## Anharmonicities of $\gamma$ vibrations in odd-mass deformed nuclei

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The  $\gamma$  vibrational states in odd-mass deformed nuclei are studied within the multiphonon method. Special attention is paid to low-energy multiphonon states in order to see if the anharmonicities observed in even-even nuclei, in which the first vibrational state  $K^{\pi} = 2^+$  appears well below the energy gap, are also found in the odd-*A* neighboring nuclei. [S0556-2813(96)03907-6]

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## I. INTRODUCTION

In most of the rare earth even-even nuclei, with  $162 \le A \le 168$ , one observes only one intrinsic excited state well below the energy gap. This state is of  $\gamma$  vibrational nature and interpreted as a "one-phonon" state. This situation arises since, in these nuclei, pairs of single-particle orbits, of same parity  $\pi$ , with quantum numbers ( $\Omega^{\pi} N n_z \Lambda$ ) satisfying the asymptotic selection rules

$$\Delta N = \Delta n_z = 0,$$
  
$$\Delta \Omega = \Delta \Lambda = \pm 2 \tag{1}$$

are available near the Fermi surface. All experimental attempts to look for the "two- $\gamma$ -phonon" vibrational states in an energy region of twice that of the one-phonon state have failed. It was therefore concluded either that the "twophonon" states do not exist or that the considered vibrations may exhibit rather strong anharmonicities. A lot of theoretical work [1-4] has been devoted to this subject. The predictions of the quasiparticle phonon nuclear model (OPNM) developed by Soloviev and his co-workers [1] are in favor of the first alternative. Practically all other theories agree with the second, which has been confirmed experimentally, at least in <sup>168</sup>Er, by Börner et al. [5] who measured the lifetime of the  $K^{\pi} = 4^+$  state at 2.55 MeV, candidate for an interpretation as a "two- $\gamma$ -phonon" state. Experimental evidence for the existence of other two-phonon  $\gamma$  vibrational states in other mass regions have also been given in [6-8].

Among the microscopic theories dealing with this topic, the multiphonon method (MPM) [3] has been systematically applied [9] to the even-even nuclei of this mass region. It was found that the  $\gamma$  vibrational spectrum is anharmonic and dilated. Furthermore, it was concluded that, in some favorable conditions, the "two-phonon"  $K^{\pi}=4^+$  states conserve some collective character, whereas their  $K^{\pi}=0^+$  partners, which are always predicted to have higher energy, lose their collectivity.

The aim of the present paper is to see how these conclusions extrapolate to the neighboring odd-mass nuclei. In these, one expects intrinsic one quasiparticle states with quantum number  $K=\Omega$ , two "one-phonon" states with K-2 and K+2, respectively, and three "two-phonon" states with K-4, K, and K+4 (respectively). It is of interest to study the relative positions of the states of such a

family and their collectivity. In particular, it will be instructive to compare the properties of the vibrational states built on different single-particle orbitals, e.g., those which contribute strongly to the  $\gamma$  vibration in even-even nuclei [see Eq. (1)] and those of unique parity, present in this region.

In Sec. II, we briefly sketch the version of the MPM suited for such a study. Some representative results are presented in Sec. III. Finally, a few interesting conclusions are drawn in a last section.

# II. SKETCH OF THE MPM FOR ODD-MASS DEFORMED NUCLEI WITH TWO BASIC PHONONS

#### A. General principles

The general principles and formulas of the MPM have been explicitly given for even-even nuclei in [3] and for odd-mass nuclei in [10]. Here only the version of the MPM which uses two phonons as building blocks is needed. For the even case this simplified method has been studied in detail in [9]. Hereafter, the important points of this approach for odd-mass nuclei will be given.

First, one introduces the quasiparticle creation  $a_m^{\dagger}$  and annihilation  $a_m$  operators where *m* summarizes all quantum numbers needed to identify the quasiparticle.

Second, phonons  $Q_i^{\dagger}$  of the Tamm-Dancoff (TDA) type

$$Q_{i}^{\dagger} = \frac{1}{2} \sum_{mn} (X_{i})_{mn} a_{m}^{\dagger} a_{n}^{\dagger}, \qquad (2)$$

are considered. Note that the matrices  $X_i$  are antisymmetric. These phonons fulfill the following commutation rule:

$$[Q_1, Q_2^{\dagger}] = -\frac{1}{2} \operatorname{Tr}(X_1 X_2) + \sum_{mn} (X_2 X_1)_{mn} a_m^{\dagger} a_n.$$
(3)

Note that in the usual quasiboson (and harmonic) approximation only the first term of Eq. (3) is retained, whereas in the MPM the full commutation relation is taken into account.

Third, one builds multiphonon states. In even-even nuclei a state with p phonons of the first type and q phonons of the second type reads

$$|pq\rangle = \frac{1}{p!q!} Q_1^{\dagger p} Q_2^{\dagger q} |0\rangle.$$
(4)

Similarly, in odd-mass nuclei one considers the states:

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$$|pq\lambda\rangle = a^{\dagger}_{\lambda}|pq\rangle,$$
 (5)

where a quasiparticle  $\lambda$  has been added to the phonons. In Eq. (4) the denominator p!q! has been introduced for numerical convenience and  $|0\rangle$  is the phonon vacuum, which, by construction, coincides with the fermion vacuum. The sets of states (4) or (5) do not form an orthonormalized basis in the mathematical sense. Therefore the first problem encountered in the MPM is the determination of the overlap matrix of the multiphonon states. Due to the Pauli principle, this is by no means an easy task. Similarly, the second problem of the MPM is the calculation of the one- and two-body operator matrix elements, which are needed to evaluate the eigenstates of a model Hamiltonian and the electromagnetic transitions.

It has been shown [10] that all these matrix elements of the odd case can be given in terms of the overlap matrix elements of states (4):

$$F(p'q';pq) = \langle p'q' | pq \rangle \tag{6}$$

(with p' + q' = p + q), the matrices

$$A_{mn}(p'q';pq) = \langle p'q' | a_n a_m | pq \rangle \tag{7}$$

(with p' + q' = p + q - 1), the quantities

$$B_{stuv}(p'q';pq) = \langle p'q' | a_v a_u a_t a_s | pq \rangle \tag{8}$$

(where p' + q' = p + q - 2), which we had in the even nuclei, and

$$D_{stuvwx}(p'q';pq) = \langle p'q' | a_x a_w a_v a_u a_t a_s | pq \rangle \qquad (9)$$

(where p'+q'=p+q-3) which are needed in addition. The quantities A, B, and D have, of course, the symmetry properties of the fermion operators product they contain. Note the relative indices order in both sides of these equations.

