Multiphonon $K^\pi = 0^+$ states in even-even deformed nuclei. III. Comparison with boson expansions in a realistic case

B. Silvestre-Brac and R. Piepenbring
Institut des Sciences Nucléaires, 38026 Grenoble-Cédex, France
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Collective $K^\pi = 0^+$ multiphonon states are studied in a realistic case and compared to those obtained by use of two different boson expansions.

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I. INTRODUCTION

In two recent papers[1,2] (quoted hereafter as I and II) we developed a microscopic theory allowing the study of the anharmonicity of the collective multiphonon $K^\pi = 0^+$ states in even-even axially deformed nuclei. Taking properly into account the Pauli principle we gave recursion formulas allowing an exact calculation of the norms of these multiphonon states (paper I) and of the matrix elements of a general Hamiltonian (paper II). Since, in an application to real nuclei, this approach may be very time consuming on a computer, we also developed an approximate method generalizing to higher order the modified Marumori boson expansion suggested by Holzwarth *et al.*[3] These exact and approximate treatments were applied to a simple solvable model of $2m$ identical particles filling $2m$ equidistant pairwise degenerate levels and interacting via a pure constant monopole pairing force. In this schematic model we could test, to different orders, the proposed approximations and observe some properties, the most specific of which are summarized here.

In the "exact" calculation (i.e., where the Pauli principle is correctly fulfilled) the energy of the two-phonon states $E(0_2^+)$ was always found to be larger than twice the energy of the one-phonon level. This is generally not the situation observed in the nuclei of the rare earth region.

In the different approximations it was found that there exists a cutoff factor N_c in the dimension of the basis of diagonalization, i.e., a critical value beyond which the energy spectrum becomes wrong.

In some conditions we obtained some "dangerous" or "intruder" states, low in energy, the wave function of which is predominantly composed of a large number of phonons.

It seemed interesting to us to see whether these properties are conserved, or how they are modified, in a more realistic model (e.g., two kinds of particles in a Nilsson potential interacting by a monopole pairing plus quadrupole-quadrupole residual force). Lastly, according to the recent success of the boson expansion techniques developed by Kishimoto and Tamura[4] (KT) in the spherical and transitional nuclei, it seemed also worthwhile to compare this kind of approach to the exact and/or approximate method mentioned before. In Sec. II we review the essential points of the theory developed in the two preceding papers I and II. In Sec. III we summarize the method of the boson expansion of KT for deformed nuclei. In Sec. IV we apply, successively, the exact multiphonon theory and the modified Marumori and KT boson expansion techniques to the more realistic model chosen here, and compare the different results obtained. Our conclusions are finally drawn in the last section.

II. SUMMARY OF THE THEORY DEVELOPED IN PAPERS I AND II

A. The starting point

We introduce an orthonormal basis of quasiparticles fulfilling the usual anticommutation rules

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

The Hamiltonian of the system is expressed in terms of these basic operators as

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

with

$$H_{11} = \sum_\nu E_\nu \alpha_\nu^\dagger \alpha_\nu,$$

$$H_{22} = \sum_{\alpha\beta\gamma\delta} S_{\alpha\beta\delta\gamma} \alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma \alpha_\delta, \tag{3}$$

$$H_{31} = \sum_{\alpha\beta\gamma\delta} R_{\alpha\beta\gamma\delta} (\alpha_\alpha^\dagger \alpha_\beta^\dagger \alpha_\gamma^\dagger \alpha_\delta + \alpha_\delta^\dagger \alpha_\gamma \alpha_\beta \alpha_\alpha),$$

$$H_{40}=\sum_{\alpha\beta\gamma\delta} P_{\alpha\beta\gamma\delta}(\alpha^{\dagger}_{\alpha}\alpha^{\dagger}_{\beta}\alpha^{\dagger}_{\gamma}\alpha^{\dagger}_{\delta}+\alpha_{\delta}\alpha_{\gamma}\alpha_{\beta}\alpha_{\alpha}).$$

The coefficients P, R, and S are assumed to be real and verify all symmetry properties of the quasiparticle operators.

We suppose that in the two-quasiparticle space it is possible to find a collective state described by

$$Q^{\dagger}_{K}(i)=\tfrac{1}{2}\sum_{\mu\nu} X^{K}_{\mu\nu}(i)\,\alpha^{\dagger}_{\mu}\alpha^{\dagger}_{\nu}, \tag{4}$$

where K is the projection of the intrinsic angular momentum on the symmetry axis and where i stands for all other quantum numbers. The X matrix may, for instance, be chosen as the collective solution of the Tamm-Dancoff approximation (TDA). One could also take any other unitary matrix fulfilling the condition $X_{\mu\nu}=-X_{\nu\mu}$. Without any loss of generality we assume the X matrix to be real.

In order to simplify the treatment we restrict ourselves to $K^{\pi}=0^{+}$ collective states and henceforth omit indices i and K. By this restriction we neglect states built on couples of $Q^{\dagger}_{L}Q^{\dagger}_{-L}$ with $L\neq 0$, which may be important when one wants to compare to the experimental situation.

Finally, we introduce the normalized multiphonon states $|n\rangle=N_n(Q^{\dagger})^n|0\rangle$.

B. Norms and matrix elements

Owing to the Pauli principle, the calculation of the norm N_n and of the matrix elements $\langle n|H|m\rangle$ is not easy. In I and II recursion formulas were established for these quantities. To write those in a simple form we introduced the following tools:

(1) The successive powers of the X matrix,

(2) The "reduced norm" $\mathfrak{N}_n=(n!\,N_n)^{-2}$.

It was shown in I that the norms can be obtained by

$$n\mathfrak{N}_n=\mathfrak{N}_{n-1}-\tfrac{1}{2}\sum_{l=1}^{n-1}\mathrm{Tr}(X^{2l+2})\mathfrak{N}_{n-l-1}, \tag{5}$$

where the existence of the second term shows clearly that $Q^{\dagger}$ is not a pure boson.

