization in the collective subspace $\mathcal{F}_C$; C, Second approximation in $\mathcal{F}_C$; D, Diagonalization in $\mathcal{B}_C$ with dimension $2m+1$ : second approximation; E, Same as D with dimension $N_c$; F, Same as D for fourth approximation; and G, Same as E for fourth approximation. $E$ is expressed in MeV and the parameters $2m=6$, $D=0.3$ MeV, and $\Delta=1$ MeV.

require going further than the second approximation.

All kinds of approximations done in this work are summarized in the spectra described by Fig. 3. Several interesting conclusions may be drawn. The second approximation is much better in the fermion space $\mathcal{F}_C$ than in the boson space $\mathcal{B}_C$. An important point to emphasize is that to obtain a correct spectrum with the second approximation in boson space it is necessary to perform the diagonalization in a space including less than $N_c$ phonons [compare spectra $D$ and $E$ to $A$. This fact justifies the interpretation of $N_c$ as the cutoff factor of a SU(3) scheme[11]]: it is meaningless to consider boson space including more than $N_c$ phonons. The fourth order approximation in boson space is definitively superior to any approximation in fermion space; the modified Marumori boson expansion is converging very rapidly in the collective subspace. This suggests that the third order boson approximation which was not considered here because it has no counterpart in fermion space, is probably[4] accurate enough to give a good description of the collective properties.

## IV. CONCLUSIONS

In order to describe the anharmonicities in the spectrum of $K^\pi = 0^+$ vibrations in deformed nuclei (the so called $\beta, \beta\beta, \beta\beta\beta, \ldots$ vibrations) we have developed the necessary tools for such a program. The matrix elements of the Hamiltonian in a subspace spanned by the collective $Q_0^\dagger$ TD phonon operator are derived as well as approximations for them. The role of the cutoff factor $N_c$ and the reduced norm $\mathcal{N}_n$ is emphasized all along the paper. With the help of a simple model several interesting features have emerged. In the fermion space the coupling between collective and noncollective degrees of freedom is in general weak (however, a peculiar care must be taken when transposing this formalism to realistic cases). To avoid tremendous computational work a second approximation in the fermion space has been suggested (in fact, it is Holzwarth's approximation) which is rather good especially if $Q_0^\dagger$ is very collective. If a further accuracy in the method is needed it would be more convenient to deal with the modified Marumori boson expansion; in this case the dimension of the basis must not include states with more than $N_c$ phonons.

Further developments may be expected within this formalism:

1. Introduction of two kinds of particles in an average deformed field interacting by more realistic forces (pairing and quadrupole quadrupole forces for instance).

2. Coupling between collective vibrations $K^\pi = 0^+$ and $K^\pi = 2^+$. *A priori* the same techniques are available but we are faced with the difficulty that the states $Q_{K_1}^\dagger Q_{K_2}^\dagger \cdots Q_{K_n}^\dagger |0\rangle$ do not form an orthogonal basis.

[1]T. Kishimoto and T. Tamura, Nucl. Phys. A192, 246 (1972); A270, 317 (1976).

[2]P. Aguer, C. F. Liang, J. Libert, P. Paris, A. Charvet, R. Duffait, and G. Marguier, Nucl. Phys. A249, 239 (1975); A252, 293 (1975); J. J. Kolata and M. Oothoudt, Phys. Lett. 65B, 116 (1976).

[3]B. Sørensen, Nucl. Phys. A97, 1 (1967); A119, 65 (1968); A142, 392 (1970); A217, 505 (1973).

[4]G. Holzwarth, D. Janssen, and R. V. Jolos, Nucl. Phys. A261, 1 (1976).
[5]S. Iwasaki, F. Sakata, and K. Takada, Prog. Theor. Phys. 57, 1289 (1977).
[6]B. Silvestre-Brac and R. Piepenbring, Phys. Rev. C 16, 1638 (1977).
[7]M. Kleber, Phys. Lett. 30B, 588 (1969).
[8]S. G. Lie and G. Holzwarth, Phys. Rev. C 12, 1035 (1975).
[9]W. F. Van Gunsteren and K. Allaart, Nucl. Phys. A236, 317 (1974); Z. Physik A276, 1 (1976).
[10]S. Iwasaki, T. Marumori, F. Sakata, and K. Takada, Prog. Theor. Phys. 56, 846 (1976).
[11]D. Janssen, R. V. Jolos, and F. Dönau, Nucl. Phys. A225, 93 (1974); A. Arima and F. Iachello, Phys. Rev. Lett. 35, 1069 (1975).