The quantities F, A, and B are related by the following recursion formulas:

$$[(1+\varepsilon)p' + (1-\varepsilon)q']F(p'q';pq)$$
  
= -Tr{X(\varepsilon)A[p'(\varepsilon),q'(\varepsilon);pq]}, (10)

where  $\varepsilon = \pm 1$ ,  $X(\varepsilon) = X_1$  if  $\varepsilon = +1$ , and  $X(\varepsilon) = X_2$  if  $\varepsilon = -1$ ;

$$A_{mn}(p'q';pq) = \sum_{\varepsilon_1} \left( X(\varepsilon_1)F[p'q';p(\varepsilon_1)q(\varepsilon_1)] + \sum_{\varepsilon_2} X(\varepsilon_2)A[p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2);p'q']X(\varepsilon_2) \right)_{mn},$$
(11)

$$B_{abcd}(p'q';pq) = -\sum_{\varepsilon_{1},\varepsilon_{2}} [X(\varepsilon_{1})^{*}X(\varepsilon_{2})]_{abcd} F[p'q';p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2})] + \sum_{\varepsilon_{1}} (\{X(\varepsilon_{1})^{*}A[p'q';p(\varepsilon_{1})q(\varepsilon_{1})]\}_{abcd} + \{A[p'q';p(\varepsilon_{1})q(\varepsilon_{1})]^{*}X(\varepsilon_{1})\}_{abcd}) + \sum_{\varepsilon_{1},\varepsilon_{2},\varepsilon_{3},\varepsilon_{4}} \sum_{stuv} X_{as}(\varepsilon_{1})X_{bt}(\varepsilon_{2})X_{cu}(\varepsilon_{3})X_{dv}(\varepsilon_{4})B_{stuv}[p(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3},\varepsilon_{4})q(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3},\varepsilon_{4});p'q'], (12)$$

where  $\varepsilon_i = \pm 1$ ,

$$p(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \dots, \varepsilon_n) = p - \frac{1}{2} \sum_{i=1}^n (1 + \varepsilon_i),$$
$$q(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \dots, \varepsilon_n) = q - \frac{1}{2} \sum_{i=1}^n (1 - \varepsilon_i).$$

$$q(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \dots, \varepsilon_n) = q - \frac{1}{2} \sum_{i=1}^{n} (1)$$

Note that

$$p(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \dots, \varepsilon_n) + q(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \dots, \varepsilon_n)$$

and that

$$(f^*g)_{abcd} = f_{ab}g_{cd} - f_{ac}g_{bd} + f_{ad}g_{bc}$$

$$D_{abcdef}(p'q';pq) = \sum_{\varepsilon_{1},\varepsilon_{2},\varepsilon_{3}} [X(\varepsilon_{1}) \star X(\varepsilon_{2}) \star X(\varepsilon_{3})]_{abcdef} F[p'q';p(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3})q(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3})]$$

$$= \sum_{\varepsilon_{1},\varepsilon_{2}} \{A[p'q';p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2})] \otimes [X(\varepsilon_{1}) \star X(\varepsilon_{2})]\}_{abcdef}$$

$$+ \sum_{\varepsilon_{1}} \{X(\varepsilon_{1}) \otimes B[p'q';p(\varepsilon_{1})q(\varepsilon_{1})]\}_{abcdef}$$

$$= \sum_{\varepsilon_{1},\varepsilon_{2},\varepsilon_{3},\varepsilon_{4},\varepsilon_{5},\varepsilon_{6}} \sum_{stuvwx} X_{as}(\varepsilon_{1})X_{bt}(\varepsilon_{2})X_{cu}(\varepsilon_{3})X_{dv}(\varepsilon_{4})X_{ew}(\varepsilon_{5})X_{fx}(\varepsilon_{6})$$

$$\times D_{stuvwx}[p(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3},\varepsilon_{4},\varepsilon_{5},\varepsilon_{6})q(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3},\varepsilon_{4},\varepsilon_{5},\varepsilon_{6});p'q'], \qquad (13)$$

where

$$[f \star g \star h]_{abcdef} = f_{ab}(g \star h)_{cdef} - f_{ac}(g \star h)_{bdef} + f_{ad}(g \star h)_{bcef} - f_{ae}(g \star h)_{bcdf} + f_{af}(g \star h)_{bcde}$$
(14)

and

$$[f \otimes g]_{abcdef} = f_{ab}g_{cdef} - f_{ac}g_{bdef} + f_{ad}g_{bcef} - f_{ae}g_{bcdf} + f_{af}g_{bcde} + f_{bc}g_{adef} - f_{bd}g_{acef} + f_{be}g_{acdf} - f_{bf}g_{acde} + f_{cd}g_{abef} - f_{ce}g_{abdf} + f_{cf}g_{abde} + f_{de}g_{abcf} - f_{df}g_{abce} + f_{ef}g_{abcd}.$$
(15)

From the quantities F and A one can calculate the overlap matrix through:

$$\langle p'q'\lambda'|pq\lambda \rangle = \delta_{\lambda\lambda'}F(p'q';pq)$$
  
+  $\sum_{\varepsilon_1} \{X(\varepsilon_1)A[p(\varepsilon_1)q(\varepsilon_1);p'q']\}_{\lambda'\lambda}.$  (16)

In the special case which is under consideration in this paper, the two phonons 1 and 2 correspond to  $\gamma$  and  $\overline{\gamma}$ , respectively. As a consequence, the matrix  $X_2$  can be deduced from  $X_1$  by time reversal properties. To go further on, one needs to choose a model Hamiltonian. The main aim of this paper is to look for the general trends of the  $\gamma$  motion in odd-mass nuclei and not to look for a fine agreement between theory and experiment. Therefore, we chose the simplest model Hamiltonian containing the interactions known to play the major roles in the considered nuclei. We assume an axially deformed nuclear potential ( $H_{sp}$ ) of the Nilsson or Woods-Saxon type, a constant monopole pairing force of strength  $G_{\tau}$  for each kind  $\tau$  of particles (protons and neutrons), and a charge independent quadrupole-quadrupole (QQ) interaction

$$H = H_{sp} + H_P + H_{QQ}$$

As usual, the pairing is treated by introduction of the canonical Bogolyubov-Valatin transformation, which separates the model Hamiltonian into its different parts:

$$H = H_{00} + H_{11} + H_{22} + H'_{22} + H_{31} + H_{13} + H_{40} + H_{04},$$

where  $H_{ij}$  contains *i* creation operators  $a^{\dagger}$  and *j* annihilation operators *a*. Similarly, the electromagnetic operators split into four parts

$$T = T_{00} + T_{11} + T_{20} + T_{02}$$

The contribution of the constant term  $T_{00}$  to nondiagonal matrix elements vanishes. It has been shown in [10] that the matrix elements of the one-body operators  $H_{11}$  and  $T_{11}$  can be deduced from the knowledge of the quantities F, A, and B, whereas for  $T_{20}$  and  $T_{02}$  only A and B are needed. For the evaluation of the matrices of the two-body parts of the model Hamiltonian the quantities D are required in addition. The recursion formulas for these matrix elements are rather sophisticated and their explicit form will be postponed to the Appendices. To summarize, the MPM is an *exact* diagonalization of the *complete* model Hamiltonian within the space spanned by the multiphonon states (5). Note also that, in contrast to the case of the  $\gamma$  motion in even-even nuclei, the parts  $H_{31}$  and  $H_{13}$  of H contribute in odd-mass nuclei.