In II we established recursion formulas for the different matrix elements involved in (2). Explicitly one has

$$\begin{aligned}
&\mathfrak{N}_n\langle n|H_{11}|n\rangle=-\sum_{l=1}^{n}\mathrm{Tr}(EX^{2l})\mathfrak{N}_{n-l},\\
&(\mathfrak{N}_{n+2}\mathfrak{N})^{1/2}\langle n+2|H_{40}|n\rangle=3\sum_{l=0}^{[n/2]}\mathcal{P}(2l+1,2l+1)\mathfrak{N}_{n-2l}+6\sum_{l=0}^{[(n-1)/2]}\sum_{k=0}^{n-1-2l}\mathcal{P}(2l+3+2k,2l+1)\mathfrak{N}_{n-1-2l-k},\\
&(\mathfrak{N}_{n+1}\mathfrak{N}_n)^{1/2}\langle n+1|H_{31}|n\rangle=-3\sum_{l=1}^{[(n+1)/2]}\mathcal{R}(2l-1,2l)\mathfrak{N}_{n+1-2l}\\
&\qquad\qquad-3\sum_{l=1}^{[n/2]}\sum_{k=0}^{n-2l}[\mathcal{R}(2l+1+2k,2l)+\mathcal{R}(2l-1,2l+2+2k)]\mathfrak{N}_{n-2l-k},\\
&\mathfrak{N}_n\langle n|H_{22}|n\rangle=-\sum_{l=0}^{n-1}\mathcal{S}_{I}(2l+1,1)\mathfrak{N}_{n-l-1}-\sum_{l=1}^{[n/2]}\mathcal{S}_{I}(2l-1,2l+1)+2\mathcal{S}_{II}(2l,2l)\,\mathfrak{N}_{n-2l}\\
&\qquad-\sum_{l=1}^{[(n-1)/2]}\sum_{k=0}^{n-2l-1}\mathcal{S}_{I}(2l+1+2k,2l+1)+\mathcal{S}_{I}(2l-1,2l+3+2k)+4\mathcal{S}_{II}(2l+2+2k,2l)]\mathfrak{N}_{n-2l-1-k},
\end{aligned} \tag{6}$$

where the symbol $[x]$ stands for integer m such that $m\leq x<m+1$. The quantities $\mathcal{P}$ and $\mathcal{R}$ are defined by a relation of the type

$$\mathcal{T}(l,m)=\sum_{\alpha\beta\gamma\delta}T_{\alpha\beta\gamma\delta}(X^{l})_{\alpha\beta}(X^{m})_{\gamma\delta},$$

whereas

$$\mathcal{S}_{I}(l,m)=\sum_{\alpha\beta\gamma\delta}S_{\alpha\beta\gamma\delta}(X^{l})_{\alpha\beta}(X^{m})_{\gamma\delta}$$

and

$$\mathcal{S}_{II}(l,m)=\sum_{\alpha\beta\gamma\delta}S_{\alpha\beta\gamma\delta}(X^{l})_{\alpha\gamma}(X^{m})_{\beta\delta}.$$

C. The modified Marumori boson expansion

The numerical evaluation of the powers of the matrix X and of the quantities $\mathcal{P}$, $\mathcal{R}$, and $\mathcal{S}$ involved in the preceding recursion formulas may be, in some cases (large number of levels, for instance) very time consuming. To avoid the exact calculation of $\langle n|H|m\rangle$ for large values of m and/or n it is possible to work with the boson representation of the Hamiltonian through the modified Marumori expansion. In the boson space we define the image of the multiphonon state $|n\rangle$ by

$$|n\rangle=(n!)^{-1/2}(B^{\dagger})^n|0\rangle,$$

where $B|0\rangle\equiv 0$. According to a suggestion of Holzwarth *et al.*[3] this can be achieved by use of the pth approximation of the boson Hamiltonian given in II:

$$H_B^{(p)}=\sum_{n=0}^{p}\frac{\langle n|H|n\rangle}{n!}\sum_{k=0}^{p-n}\frac{(-1)^k}{k!}(B^\dagger)^{n+k}B^{n+k}$$
$$+\sum_{n=0}^{p-1}\frac{\langle n+1|H|n\rangle}{[n!\,(n+1)!]^{1/2}}\sum_{k=0}^{p-n-1}\frac{(-1)^k}{k!}[(B^\dagger)^{n+k+1}B^{n+k}+(B^\dagger)^{n+k}B^{n+k+1}]$$
$$+\sum_{n=0}^{p-2}\frac{\langle n+2|H|n\rangle}{[n!\,(n+2)!]^{1/2}}\sum_{k=0}^{p-n-2}\frac{(-1)^k}{k!}[(B^\dagger)^{n+k+2}B^{n+k}+(B^\dagger)^{n+k}B^{n+k+2}]. \tag{7}$$

One can see that in this kind of approximation one only needs to calculate matrix elements $\langle m|H|n\rangle$ with $n\leq m\leq p$.

The boson Hamiltonian (7) can be written in the simple form

$$H_B^{(p)}=\sum_{i,j=0}^{p}c(i,j)\,B^{\dagger i}B^j, \tag{8}$$

where

$$c(i,i)=\sum_{m=0}^{i}(-1)^{i-m}\frac{\langle m|H|m\rangle}{m!(i-m)!},$$
$$c(i,i-1)=c(i-1,i)=\sum_{m=1}^{i}(-1)^{i-m}\frac{\langle m|H|m-1\rangle}{(i-m)!\,[m!\,(m-1)!]^{1/2}},$$
$$c(i,i-2)=c(i-2,i)=\sum_{m=2}^{i}(-1)^{i-m}\frac{\langle m|H|m-2\rangle}{(i-m)!\,[m!\,(m-2)!]^{1/2}},$$
$$c(i,j)=0 \text{ otherwise}.$$

If one considers the approximations up to order $p=4$ one gets 11 nonvanishing coefficients.

The matrix elements $(n|H_B^{(p)}|m)$ in the boson space depend on these coefficients $c(i,j)$ and on the geometrical factors $(n|B^{\dagger r}B^q|m)$. After some simple algebra one can, however, express the interesting matrix elements in the boson space directly in terms of those in the fermion space. Explicitly one gets

$$(n|H_B^{(p)}|n)=\langle n|H|n\rangle \text{ for } n\leq p$$
$$=A_n^{p+1}\sum_{m=0}^{p}(-1)^{p-m}\frac{\langle m|H|m\rangle}{(n-m)m!\,(p-m)!} \text{ if } n>p,$$
$$(n|H_B^{(p)}|n-1)=\langle n|H|n-1\rangle \text{ for } n\leq p$$
$$=\sqrt{n}\,A_{n-1}^{p}\sum_{m=1}^{p}(-1)^{p-m}\frac{\langle m|H|m-1\rangle}{(n-m)(p-m)!\,[m!\,(m-1)!]^{1/2}} \text{ if } n>p, \tag{9}$$

and

$$(n|H_B^{(p)}|n-2)=\langle n|H|n-2\rangle \text{ for } n\leq p$$
$$=[n(n-1)]^{1/2}A_{n-2}^{p-1}\sum_{m=2}^{p}(-1)^{p-m}\frac{\langle m|H|m-2\rangle}{(n-m)(p-m)!\,[m!\,(m-2)!]^{1/2}} \text{ if } n>p,$$

where

$$A_n^p=n(n-1)(n-2),\ldots,(n-p+1).$$

These relations demonstrate the existence of a cutoff factor empirically observed in II. As a matter of fact let us consider as an example $(n|H^{(2)}|n-2)$. According to (9) one has

$$(n|H^{(2)}|n-2)=\tfrac{1}{2}[n(n-1)]^{1/2}\langle 2|H|0\rangle$$

which shows that this matrix element goes to infinity for large n, whereas, according to the Pauli principle $\langle n|H|n-2\rangle$ goes to zero. In the same way, for any matrix element (9) to any order it is possible to see that $(n|H_B^{(p)}|m)$ behaves asymptotically as a "polynomial" in n and consequently goes to $\pm\infty$ for large n, contrary to the fermion matrix element $\langle n|H|m\rangle$ which necessarily goes to zero beyond a given value of n.

III. THE KISHIMOTO AND TAMURA BOSON EXPANSION APPLIED TO DEFORMED NUCLEI

A. The principle of the KT boson expansion

The transcription of the boson expansion (BE) techniques of KT to deformed nuclei has been achieved in a previous paper.[5] We therefore review only briefly the principle of this method. The BE consists of introducing pure boson creation

(annihilation) operators $C_{12}^\dagger$ (C_{12}) and in writing $\alpha_1^\dagger\alpha_2^\dagger$ and $\alpha_1^\dagger\alpha_2$ in terms of $C_{ij}^\dagger$ and C_{ij}. The only requirement for the determination of the expansions is that the commutation properties

$$
\begin{aligned}
&[\alpha_1^\dagger\alpha_2^\dagger,\ \alpha_3^\dagger\alpha_4] = \alpha_3^\dagger\alpha_1^\dagger\delta_{24} - \alpha_3^\dagger\alpha_2^\dagger\delta_{14},\\
&[\alpha_1^\dagger\alpha_2,\ \alpha_3^\dagger\alpha_4] = \alpha_1^\dagger\alpha_4\delta_{23} - \alpha_3^\dagger\alpha_2\delta_{14},\\
&[\alpha_1^\dagger\alpha_2^\dagger,\ \alpha_3^\dagger\alpha_4^\dagger] = [\alpha_2\alpha_1,\ \alpha_4\alpha_3] = 0,\\
&[\alpha_2\alpha_1,\ \alpha_3^\dagger\alpha_4^\dagger] = \delta_{13}\delta_{24} - \delta_{23}\delta_{14} + \alpha_3^\dagger\alpha_2\delta_{14} - \alpha_4^\dagger\alpha_2\delta_{13}\\
&\qquad\qquad + \alpha_4^\dagger\alpha_1\delta_{23} - \alpha_3^\dagger\alpha_1\delta_{24},
\end{aligned}
\tag{10}
$$

are exactly satisfied order by order. It has been shown[4,6] that it is possible to choose a finite expansion for $\alpha^\dagger\alpha$. As suggested by Sørensen,[6] it is convenient to deal with an operator which changes by one the number of bosons for the mapping of $\alpha^\dagger\alpha^\dagger$ and which does not change the number of bosons for $\alpha^\dagger\alpha$.

In expanding $\alpha_1^\dagger\alpha_2^\dagger$ we choose all possible combinations of $C^\dagger$ and C which contain the indices 1 and 2 in creation operators $C_{ij}^\dagger$ and sum over all other indices. A similar rule holds for the expansion of $\alpha_1^\dagger\alpha_2$. Up to the sixth order defined by KT (equivalent to the fifth order of Ref. 5) the image of fermion pairs can be written as

$$
\begin{aligned}
&(\alpha_1^\dagger\alpha_2)_B = x_0\delta_{12} + x_2\sum_3 C_{13}^\dagger C_{23},\\
&(\alpha_1^\dagger\alpha_2^\dagger)_B = xC_{12}^\dagger + aC_{12}^\dagger\sum_{34} C_{34}^\dagger C_{34} + b\sum_{34} C_{13}^\dagger C_{24}^\dagger C_{34} + pC_{12}^\dagger\sum_{3456} C_{34}^\dagger C_{56}^\dagger C_{56}C_{34} + q\sum_{3456} C_{13}^\dagger C_{24}^\dagger C_{56}^\dagger C_{56}C_{34}\\
&\qquad + r\sum_{3456} C_{13}^\dagger C_{24}^\dagger C_{56}^\dagger C_{35}C_{46} + sC_{12}^\dagger\sum_{3456} C_{34}^\dagger C_{56}^\dagger C_{35}C_{46}.
\end{aligned}
\tag{11}
$$

In Ref. 5 it has been shown that we can restrict ourselves to real coefficients x_0, x, x_2, a, b, p, q, r, and s. Furthermore, it was found that $x_2 = 1$, $x = (1 - 2x_0)^{1/2}$, and that all the other coefficients can be expressed in terms of x (or x_0) which can be considered as a "convergence parameter." The third order coefficients a and b are obtained by solving Eq. (2.12) of Ref. 5 which contain terms such as a^2, b^2, and ab coming from contractions of six operators (e.g., $C^\dagger C^\dagger C\,C^\dagger C\,C$) to four operators ($C^\dagger C^\dagger C\,C$). There exist four real solutions from which we retain the unique one where a and b behave as const$/x^p$ (where p is an integer larger than one), i.e.,

$$
\begin{aligned}
&a = \tfrac{1}{6}[2(x^2-1)^{1/2} + (x^2+2)^{1/2} - 3x] \simeq -\frac{1}{8x^3},\\
&b = \tfrac{1}{3}[(x^2-1)^{1/2} - (x^2+2)^{1/2}] \simeq -\frac{1}{2x}.
\end{aligned}
\tag{12}
$$