#### B. The different steps of the MPM in realistic calculations

Once the model Hamiltonian has been chosen, the different steps of the MPM go as follows.

(1) Using some physical arguments, one has to select the multiphonon "basis." This includes first the choice of the phonons which are expected to play a major role in the collective subspace. In the present paper, we restrict ourselves to the two phonons  $\gamma$  and  $\overline{\gamma}$ . As a consequence, the version of the MPM used here can only be applied with confidence in a mass region where the  $\gamma$  vibration is much lower in energy than any other *intrinsic* excitation below the energy gap, observed in even-even nuclei. To build the retained phonon (2) one has to fix the number  $n_1$  of active, two times degenerate, single-particle orbitals for each kind of particle (protons and neutrons). One generally chooses the same number of levels (e.g.,  $n_1 = 20$ ) for each kind, equitably distributed on each side of the Fermi surface. A Tamm-Dancoff calculation gives then a reasonable choice for the matrices  $X_1$  and  $X_2$ .

(2) The second step consists of calculating and storing the quantities F, A, B, and D using the recursion formulas up to some given maximum number  $n_{\rm ph}$  of phonons. To minimize the effort only nonequivalent (i.e., quantities which cannot be deduced by symmetry properties from a previous calculated one) are evaluated and only nonzero values are stored. To give a rough idea of this first problem, if one considers two types of phonons,  $n_l = 20$  and  $n_{ph} = 8$ , one has  $3 \times 85 = 255$  quantities B each of which has a maximum of  $(2 \times 20)^4$  elements, leading to a total number of  $\simeq 6.5 \times 10^8$ elements. If one eliminates those which vanish and calculate only the nonequivalent quantities one remains with  $\simeq 5 \times 10^{5}$  elements. In this counting, the factor 3 comes from the following three possibilities: either four protons, or four neutrons, or two protons and two neutrons, can appear among the four operators a in the definition (8). The second factor, 85, results from the sum over the current number of initial n and final n' phonon numbers of all combined possible partitions of *n* between *p* and *q* and n' between p' and q', with the constraint n' = p' + q' = n - 2 = p + q - 2. In a completely similar way, and in the same conditions for  $n_{\rm ph}$ and  $n_1$ , one gets  $4 \times 394 = 1576$  entities D, each of which having  $(2 \times 20)^6$  elements, leading to a total amount of  $\approx 6.5 \times 10^{12}$  elements. Fortunately, here too a lot of these elements vanish according to the conservation of parity and/or K quantum numbers or to the Pauli principle. One remains however with  $\simeq 2 \times 10^7$  nonequivalent D values. It appears therefore that their evaluation is very time consuming, even on modern computers. Furthermore, the computer memory needed to store all what one has to keep for further calculations is of the order of 285 megaoctets.

(3) The next step is the determination, for each chosen  $K^{\pi}$  value, of the overlap matrix and the Hamiltonian matrix in the nonorthonormalized MPM basis (5), by an extensive use of the recursion formulas given in (16) and in the Appendices. Then follows the diagonalization of the obtained H matrix within an appropriate method for non-orthonormalized bases. Special attention is paid to the lowest eigenvalues. According to the numerous contributions  $H_{ij}$  entering the model Hamiltonian, this step constitutes a second rather tremendous numerical task.

These steps are repeated for successive increasing values of the maximum number  $n_{\rm ph}$  of phonons. The procedure stops once a reasonable numerical stability of the lowest eigenvalues is observed. It is worthwhile to note that the value of  $n_{\rm ph}$  depends mainly on the collectivity of the building phonons, i.e., on the choice of the antisymmetric matrices  $X_1$  and  $X_2$ . In practical situations, where these are taken from the Tamm-Dancoff approximation, the value of  $n_{\rm ph}$  is of the order of 8 when realistic values of the QQ strength  $\chi$  are used. We emphasize that the whole procedure just described has to be repeated from the very beginning if one wants to change any of the parameters entering the model Hamiltonian (e.g., deformation of the single-particle field, pairing strength  $G_{\tau}$ , or quadrupole-quadrupole interaction). The same holds if one wants to select another number  $n_1$  of active orbitals entering the pairing and TDA calculations. We may remark here that there is, a priori, no fundamental reason to use the same value of the quadrupole strength parameter  $\chi$  in the model Hamiltonian and in the resolution of the secular TDA equation. According to this, if one only wants to study the effect of the variation of the QQ interaction strength  $\chi$ , one may restart the procedure only at the third step.

It is necessary to add a few words concerning the interpretation of the eigenstates resulting from the MPM calculation. After the diagonalization of the H matrix, the eigenvectors appear as superpositions of the multiphonon states (5)and one can no longer speak about states containing a fixed number of phonons. According to the nonorthogonality of the MPM "basis" their interpretation may not be easy. It has therefore appeared to be worthwhile to study the E2 transitions with  $|\Delta K| = 2$  between the obtained eigenstates, in order to detect possible collective transitions. Two states related by a collective transition will therefore be considered as "differing by one phonon." As a consequence, we shall speak in our further analyses about "one-phonon" or "twophonon'' states (with quotes) built on a given " $K^{\pi}$  state." Note that, since we have to restrict ourselves to a definite number of active levels for each kind of particle, some effective charge  $e_n = e(1 + \epsilon)$  and  $e_n = e\epsilon$  (where  $\epsilon$  is a small free parameter) have to be introduced in the evaluation of the E2 matrix elements.

### **III. SOME REPRESENTATIVE RESULTS**

In the considered mass region,  $162 \le A \le 168$ , two kinds of single-particle states can be found in the neigborhood of the Fermi surface.