In the same spirit the five order coefficients p, q, r, and s are solutions of Eq. (2.13) of Ref. 5, where terms such as p^2, q^2, r^2, $pq\ldots$, and ap, $bq\ldots$ come from contractions. There are eight real solutions among which only one behaves as required:

$$
\begin{aligned}
&p = \tfrac{1}{120}[5(x^2-2)^{1/2} - 16(x^2-1)^{1/2} - 5(x^2+2)^{1/2} + (x^2+4)^{1/2} + 15x] \simeq -\frac{5}{64x^7},\\
&q = 2s = \tfrac{1}{60}[5(x^2-2)^{1/2} - 8(x^2-1)^{1/2} + 5(x^2+2)^{1/2} - 2(x^2+4)^{1/2}] \simeq -\frac{1}{8x^5},\\
&r = \tfrac{1}{60}[5(x^2-2)^{1/2} - 4(x^2-1)^{1/2} - 5(x^2+2)^{1/2} + 4(x^2+4)^{1/2}] \simeq -\frac{1}{8x^3}.
\end{aligned}
\tag{13}
$$

B. Conditions of existence of KT boson expansions

The relation $x = (1 - 2x_0)^{1/2}$ shows that x_0 must be chosen so that $x_0 < \frac{1}{2}$. The fourth order expansion (12), hereafter noted KT4, exists only if the condition $x^2 \geq 1$ or $x_0 \leq 0$ is fulfilled. The sixth order expansion KT6 defined by (13) further implies $x^2 \geq 2$ or $x_0 \leq -\frac{1}{2}$. We see that to extend the BE to higher orders one needs to take larger values of $|x_0|$. This leads to a severe limitation of the KT techniques, namely, when $|x_0|$ increases the boson vacuum $|0)$ diverges considerably from the fermion vacuum since $\alpha_i^\dagger\alpha_i|0\rangle \equiv 0$ while $(\alpha_i^\dagger\alpha_i)_B|0) = x_0|0) \neq 0$. According to this Kishimoto and Tamura[4] have suggested some approximate solutions to KT4 and KT6, respectively, noted A4 and A6. These approximations are obtained by removing the terms coming from the contractions in the previously mentioned equations. More precisely A4 leads to $a = 0$ and $b = -(1/2x)$ with the only condition $x_0 < \frac{1}{2}$. The approximate sixth order A6 uses the exact solutions (12) for a and b and the approximate values

$$p = -\frac{a^2}{2x} \simeq -\frac{1}{128x^7},$$

$$q = -\frac{ab}{x} \simeq -\frac{1}{16x^5},$$

$$r = -\frac{b^2}{2x} \simeq -\frac{1}{8x^3},$$

$$s = 0,$$

implying simply $x_0 \leq 0$. We note that these approximate BE have coefficients the asymptotic behaviors of which only slightly differ from those of the exact solutions. Finally we summarize the conditions of existence of the different boson expansion we shall consider:

KT2: $x_0 \leq \frac{1}{2}$, KT4: $x_0 \leq 0$, KT6: $x_0 \leq -\frac{1}{2}$;

A4: $x_0 < \frac{1}{2}$, A6: $x_0 \leq 0$.

C. Hamiltonian in boson operators

The general procedure consists, first, in writing the chosen Hamiltonian in terms of quasiparticle operators, second, in replacing the fermion pairs $\alpha^\dagger\alpha^\dagger$ and $\alpha^\dagger\alpha$ by their expansions (11). Since we are mainly interested in a comparison with the methods developed in Sec. II, we then introduce collective Tamm-Dancoff phonons of the form

$$B^\dagger = \tfrac{1}{2} \sum X_{\mu\nu} C^\dagger_{\mu\nu}. \tag{14}$$

It is easy to invert Eq. (14) and finally to express H in terms of the collective operators in the normal order as in relation (8).

Such a procedure presents some ambiguities on the part of the Hamiltonian containing two body interaction since there exist several possibilities of forming pairs of fermion operators. In this part of our work, and with the simple force we shall introduce, it is possible to use a rather "natural" way of selecting these pairs. This implies that we shall not necessarily use the normal ordered form (2) for H. The aim is to postpone the contractions to the final step of the procedure (see Ref. 7). We end up with a Hamiltonian written in the form (8).

Explicitly expansions of order 4 contain terms with coefficients $c(0,0)$; $c(1,0) = c(0,1)$; $c(1,1)$; $c(2,0)$; $c(2,1) = c(1,2)$. Expansions of order 6 add terms with $c(2,2)$; $c(3,1) = c(1,3)$ and $c(3,2) = c(2,3)$. We point out that contrary to the modified Marumori BE, the present one contains a linear term $B^\dagger + B$ but no terms $B^{\dagger 2}B^2$ in the fourth order nor $B^{\dagger 3}B^3$ in the sixth order. As a consequence the direct comparison of these two boson Hamiltonians is meaningless. We finally mention here that the determination of the coefficients $c(i,j)$ needs the knowledge of quantities which also arise, at least partially, in the multiphonon approach.

IV. APPLICATION AND DISCUSSION

A. Choice of the model examples and parameters

The general formalism developed in Secs. II and III is applied to a realistic model of two kinds of particles in a Nilsson potential interacting by a constant monopole pairing plus charge independent quadrupole-quadrupole residual force. Since we restricted the formalism to $K^\pi = 0^+$ collective phonons only, this model will not yet allow any reasonable comparison to the experimental results. However, it is sufficiently realistic and tractable to allow an interesting comparison of the three suggested methods.

For such a type of model the detailed form (2) of the Hamiltonian is well known. Therefore we shall not give the explicit expressions of the quantities P, R, S nor the form deduced for the Hamiltonian in the KT expansion. They can be found in Ref. 7.

As usual, the pairing force is treated within the BCS approximation. This introduces some fluctuations in the number of particles. We suppose that these have similar effects in the three proposed approaches. Various examples of real nuclei are chosen in the rare earth region: ^{154}Gd, ^{164}Er, ^{172}Yb, and ^{182}W for their diversity. They present the following characteristics: The density of the individual levels around the Fermi surface are quite different and so are the pairing gaps, the measured energies of the two first collective 0^+ states, and the observed anharmonic effects. Furthermore, these examples cover practically the whole well deformed rare earth region. Table I summarizes the experimental data.

The parameters of the Nilsson model are taken from Lamm,[8] the deformation fixed to $\epsilon_2 = 0.25$, and the single particle matrix elements of r^2Y_{20} calculated according to the prescriptions of Boisson and Piepenbring.[9] The usual BCS equations are solved using 30 active levels, 15 on each side of the Fermi level. The strength of the pairing force G is obtained by fixing the gaps of Table I. The TDA secular equation is solved for different values of the strength χ_0^{TDA} of the residual quadrupole force. It is convenient to express the lengths in $(\hbar/m\omega)^{1/2}$ units and χ_0 in MeV. The choice of the number of active particles may be of some importance. It must be chosen in a suitable way—sufficiently large to give stable results and not too large to avoid effects of states which would be unbound in a finite potential well. Our present choice is a good compromise.

TABLE I. Experimental data for the chosen nuclei. All energies are given in keV. When there are several candidates for the two-phonon state we indicate the possible energies $E(0_2^+)$, the most probable one being indicated by an asterisk. One observes that $E(0_2^+) < 2E(0_1^+)$. The gaps Δ are deduced, as usual, from the odd-even mass difference (Ref. 10).

Nucleus	$E(0_1^+)$	$E(0_2^+)$	Δ_p	Δ_n
$^{154}_{64}Gd_{90}$	680.64	1214.6	1020.0	1110.0
$^{164}_{68}Er_{96}$	1246.0	1698.0* 1766.0 2172.0 2185.0	900.0	940.0
$^{172}_{70}Yb_{102}$	1042.9	1404.0* 1794.0 1896.0	830.0	700.0
$^{182}_{74}W_{108}$	1137.0	2239.5	830.0	660.0

B. The "exact" multiphonon approach

The norms of the multiphonon states and the matrix elements of the model Hamiltonian between them are calculated according to the formalism of Sec. II. The eigenstates of H are obtained by the diagonalization in a basis containing all collective multiphonons up to $n=9$. The stability of the three lowest eigenstates are checked by comparing the results obtained with a basis using one state more.

1. Some remarks on the norms

As for the simple example treated in I, we again find that the exchange term in relation 5, due to the Pauli principle, is mainly sensitive to the collectivity of the phonon we introduce. To this purpose we consider the variable

$$(\mathfrak{N}_n)_H = (N_n^B)^2/(N_n^2) = n!\,\mathfrak{N}_n ,$$

introduced by Holzwarth *et al.*[3] to measure the deviation of the fermion state $(Q^\dagger)^n|0\rangle$ from a pure boson $(B^\dagger)^n|0\rangle$. In the case of ^{154}Gd where the basic phonon is strongly collective we get typical values

$$(\mathfrak{N}_7)_H = 0.057 ,$$

$$(\mathfrak{N}_{10})_H = 0.0025 .$$

On the other hand, for ^{172}Yb, where the TDA phonon is less collective, the corresponding values of $\mathfrak{N}_H$ are, respectively, 0.0017 and 0.000 004 6.

2. Some remarks on the different matrix elements of H

Two parts of H, H_{11}, and H_{22} contribute to the diagonal matrix elements. As expected, the element $\langle n|H_{11}|n\rangle$ is always positive and increases regularly with n; the contribution of $\langle n|H_{22}|n\rangle$ is always negative and much smaller than $\langle n|H_{11}|n\rangle$ leading to positive values of $\langle n|H|n\rangle$ which are always found greater than n times $\langle 1|H|1\rangle$. In the four studied cases the deviation from the harmonic situation increases with n. It is only in the case of ^{182}W that this deviation remains small. Concerning the nondiagonal matrix elements $\langle n|H_{31}|n-1\rangle$ and $\langle n|H_{40}|n-2\rangle$, it is worthwhile to note that the pairing and quadrupole forces contribute with opposite signs. Consequently, for a fixed value of the pairing strength, it is possible to change considerably these nondiagonal terms by varying the quadrupole parameter χ_0. Typical values of the exact matrix elements of H are given in Table II.

TABLE II. Exact $\langle m|H|n\rangle$ and approximate $(m|H|n)^{(p)}$ matrix elements of H obtained in the multiphonon and modified Marumori approaches for the case of ^{154}Gd. The strength of the quadrupole-quadrupole interaction was $\chi_0^{\mathrm{TDA}} = \chi_0^H = 0.035$ MeV. All elements are given in MeV.

n	1	2	3	4	5	6	7	8	9
$(n\|H\|n)^{(2)}$	0.6596	1.595	2.806	4.293	6.056	8.094	10.41	13.00	15.86
$(n\|H\|n)^{(3)}$	0.6596	1.595	2.785	4.209	5.846	7.675	9.675	11.82	14.10
$(n\|H\|n)^{(4)}$	0.6596	1.595	2.785	4.215	5.877	7.766	9.889	12.25	14.87
$\langle n\|H\|n\rangle$	0.6596	1.595	2.785	4.215	5.878	7.772	9.897	12.25	14.85
$(n\|H\|n-1)^{(2)}$	0.0	0.2110	0.5169	0.8953	1.335	1.827	2.369	2.954	3.581
$(n\|H\|n-1)^{(3)}$	0.0	0.2110	0.4810	0.7708	1.056	1.319	1.545	1.721	1.838
$(n\|H\|n-1)^{(4)}$	0.0	0.2110	0.4810	0.7709	1.057	1.321	1.549	1.728	1.850
$\langle n\|H\|n-1\rangle$	0.0	0.2110	0.4810	0.7709	1.061	1.340	1.599	1.832	2.032
$(n\|H\|n-2)^{(2)}$		−0.1724	−0.2985	−0.4222	−0.5451	−0.6675	−0.7899	−0.9120	−1.034
$(n\|H\|n-2)^{(3)}$		−0.1724	−0.1754	−0.0738	0.1296	0.4340	0.8394	1.346	1.952
$(n\|H\|n-2)^{(4)}$		−0.1724	−0.1754	−0.0985	0.0341	0.2003	0.3786	0.5473	0.6852
$\langle n\|N\|n-2\rangle$		−0.1724	−0.1754	−0.0985	0.0384	0.2224	0.4445	0.6973	0.9742

3. On the relative values of $E(0_2^+)$ and $2E(0_1^+)$

Even if the restriction to $K^\pi = 0^+$ modes does not yet allow a comparison with the experimental situation, it is interesting to see whether the deviation from the harmonicity introduced by the correct treatment of the Pauli principle is going in the same direction as that observed in actual nuclei.