The first kind contains the states originating from the "unique parity" subshell  $i_{13/2}$  for neutrons or  $h_{11/2}$  for protons. Since the coupling to the  $\gamma$  and  $\overline{\gamma}$  phonons conserves the parity, the single-particle orbitals to be considered in the MPM basis arise mainly from the same spherical subshells. As a consequence, no pairs of orbitals satisfying (1) exist among the unique parity states and one may, *a priori*, expect rather pure vibrational excited states.

The second kind concerns the orbitals of "natural parity." Among those one finds several pairs of states which fulfill the asymptotic selection rules (1) and contribute therefore strongly to the  $\gamma$  phonon. For the proton field one has, near the Fermi surface, the pairs  $1/2^+411$  and  $5/2^+413$ , or  $-(1/2^+411)$  and  $3/2^+411$ , whereas for the neutrons the pairs  $1/2^-521$  and  $5/2^-523$  or  $-(1/2^-521)$  and  $3/2^-521$  are expected. It is therefore of interest to study the blocking effect of an odd quasiparticle of such pairs on the collectivity of the vibrational states in odd-mass nuclei.

For a considered  $K^{\pi}$ , we study first the "one-phonon" states with K-2 and K+2. Special attention will be paid to the energy splitting  $\Delta E = E(K+2) - E(K-2)$  and to the *E*2 transitions with  $|\Delta K| = 2$ , which relay these "one-phonon" states to the  $K^{\pi}$  state. In a second step, we search for the "two-phonon" states with K-4, K, and K+4, respectively, by careful analysis of their *E*2 decay to the "one-phonon" states.

Since we are not aimed at looking for a fine adjustment between theory and experiment, we shall use for the studied odd-A nuclei the parameter sets of their doubly even core as given in [9]. More precisely, we use a Nilsson potential with a fixed quadrupole deformation parameter for each core, BCS gap parameters deduced from the experimental masses [12], and a quadrupole strength parameter  $\chi$ , fitted, within

TABLE I. Absolute energies of the first lowest negative parity states in  $^{165}$ Ho. The last column indicates the nature of the level, as deduced from analysis of the *E*2 transitons.

$I^+$	$n_{\rm ph} = 4$	$n_{\rm ph} = 5$	$n_{\rm ph} = 6$	$n_{\rm ph} = 7$	$n_{\rm ph} = 8$	Identification
$(7/2)_1$	-480	-489	- 565	- 566	- 574	7/2-523
(3/2) <sub>1</sub>	405	106	93	48	47	$(7/2)_1 + \overline{\gamma}$
(11/2) <sub>1</sub>	500	181	174	126	126	$(7/2)_1 + \gamma$
(9/2) <sub>1</sub>	437	437	367	367	361	$9/2^{-}514$
(5/2)1	501	474	410	406	400	5/2-532
(1/2) <sub>1</sub>	585	564	491	487	480	$1/2^{-}541$
$(1/2)_2$	1106	903	851	821	815	$(5/2)_1 + \overline{\gamma}$
$(3/2)_2$	1173	997	947	918	913	$(1/2)_1 + \overline{\gamma}$
$(5/2)_2$	1418	1106	1105	1060	1060	$(9/2)_1 + \overline{\gamma}$
(13/2) <sub>1</sub>	1438	1127	1127	1081	1081	$(9/2)_1 + \gamma$
(9/2) <sub>2</sub>	1504	1217	1200	1159	1157	$(5/2)_1 + \gamma$
(5/2) <sub>3</sub>	1584	1270	1257	1210	1209	$(1/2)_1 + \gamma$
(3/2) <sub>3</sub>	1395	1298	1237	1220	1214	$3/2^-541$ ?
(1/2) <sub>3</sub>	1590	1455	1292	1272	1252	$(7/2)_1 + \overline{\gamma}\overline{\gamma}$
(15/2) <sub>1</sub>	1747	1724	1465	1460	1430	$(7/2)_1 + \gamma \gamma$

the MPM, to the one-phonon state in the core when 20 active levels are introduced. With such a choice, one has a parameter free problem in the considered odd-mass nuclei, which allows one to go only once through the different steps of the MPM described in Sec. II B. As a consequence, it is clear that only the general trends of the  $\gamma$  vibrational motion in odd-mass nuclei can be reached. According to the status of the experimental information available at the present time, this seems sufficient.

## A. Unique parity vibrational states

The  $K=7/2^-$  orbital originating from the  $h_{11/2}$  proton subshell appears as the ground state for the Ho isotopes. Concerning the neutron subshell  $i_{13/2}$ , the  $K=7/2^+$  member is the ground state for <sup>167</sup>Er, whereas the  $K=5/2^+$  is found as such in <sup>161</sup>Dy. Preliminary results for the K=7/2 in <sup>167</sup>Er and <sup>167</sup>Ho have been published recently in [11]. Representative results for three nuclei, where the ground state is of unique parity, are given below.

In <sup>165</sup>Ho, the ground state is  $7/2^{-}523$ . All the other orbitals originating from the subshell  $h_{11/2}$  are found in the chosen single-particle proton field as well as the  $1/2^{-}541,3/2^{-}532$ , and  $1/2^{-}530$  orbitals. The quasiparticle energies of these unique parity states are all lower than 3.5 MeV. Table I gives the calculated absolute energies of the first 15 levels versus the maximum number  $n_{\rm ph}$  of the phonons introduced in the MPM basis (5).

The displayed results show clearly that a general and reasonable stability of the energies is obtained when  $n_{\rm ph}=8$  is used. As expected, the binding energy of the ground state gets larger with larger  $n_{\rm ph}$ . The ground state energy stays stable for  $n_{\rm ph}=6$  and  $n_{\rm ph}=7$ , whereas the "one-phonon" states with K=3/2 and K=11/2 keep stable for  $n_{\rm ph}=7$  and  $n_{\rm ph}=8$ . This result, which is similar to that obtained in the doubly even nuclei [9], shows that the parts  $H_{40}$  and  $H_{04}$  of H, which couple multiphonons states where  $\Delta n = \pm 2$ , play a dominant role. As for even-even nuclei, it is also found that,

TABLE II. Calculated values of some typical  $|\langle K_f | E2 | K_i \rangle|$  matrix elements for different values of the effective charge  $\epsilon$  and  $n_{\rm ph} = 8$  in <sup>165</sup>Ho and unique parity.