As mentioned in the previous subsection the diagonal matrix elements are such that $\langle n|H|n\rangle > n\langle 1|H|1\rangle$. To obtain the observed situation $E(0_2^+) < 2E(0_1^+)$, the off-diagonal elements $\langle n|H_{31}|n-1\rangle$ and $\langle n|H_{40}|n-2\rangle$ must play an important role. If the anharmonicity of the diagonal elements is too large, it seems that the off-diagonal effects are not able to compensate the diagonal one. It was suggested[6] that one may choose for χ_0 in H a value χ_0^H slightly different from that χ_0^{TDA} used in the TDA. This is possible since the only condition for X in our formalism is to be a unitary transformation. Such a choice may help to obtain the expected effect. Figure 1 illustrates this discussion in the case of ^{182}W where for certain appropriate choices of χ_0^H and χ_0^{TDA} the energy $E(0_2^+)$ can be brought lower than $2E(0_1^+)$. A careful observation of the matrix elements of H seems to show (empirically) that the conditions $\langle n|H|n-1\rangle \cdot \langle n|H|n-2\rangle < 0$ and $|\langle n|H|n-1\rangle| > |\langle n|H|n-2\rangle|$ for rather low values of n favor the expected effect. It has been further checked that this situation is not affected by a slight change of the deformation ϵ_2 of the Nilsson field.

C. The modified Marumori boson expansion

Using the formalism of Sec, II C, we have calculated the matrix elements $(n|H^{(p)}|n)$,

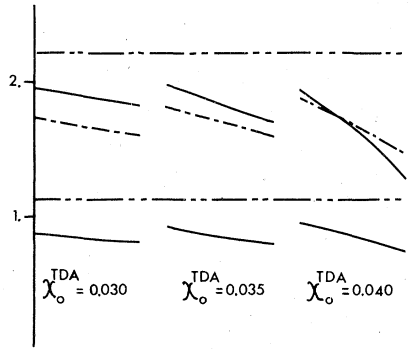

FIG. 1. Comparison of the relative values of $E(0_2^+)$ and $2E(0_1^+)$ in the case of the case of ^{182}W. The full and horizontal double-dotted lines represent,, respectively, the calculated and observed energies $E(0_1^+)$ and $E(0_2^+)$; the single-dotted lines represent $2E(0_1^+)$. These different quantities are plotted for three values of χ_0^{TDA} versus χ_0^{H} varying from 0.8 χ_0^{TDA} to 1.2 χ_0^{TDA}. All quantities E and χ_0 are expressed in MeV.

$(n|H^{(p)}|n-1)$, and $(n|H^{(p)}|n-2)$ for the three orders $p = 2$, 3, and 4 and $1 \leq n \leq 9$. The eigenproblem is solved by diagonalization of the matrix of $H^{(p)}$, the dimension of which is varied from 3 to 10.

1. Comparison of the approximate solutions to the exact one

In Table II we give the calculated matrix elements of orders 2, 3, and 4 as well as their exact values obtained in subsection B in the case of ^{154}Gd for $\chi_0^{\mathrm{TDA}} = \chi_0^H = 0.035$ MeV. In this example it is seen that the diagonal matrix elements are very well reproduced whatever the order of the approximation (the largest deviation for $n = 9$ being of the order of 7%). The situation is much different for the off-diagonal matrix elements. It is easily seen that the second order approximation deviates very rapidly from the exact value: The order of magnitude and even the sign of these elements (e.g., $\langle 5|H^{(2)}|3\rangle$) can be wrong. The situation is improved by the higher order approximations and it appears that the fourth order one gives a satisfactory overall agreement. These conclusions are better illustrated in Table III where we give the three lowest eigenvalues $E(0_i^+)$. Peculiarly it is seen that these eigenvalues are exactly reproduced by a fourth order calculation where the basis of diagonalization is restricted to the six lowest collective phonons. Furthermore, for each order of the approximation, one gets a stability of these energies with increasing n, the values of which may be either less or greater than the exact values. It is also interesting to see the values of the $c(i,j)$ coefficients of Eq. (8). In the case studied, one has $c(1,1) = 0.6596$; $c(2,2) = 0.1379$; $c(3,3) = -0.0035$; $c(4,4) = 0.00025$; $c(2,1) = 0.1492$; $c(3,2) = -0.0104$; $c(4,3) = 0.000011$; $c(2,0) = -0.1219$; $c(3,1) = 0.0503$; $c(4,2) = -C\ 0036$ showing a certain convergence of the expansion, since

$$c(i+1, j+1) < c(i,j), \quad \forall i \text{ and } j .$$

2. Discussion of the cutoff factor N_c

In Sec. II C we proved the existence of a cutoff factor, i.e., a critical value of n noted N_c such that the approximations fail for $n > N_c$. In paper I we suggested that N_c is intimately related to the parameter

$$\eta = \left| \frac{\mathrm{Tr}(X^4)}{\mathrm{Tr}(X^2)} \right| = \tfrac{1}{2} |\mathrm{Tr}(X^4)| ,$$

and in paper II we plotted N_c as a function of η. In the example treated in Tables II and III, $\mathrm{Tr}(X^4) = 0.135$ and no cutoff factor appeared, at least for $p = 3$ and 4, within the studied range of n. In Table IV, which corresponds to Table III for ^{182}W with

TABLE III. Exact E and approximate $E^{(p)}$ values of the energies (in keV) of the three lowest eigenvalues of H in the same case as in Table II.