	$\epsilon = 0$	$\epsilon = 0.2$	$\epsilon = 0.4$
$\overline{(3/2)_1 \rightarrow (7/2)_1}$	2.69	3.93	5.18
$(11/2)_1 \rightarrow (7/2)_1$	2.65	3.90	5.15
$(5/2)_1 \rightarrow (9/2)_1$	0.006	0.008	0.011
$(5/2)_2 \rightarrow (9/2)_1$	2.57	3.79	5.02
$(13/2)_1 \rightarrow (9/2)_1$	2.55	3.78	5.00
$(1/2)_1 \rightarrow (5/2)_1$	0.026	0.041	0.057
$(1/2)_2 \rightarrow (5/2)_1$	2.57	3.72	4.87
$(9/2)_2 \rightarrow (5/2)_1$	2.67	3.92	5.17
$(15/2)_1 \rightarrow (11/2)_1$	2.94	4.30	5.66
$-(1/2)_1 \rightarrow (3/2)_1$	0.14	0.22	0.30
$-(1/2)_2 \rightarrow (3/2)_1$	1.01	1.47	1.92
$-(1/2)_3 \rightarrow (3/2)_1$	2.70	3.93	5.16

for spaces restricted to  $n_{\rm ph} < 5$ , some states (in fact the vibrational states) have strongly overestimated energies. As a consequence, model calculations restricted to a too small multiphonon basis may not be considered as really meaningful. On the other way round, the variation of the absolute energies with  $n_{\rm ph}$  may give a serious indication on the nature of the eigenstates. Energies which vary by  $\leq 100$  keV correspond to states of rather pure quasiparticle nature; energies which are stable for  $n_{\rm ph}=7$  and  $n_{\rm ph}=8$  indicate a main component with "one phonon." These indications on the nature of the different excited levels are to be checked through the analysis of the *E*2 transitions with  $|\Delta K|=2$ . Table II gives the values of  $|\langle K_f | E2 | K_i \rangle|$  matrix element for different values of the effective charge  $\epsilon$  and  $n_{\rm ph}=8$ , for some typical transitions.

First, it is found that the  $|\langle K_f | E2 | K_i \rangle|$  vary linearly with  $\epsilon$ . Second, it is easy to separate the collective transitions from the noncollective ones. Consequently, it becomes clear that the "one-phonon" states built on the ground state  $(7/2)_1$  are  $(3/2)_1$  and  $(11/2)_1$ , the "one-phonon" states built on the  $(9/2)_1$  are  $(5/2)_2$  and  $(13/2)_1$  while the "onephonon'' states built on the  $(5/2)_1$  are  $(1/2)_2$  and  $(9/2)_2$ . Concerning the  $K \pm 4$  "two-phonon" states built on the ground state, the candidates are  $(1/2)_3$  and  $(15/2)_1$ . None of the first three excited states with K = 7/2 are linked to the  $(3/2)_1$  and  $(11/2)_1$  by a collective E2 transition. Therefore, no candidate for the label "two-phonon" state with K = 7/2clearly appears. It is also quite interesting to have a look to the splitting  $\Delta E = E(K+2) - E(K-2)$  of the two "onephonon'' states for several values of K. All calculated values of  $\Delta E$  are positive: e.g., one gets 79, 21, and 342 keV, respectively, for  $(7/2)_1$ ,  $(9/2)_1$ , and  $(5/2)_1$ . For the two last cases it is clear that these splittings are (rather strongly) influenced by the repulsion of the states  $(9/2)_1$  and  $(5/2)_1 + \gamma$  on one hand and  $(5/2)_1$  and  $(9/2)_1 + \overline{\gamma}$  on the other hand. For well-defined "two-phonon" states, built on the same K state, one may also evaluate the anharmonicity ratios

$$R_{\pm}(K) = \frac{E(K \pm 4) - E(K)}{E(K \pm 2) - E(K)}.$$

TABLE III. Relative energies of the first excited positive parity states in  $^{167}$ Er.

$I^+$	$n_{\rm ph}=4$	$n_{\rm ph} = 5$	$n_{\rm ph} = 6$	$n_{\rm ph} = 7$	$n_{\rm ph} = 8$	Expt.
(3/2) <sub>1</sub>	866	607	657	617	621	531
$(11/2)_1$	1017	720	780	735	741	711
$(5/2)_1$	755	734	741	737	738	810
$(1/2)_1$	1303	1134	1147	1121	1122	
(9/2) <sub>1</sub>	1021	1034	1039	1042	1042	1253
$(3/2)_2$	1637	1521	1542	1522	1524	
$(9/2)_2$	1795	1518	1567	1528	1532	
$(1/2)_2$	1766	1773	1766	1757	1751	
$(5/2)_2$	2043	1749	1820	1776	1783	
$(13/2)_1$	2088	1796	1867	1824	1831	
$(1/2)_3$	2057	1858	1843	1826	1824	
$(15/2)_1$	2355	2323	2140	2133	2109	
(7/2) <sub>2</sub>	2544	2269	2287	2244	2243	

For the ground state K=7/2, one gets  $R_+ \approx R_- \approx 2.9$ . Another instructive quantity, which concerns the *E*2 transitions is

$$Q_{\pm}(K) = \frac{|\langle K \pm 2|E2|K \pm 4\rangle|}{|\langle K|E2|K \pm 2\rangle|}$$

It appears that  $Q_+(K)$  is stable versus variation of  $\epsilon$  and practically independent of *K*. Its value, 1.1, is slightly larger than 1. This last property shows that the vibrational character of the *K*+4 states is somehow larger than that of the *K*+2 as expected from the absence of high *K* quasiparticle levels in the mean field. No general conclusions can be given for  $Q_-(K)$ .

For  ${}^{167}$ Er, the ground state is  $7/2^+633$ . The other positive parity single-particle states present among the 20 retained active neutron levels are  $1/2^+660$ ,  $3/2^+651$ ,  $5/2^+642$ ,  $9/2^+624$ , and  $11/2^+651$  from the  $i_{13/2}$  subshell to which the  $3/2^+402$ , which is known to pseudocross with  $3/2^+651$ , is added. All these orbitals have quasiparticle energies lower than 3.3 MeV. Table III gives the calculated energies of the first 13 excited positive parity levels relative to the ground state versus the maximum  $n_{\rm ph}$  of the phonons introduced in the MPM basis. The last column gives the experimental energy (which contains some rotational and Coriolis contributions) when available. As for the case of  $^{165}$ Ho, a reasonable stability of the energies is obtained for  $n_{\rm ph} = 8$ . It is interesting to notice that within 2.3 MeV all expected levels are found. First, one finds candidates for the "one-phonon" states with K=3/2 and K=11/2 and for the "two-phonon" states with K = -1/2, 7/2, and 15/2 built on the K = 7/2ground state. Second, one also finds the "quasiparticle" states corresponding to  $5/2^+642$  and  $9/2^+624$  and candidates for the "one-phonon" states built on these orbitals with K = 1/2 and 9/2, 5/2, and 13/2. Two additional levels with K=1/2 and 3/2 are also obtained. It is worthwhile to note that for a completely parameter free calculation the comparison with the available experimental results are rather good. Again, the nature of the different excited levels can be checked by the analysis of a few typical E2 transitions with  $|\Delta K| = 2$  given in Table IV for  $n_{\rm ph} = 8$  and different values

TABLE IV. Values of  $|\langle K_f | E2 | K_i \rangle|$  matrix element for different values of the effective charge  $\epsilon$  and  $n_{\rm ph} = 8$  in <sup>167</sup>Er and unique parity.