	2	3	4	5	6	7	8	9	10
$E^{(2)}(0_1^+)$	635.4	562.6	539.9	528.4	524.3	522.9	522.5	522.4	
$E^{(3)}(0_1^+)$	635.4	601.5	597.4	597.3	597.3	597.3	597.3	597.3	
$E^{(4)}(0_1^+)$	635.4	601.5	597.0	596.8	596.8	596.8	596.8	596.8	
$E(0_1^+)$								596.8	596.8
$E^{(2)}(0_2^+)$	1677.0	1545.0	1397.0	1336.0	1306.0	1295.0	1291.0	1290.0	
$E^{(3)}(0_2^+)$	1677.0	1540.0	1502.0	1500.0	1500.0	1500.0	1500.0	1500.0	
$E^{(4)}(0_2^+)$	1677.0	1540.0	1497.0	1493.0	1493.0	1493.0	1493.0	1493.0	
$E(0_2^+)$								1493.0	1493.0
$E^{(2)}(0_3^+)$		3038.0	2780.0	2541.0	2428.0	2371.0	2349.0	2341.0	
$E^{(3)}(0_3^+)$		2981.0	2679.0	2644.0	2644.0	2642.0	2642.0	2642.0	
$E^{(4)}(0_3^+)$		2981.0	2688.0	2636.0	2634.0	2634.0	2634.0	2634.0	
$E(0_3^+)$								2635.0	2635.0

$\chi_0^{\mathrm{TDA}} = \chi_0^H = 0.030$ MeV and $\mathrm{Tr}(X^4) = 0.239$, there is some evidence for $N_c \simeq 6$ in rough agreement with the estimate $N_c = N_c(\eta)$ of II. In the cases where the exact solution is not reachable for computational reasons it is necessary to have an estimate of N_c. The value of the parameter η, or more simply the $\mathrm{Tr}(X^4)$, still seems to be, in this realistic model, a good criterion for fixing N_c.

3. *On the observation of intruder states*

In analyzing the energy spectra obtained in the modified Marumori approach we also found in some cases (e.g., ^{182}W, $\chi_0 = 0.040$ MeV, and $p = 3$) some intruder states. They appeared for $n = 8$ (and $n = 9$) between 0_2^+ and 0_3^+ (0_1^+ and 0_2^+), respectively. These states were composed predominantly of a great number of phonons and may be due to the fact that for $n > N_c$ the modified Marumori approach is misleading.

D. The Kishimoto and Tamura boson expansion

Following the theory summarized in Sec. III we studied the different boson expansions KT4, KT6, A4, and A6 for several values of the convergence

TABLE IV. Same as Table III but for ^{182}W and $\chi_0^{\mathrm{TDA}} = \chi_0^H = 0.030$ MeV.

	2	3	4	5	6	7	8	9	10
$E^{(2)}(0_1^+)$	1176.0	847.3	867.0	800.3	802.0	791.0	790.9	789.6	
$E^{(3)}(0_1^+)$	1176.0	875.1	892.7	847.6	849.2	845.2	845.2	845.0	
$E^{(4)}(0_1^+)$	1176.0	875.1	893.1	842.2	844.2	837.1	837.2	836.4	
$E(0_1^+)$								840.0	840.0
$E^{(2)}(0_2^+)$	2463.0	2444.0	1926.0	1914.0	1793.0	1787.0	1765.0	1763.0	
$E^{(3)}(0_2^+)$	2463.0	2455.0	2008.0	2008.0	1935.0	1934.0	1928.0	1928.0	
$E^{(4)}(0_2^+)$	2463.0	2455.0	1995.0	1993.0	1898.0	1897.0	1881.0	1880.0	
$E(0_2^+)$								1898.0	1897.0
$E^{(2)}(0_3^+)$		3933.0	3891.0	3155.0	3122.0	2937.0	2920.0	2884.0	
$E^{(3)}(0_3^+)$		3896.0	3909.0	3291.0	3291.0	3191.0	3187.0	3180.0	
$E^{(4)}(0_3^+)$		3896.0	3904.0	3237.0	3234.0	3075.0	3071.0	3038.0	
$E(0_3^+)$								3109.0	3109.0

parameter x_0. This one was varied from $x_0 = 0$ to $x_0 = -0.6$ by steps of -0.1. In the region $-0.5 < x_0 \leq 0$ the sixth order coefficients p, q, r, and s of the boson expansion are not defined; we put them equal to zero. This method permits us to evaluate the effects of the terms of H_B with coefficients $c(2, 2)$, $c(3, 2) = c(2, 3)$ and $c(3, 1) = c(1, 3)$ due to the contractions of higher order terms depending on the fourth order coefficients a and b, and to define an expansion hereafter noted KT4′.

1. *Comparison of the different expansions*

Table V illustrates a typical case ^{164}Er, where $\chi_0^{TDA} = \chi_0^H = 0.040$ MeV, and from which some definite conclusions can be drawn. First of all, it is seen that for the same value of the convergence parameter x_0 the different expansions give completely different results. Only the lower order approximations KT4 and A4 can give values of $E(0_1^+)$ and $E(0_2^+)$ which have something in common with the exact values obtained in the multiphonon approach. The approximate calculation A4 gives an agreement for small values of $x_0 \simeq -0.1$, and it is worthwhile to note that it is just for this approximation and this order of magnitude of x_0 that Kishimoto and Tamura got their good agreement with the experimental results.[4] Another possible way of getting an agreement is to take $x_0 < -0.6$ in the approximation KT4. But an examination of the wave function then shows clearly that one has very strong mixing of the multiphonon states, even if the energy spectrum seems very near to harmonicity. We also observe that the latter property is only possible for fourth order expansions, and that in some cases one may have $E(0_2^+) < 2E(0_1^+)$. For $-0.5 < x_0 \leq 0$ the results of KT6 ≡ KT4′ and A6 are quite equivalent, showing that the values of the p, q, r, and s coefficients in A6 are small enough to introduce only slight differences with KT4′ where these coefficients are arbitrarily put equal to zero. For $-0.5 < x_0 \leq 0$ the comparison of KT4 and KT4′ show that the contributions of the contractions of higher order terms mainly affect the energy of the second (and higher lying) 0^+ state. It may be that contractions of eighth order terms, but depending only on sixth order coefficients, also alter the results of KT6.