	$\epsilon = 0$	$\epsilon = 0.2$	$\epsilon = 0.4$
$(3/2)_1 \rightarrow (7/2)_1$	2.67	3.89	5.11
$(11/2)_1 \rightarrow (7/2)_1$	2.75	3.99	5.23
$(1/2)_1 \rightarrow (-3/2)_1$	0.96	1.40	1.84
$(1/2)_1 \rightarrow (5/2)_1$	2.41	3.56	4.72
$(9/2)_1 \rightarrow (5/2)_1$	0.24	0.36	0.48
$(9/2)_2 \rightarrow (5/2)_1$	2.75	4.01	5.28
$(1/2)_2 \rightarrow (-3/2)_1$	1.89	2.74	3.58
$(1/2)_2 \rightarrow (5/2)_1$	0.85	1.22	1.59
$(1/2)_3 \rightarrow (-3/2)_1$	1.57	2.31	3.05
$(1/2)_3 \rightarrow (5/2)_1$	0.63	0.89	1.16
$(15/2)_1 \rightarrow (11/2)_1$	3.01	4.37	5.73
$(7/2)_2 \rightarrow (3/2)_1$	1.11	1.58	2.05
$(7/2)_2 \rightarrow (11/2)_1$	0.40	0.65	0.90

of the effective charge  $\epsilon$ . From the displayed results it is clear that the transitions from the first 3/2 and 11/2 states to the ground state are collective. The E2 transitions also indicate that the  $(9/2)_1$  is of "quasiparticle" nature, whereas the  $(9/2)_2$  is a "one-phonon" state based on the  $(5/2)_1$  state. The  $(15/2)_1$  state is clearly the K+4 "two-phonon" state built on the ground state. The decay of the 7/2 excited state by E2 to the "one-phonon" state  $(3/2)_1$  and  $(11/2)_1$  are not really of collective character. Another interesting result deals with the 1/2 states for which the E2 transitions to the state  $(-3/2)_1$  and  $(5/2)_1$  are compared. It is seen that  $(1/2)_1$  corresponds to the "one-phonon" state built one the  $(5/2)_1$ state. The collectivity of the transition between the "onephonon'' state  $(3/2)_1$  and a "two-phonon" state (-1/2) is shared between  $(1/2)_2$  and  $(1/2)_3$ . Here too, one gets an dilated vibrational spectrum anharmonic since  $R_{+} \simeq R_{-} \simeq 2.8$ , if one adopts  $(1/2)_{2}$  for the "two-phonon" state. The analysis of  $Q_+(K)$  leads to similar conclusions than for  ${}^{165}$ Ho. Roughly speaking, the results obtained for the  $7/2^+$  system in  ${}^{167}$ Er are very similar to that of the  $7/2^{-1}$  system in <sup>165</sup>Ho , except for a parity change.

For <sup>161</sup>Dy, the ground state is  $5/2^+642$ . The other unique parity states present in the considered neutron field are  $1/2^+660$ ,  $3/2^+651$ ,  $7/2^+633$ , and  $9/2^+624$ , to which one adds the deep hole states  $1/2^+400$  and  $3/2^+402$  known to pseudocross with  $1/2^+660$  and  $3/2^+651$  (respectively). It is rather easy to follow the vibrational chain K, K+2, K+4, by looking to the involved E2 transitions (for  $\epsilon=0$  and  $n_{\rm ph}=8$  for instance).

 $|\langle (9/2)_1|E2|(5/2)_1\rangle|=2.72$  and  $|\langle (13/2)_1|E2|(9/2)_1\rangle|$ = 3.02. The ratio  $R_+$  is 2.6 and  $Q_+=1.11$ . However, the lower value of K=5/2 (compared to the 7/2 systems studied before) allows for more mixing of the MPM basic states on the K, K-2, K-4 side, resulting in lower E2 matrix elements:  $|\langle (1/2)_1|E2|(5/2)_1\rangle|=2.39$ ;  $|\langle (-3/2)_2|E2|(1/2)_1\rangle|$ = 1.69;  $|\langle (-3/2)_4|E2|(1/2)_1\rangle|=2.48$  and some sharing of the collectivity at the "two-phonon" level. The identification of the K-4 "two-phonon" state, and consequently the evaluation of  $R_-$  and  $Q_-$  are therefore less obvious. If one retains the more plausible candidate,  $(3/2)_4$ , one gets a very

TABLE V. Typical  $|\langle K_f | E2 | K_i \rangle|$  matrix elements, obtained in the MPM for <sup>163</sup>Tb, natural parity,  $n_{\rm ph}$ =8, and several values of the effective charge  $\epsilon$ .

	$\epsilon = 0$	$\epsilon = 0.2$	<i>ϵ</i> =0.4
$(7/2)_2 \rightarrow (3/2)_1$	2.80	4.13	5.46
$(11/2)_2 \rightarrow (7/2)_2$	3.77	5.49	7.21
$(9/2)_1 \to (5/2)_1$	2.61	3.86	5.10
$(13/2)_1 \rightarrow (9/2)_1$	3.38	4.94	6.51
$-(1/2)_1 \rightarrow (3/2)_1$	1.52	2.34	3.16
$-(1/2)_2 \rightarrow (3/2)_1$	0.40	0.57	0.75
$-(1/2)_3 \rightarrow (3/2)_1$	2.87	4.01	5.14
$(1/2)_1 \rightarrow (5/2)_1$	0.27	0.54	0.82
$(1/2)_2 \rightarrow (5/2)_1$	0.50	0.77	1.05
$(1/2)_3 \rightarrow (5/2)_1$	3.01	4.26	5.51
$(5/2)_4 \rightarrow (1/2)_3$	3.94	5.75	7.56
$(5/2)_4 \rightarrow (9/2)_1$	2.16	2.97	3.79

large (and may be unrealistic)  $R_-$  ratio value of 3.6. A fortiori, no 5/2 state with significant E2 transitions to both "one-phonon" states,  $(1/2)_1$  and  $(9/2)_1$  can be found (e.g., one finds  $E2[(5/2)_3 \rightarrow (1/2)_1]=1.78$  and  $E2[(5/2)_3 \rightarrow (9/2)_1]=0.40$ ). In conclusion, it appears that the situation for the K=5/2 unique parity system is somehow less clear than that discussed earlier for the two K=7/2 cases. Apparently, the reason of this comes from the lower K values (1/2, 3/2, and 5/2) involved on the K-2, K-4 side.

#### **B.** Natural parity vibrational states

We shall restrict ourselves to two typical examples, one for each kind of particle.

In <sup>163</sup>Tb, the adopted ground state label is  $3/2^+411$ . Near the Fermi surface, one expects also the two orbitals,  $5/2^+413$  and  $1/2^+411$ , which form with the ground state two pairs of orbitals fulfilling relation (1). Experimentally, one observes three  $K^{\pi}=1/2^+$  bandheads at 674, 994, and 1226 keV, the properties of which indicate a complex structure. It is therefore of fondest interest to look for the predictions of the MPM calculation.

Table V gives the most important E2 transitions needed for the analysis of the natural parity states in <sup>153</sup>Tb, with special attention paid to the vibrational states built on the  $3/2^+$  ground state and the first excited  $5/2^+$  state. The first four E2 transitions allow one to follow nicely the K, K+2, and K+4 chain built on  $K=(3/2)_1$  and  $K=(5/2)_1$ , where the collective nature of the transitions is clear. The corresponding anharmonicity ratios are  $R_{+}(3/2) = 2.4$  and  $R_{+}(5/2) = 2.7$ , i.e., somewhat lower than for the unique parity studied before. For the E2 ratios one gets again stable values versus  $\epsilon$ . The values  $Q_{+}(3/2) \approx 1.32$ and  $Q_{+}(5/2) \approx 1.28$  are larger than for the unique parity cases and they increase slightly with decreasing K. The six next E2 are given in order to discuss the nature of the three first K = 1/2 excited states. The first excited 1/2 state obtained within the MPM shows some (relatively medium) collectivity in its transition to the ground state. The calculated  $(1/2)_2$  is very weakly related to the  $(3/2)_1$  and  $(5/2)_1$  and must, thus, be of individual nature (probably a rather pure

TABLE VI. Typical  $|\langle K_f | E2 | K_i \rangle|$  matrix elements, obtained in the MPM for <sup>163</sup>Er, natural parity,  $n_{\rm ph} = 8$ , and several values of the effective charge  $\epsilon$ .

	$\epsilon = 0$	$\epsilon = 0.2$	$\epsilon = 0.4$
$(9/2)_1 \rightarrow (5/2)_1$	2.83	4.12	5.40
$(13/2)_1 \rightarrow (9/2)_1$	2.77	4.09	5.40
$(7/2)_3 \rightarrow (3/2)_1$	2.53	3.64	4.75
$(11/2)_3 \rightarrow (7/2)_3$	2.70	3.96	5.22
$(1/2)_1 \rightarrow (5/2)_1$	2.09	3.04	3.99
$(1/2)_2 \rightarrow (5/2)_1$	0.03	0.002	0.03
$(1/2)_3 \rightarrow (5/2)_1$	0.34	0.42	0.50
$-(1/2)_1 \rightarrow (3/2)_1$	0.56	0.72	0.88
$-(1/2)_2 \rightarrow (3/2)_1$	1.07	1.54	2.00
$-(1/2)_3 \rightarrow (3/2)_1$	0.72	1.02	1.31
$(5/2)_4 \rightarrow (1/2)_1$	1.32	1.84	2.37
$(5/2)_4 \rightarrow (9/2)_1$	0.01	0.02	0.06
$-(3/2)_3 \rightarrow (1/2)_1$	2.17	3.17	4.16

 $1/2^+411$ ). The calculated  $(1/2)_3$  level has the most complex structure since it presents collective decay as well to the  $(5/2)_1$  excited state as to the ground state. As a consequence, it seems meaningless to really speak about "one-phonon" K-2 states built on the  $(5/2)_1$  and  $(3/2)_1$  levels. The last two E2 given in Table V concern state  $(5/2)_4$  which decays by collective transitions to  $(1/2)_3$  and to  $(9/2)_1$ . It would be a good candidate for the "two-phonon"  $K_2=K=5/2$  state built on the  $(5/2)_1$  level if the  $(1/2)_3$  could be considered as the "one-phonon" state built on this  $(5/2)_1$  state. With such a questionable interpretation, the anharmonicity ratio would be 1.7 on the K, K-2, K way and 2.0 on the K, K+2, K side.

Our second example of natural parity deals with the oddneutron nucleus<sup>163</sup>Er, where the  $5/2^{-}523$  appears as the ground state. At 104 keV one observes the  $3/2^{-}521$  level and at 346 keV the  $1/2^{-}521$ . As for the odd-proton case studied before these orbitals form two pairs satisfying the selection rules (1), but here they appear in a different order, compared to the first given example.

The presentation of Table VI is similar to the preceding one. Again it is easy to follow the K, K+2, K+4 chain built on the ground state and the first K = 3/2 excited level, with the anharmonicity ratio  $R_{+}(5/2) = 2.6$  and  $R_{+}(3/2) = 2.5$ . The E2 ratios are  $Q_{+}(5/2) \approx 0.99$  and  $Q_{+}(3/2) \approx 1.08$ . On the other hand, the analysis of the first three 1/2 states is not obvious. If the  $(1/2)_1$  has a strong E2 to the ground state, no clear candidate for the "one-phonon" K-2 state appear for the  $(3/2)_1$  state. The  $(3/2)_3$  may be a suitable candidate for the K-4 "two-phonon" state built on the ground state, whereas the  $(5/2)_4$  presents some character of the K "twophonon'' state, but only through its decay via the  $(1/2)_1$  state [and not via the  $(9/2)_1$  state]. Note that the identification of the different calculated 1/2 states within the MPM does not correspond to that adopted in experimental compilation. This fact should not be considered as surprising, since our parameter free MPM calculation does not at all pretend to lead to a fine description of the observed energy spectrum. It is indeed sure that, for the natural parity states, slight modifications of the adopted mean field may have some consequences on the MPM results more for odd-mass nuclei than it had for eveneven nuclei.

## **IV. CONCLUSIONS**

In this paper the  $\gamma$  vibrational states have been studied in odd-mass deformed nuclei, neighbors of even nuclei where one can assume that the  $\gamma$  state is energetically well separated from all other intrinsic levels.