For $x_0 \leq 0.5$ where the KT6 expansion is, *a priori*, expected to be the best, we are forced to note that it is the worst solution, showing clearly that the boson expansion does not converge. A comparison of A4 and A6 leads to the same conclusion for the approximate boson expansions. This confirms Sørensen's conclusion[6] for the case of the low degenerate orbitals.

In Table VI we give the $c(i, j)$ coefficients of the different boson expansions of KT's type for different values of x_0 in the case discussed above. We note again that $c(0, 0)$ and $c(1, 0)$ are common to all studied expansions and that $c(1, 1)$, $c(2, 1)$, and $c(2, 0)$ are the same in KT4, KT6, and A6. The present study clearly shows that a convergence of the coefficients of the boson expansion where

$$c(i, j) > c(i+1, j+1) > c(i+2, j+2)$$

absolutely does not mean that the boson expansion method itself converges. Finally, we also want to note again that we do not have at our disposal any serious criterion to select the appropriate value of the convergence parameter.

TABLE V. Approximate values of the energies of the two lowest eigenvalues (in keV) of H obtained in the various boson expansions of Kishimoto and Tamura. The results are given for ^{164}Er and $\chi_0^{TDA} = \chi_0^H = 0.040$ MeV for which the exact values of the multiphonon approach are $E(0_1^+) = 809$ keV and $E(0_2^+) = 1789$ keV.

x_0	KT4	KT6	A4	A6
0	2158.0	2165.0	1039.0	2166.0
	4275.0	5192.0	2050.0	5242.0
−0.1	1579.0	1613.0	884.0	1615.0
	3150.0	4162.0	1745.0	4349.0
−0.2	1368.0	1490.0	717.0	1502.0
	2734.0	3814.0	1412.0	3970.0
−0.3	1221.0	1522.0	530.0	1552.0
	2443.0	3733.0	1044.0	3880.0
−0.4	1107.0	1655.0	308.0	1703.0
	2214.0	3853.0	693.0	4008.0
−0.5	1007.0	2493.0	81.0	1906.0
	2014.0	5950.0	540.0	4282.0
−0.6	912.0	2546.0	503.0	2128.0
	1858.0	5602.0	1482.0	4641.0

2. *Some remarks on the intruder states*

In subsection C the analysis of the energy spectrum was always rather simple and we observed few intruder states. In the present method there are sometimes so many of these that it is not easy to select the three lowest physical eigenstates whatever the chosen expansion. Furthermore, in some cases, their characteristics are completely different from those of the intruder states observed so far. As an example, we find for ^{154}Gd, $\chi_0 = 0.035$, $x_0 = -0.2$ in the KT4 expansion a spurious ground state of a curious "collective" nature: 8 of the 10 components of its wave function are of the order of 0.3. As a consequence, this kind of intruder state is certainly of a different nature from those seen in the modified Marumori approach. It may be a spurious state due to the violation of the Pauli principle. We may also add that there are

TABLE VI. Values of the coefficients $c(i,j)$ in MeV of the different KT boson expansions of H discussed in the text for the same case as in Table V and different values of the convergence parameter x_0.

x_0		$c(0,0)$	$c(1,0)$	$c(1,1)$	$c(2,1)$	$c(2,0)$	$c(2,2)$	$c(3,2)$	$c(3,1)$
0	KT	−1.007	−0.158	2.141	0.130	0.0713	0.450	−0.0267	−0.0611
				1.046	0.0864	0.137	0.476	−0.0227	−0.0713
−0.1	KT	−38.9	0.144	1.618	−0.0535	0.130	0.457	−0.0141	−0.0535
	A			0.979	−0.0780	0.164	0.547	−0.0204	−0.0575
−0.2	KT	−77.7	0.498	1.429	0.0216	0.164	0.415	−0.0110	−0.0470
	A			0.911	0.0714	0.191	0.481	−0.0186	−0.0493
−0.3	KT	−117.0	0.899	1.286	0.00183	0.196	0.381	−0.0091	−0.0421
	A			0.843	0.0660	0.218	0.431	−0.0167	−0.0436
−0.4	KT	−158.0	1.342	1.165	−0.0116	0.226	0.352	−0.00787	−0.0382
	A			0.774	0.0615	0.246	0.392	−0.0151	−0.0392
−0.5	KT	−200.0	1.823	1.056	−0.0213	0.255	0.843	−0.108	−0.067
	A			0.706	−0.0577	0.273	0.361	−0.0138	−0.0358
−0.6	KT	−242.0	2.342	0.956	−0.0285	0.284	0.522	−0.0515	−0.0444
	A			0.638	0.0543	0.300	0.336	−0.0127	−0.0331

also many dangerous states in the sense previously defined. This observation clearly demonstrates that for a deformed basis the Kishimoto-Tamura approach is not a clean one and that it leads, at least in some cases, to a very delicate interpretation of the obtained results.

V. CONCLUSIONS

The formalism of the multiphonon appears to be well suited for the study of the anharmonicities of the collective $K^\pi = 0^+$ vibrations in deformed nuclei. When this approach is numerically tractable it constitutes the best choice. The only recommendation consists of checking the stability of the wanted eigensolutions versus the number of basic states in order to test whether the chosen basis is large enough. When such a calculation is not feasible one can use a modified Marumori boson expansion to the fourth order, which gives a much better estimate than the second order initially suggested by Holzwarth *et al.* In such an approach one should be restricted to a basis limited to N_c multiphonons. An indication for this cutoff factor N_c can be obtained from the value of $\mathrm{Tr}(X^4)$. Finally, a treatment using the boson expansion techniques of Kishimoto and Tamura has to be avoided in deformed nuclei.

According to these conclusions further developments can be expected:

(1) The coupling of collective-noncollective phonons, as well as the coupling between collective vibrations $K^\pi = 0^+$ and $K^\pi = 2^+$ can now be studied. The formalism must be slightly extended and one has to solve the technical problem of the use of a nonorthogonal basis.

(2) A comparison with the experimental results may also be considered. It may then be necessary to introduce more sophisticated forces than in the currently used model.

Finally, there remains one fundamental open problem, the importance of the fluctuation of the number of particles.

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