A first general (and empirically expected) result concerns the two "one- $\gamma$ -phonon" states which can be built on the ground state with *K* quantum number. The MPM explains, in a microscopic way, that the K-2 vibrational level has always an energy lower than its K+2 partner. However, no general rule can be given for the positive energy splitting

$$\Delta E = E(K+2) - E(K-2)$$

It depends somehow on the presence, in the energy region of the "one- $\gamma$ -phonon" state, of other intrinsic states with K-2 and/or K+2 quantum numbers. As an example, the (rather often) presence of an intrinsic (one quasiparticle state) with K-2 a little higher than the  $K\pm 2$  vibrational states may enlarge  $\Delta E$  considerably. Note however that for some natural parity orbitals it appears difficult (if not impossible) to identify the K-2 "one phonon" state.

A second conclusion concerns the three expected "two- $\gamma$ -phonon" states with  $K_1 = K - 4$ ,  $K_2 = K$  and  $K_3 = K + 4$ . Among these three "two- $\gamma$ -phonon" states, the  $K_3 = K + 4$  is the purest vibrational state. This is particularly true for the unique parity states, since no intrinsic quasiparticle state with  $K = K_3$  arises in the level scheme. Furthermore, in all cases, the *E*2 transitions from the K+4 to the K+2 states and from K+2 to K keep a real collective character, with  $Q_+$  ratio generally greater than one. The vibrational spectrum is, as in the even nuclei, strongly anharmonic and dilated.

The situation of the "two- $\gamma$ -phonon" state with  $K_1 = K - 4$  is somehow similar for K = 7/2 and unique parity. When lower K values are involved (which is the case in particular for the natural parity states) more mixing among the basic multiphonon states appear. As a consequence, a possible sharing of the collectivity of the E2 transition between the identified K-2 "one- $\gamma$ -phonon" state and different possible K-4 states may be obtained.

Finally, it is practically impossible to assign with confidence the "two- $\gamma$ -phonon" label to any  $K_2 = K$  state. The possible candidates are generally predicted higher in energy than their identified K-4 and K+4 partners and their E2 transitions to the established "one  $\gamma$  phonon" lose practically their collective character.

In some sense, the situation is rather similar to the eveneven core. One finds that for the "two- $\gamma$ -phonon"  $K_i = K \pm 4$  states in odd-mass nuclei the situation ressembles that of the K = 4 "two- $\gamma$ -phonon" states in even-even nuclei, i.e., an anharmonic dilated energy spectrum and a collective character (may be a little less pronounced for  $K_i = K - 4$  states). Similarly, the noncollective character of the K = 0 "two-phonon" states in even-even nuclei is found again in the  $K_2 = K$  states in odd-mass nuclei. There is no great chance to identify these poor collective  $K_2 = K$  states whereas, in some favorable cases (e.g., unique parity states), one should find some evidence for the collective character of the  $K_i = K \pm 4$  "two- $\gamma$ -phonon" states in odd-mass nuclei. Experiments in this direction are therefore especially desired.

#### APPENDIX A: MATRIX ELEMENTS FOR THE SINGLE-QUASIPARTICLE HAMILTONIAN

For the part  $H_{11}$  of the model Hamiltonian one has

$$\langle p'q'\lambda'|H_{11}|pq\lambda\rangle = E_{\lambda}\delta_{\lambda\lambda'}F(p'q';pq) - \delta_{\lambda\lambda'}\sum_{\varepsilon_{1}} \operatorname{Tr}\{A[p(\varepsilon_{1})q(\varepsilon_{1});p'q']EX(\varepsilon_{1})\}$$

$$+ (E_{\lambda} + E_{\lambda'})\sum_{\varepsilon_{1}} \{X(\varepsilon_{1})A[p(\varepsilon_{1})q(\varepsilon_{1});p'q']\}_{\lambda'\lambda} + \sum_{\varepsilon_{1}} \{X(\varepsilon_{1})EA[p(\varepsilon_{1})q(\varepsilon_{1});p'q']\}_{\lambda'\lambda}$$

$$- \sum_{\varepsilon_{1}}\sum_{i,j,\tau} E_{i}^{\tau}[X(\varepsilon_{1})]_{ij}^{\tau}\sum_{\varepsilon_{2}} [X(\varepsilon_{2})]_{\lambda'\ell}B_{ij\lambda\ell}[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'],$$
(A1)

where  $E_i$  is the energy of the quasiparticle *i*. In this equation, and hereafter, the trace Tr is evaluated over protons and neutrons, the sum over  $i, j, \tau$  means that *i* and *j* are of kind  $\tau$ . On the other hand the sum over  $\ell'$  runs over particle states of the same kind than  $\lambda$ . The summation over integers has the same meaning than in the recursion formulas for the quantities F, A, B, and D, the summation over  $\tau$  indicates a sum over the two kinds of particles (protons and neutrons).

## APPENDIX B: MATRIX ELEMENTS FOR E2 TRANSITIONS

We restrict ourselves here to the  $\Delta K = +2$  transitions. Those with  $\Delta K = -2$  can be deduced by complex conjugation. The part  $T_{00}$  of the operator does not contribute. For  $T_{20}$  one has the relation

$$\langle p'q'\lambda'|T_{20}|pq\lambda\rangle = e_{\lambda} [\mathcal{F}A(pq;p'q')]_{\lambda'\lambda} - \frac{1}{2} \delta_{\lambda\lambda'} \sum_{\tau} e_{\tau} \mathrm{Tr}[\mathcal{F}A(pq;p'q')]$$
$$- \frac{1}{2} \sum_{\tau,\varepsilon_{1}} e_{\tau} \mathcal{F}_{ij} [X(\varepsilon_{1})]_{\lambda'} \mathcal{B}_{ij\lambda\ell} [p(\varepsilon_{1}),q(\varepsilon_{1});p'q'],$$
(B1)

where  $\mathcal{F}$  is the antisymmetric matrix:

$$\mathcal{F}_{ij} = \langle i | r^2 Y_{22} | \overline{j} \rangle (u_i v_j + u_j v_i). \tag{B2}$$

The single-particle state  $\overline{j}$  is the time reversed of j, with the convention  $\overline{\overline{j}} = -j$ . The elements of  $T_{02}$  can be deduced from the preceding by time reversal:

$$\langle p'q'\lambda'|T_{02}|pq\lambda\rangle = \langle pq\lambda|T_{20}|p'q'\lambda'\rangle.$$
(B3)

In a similar way, for  $T_{11}$  one has

$$\langle p'q'\lambda'|T_{11}|pq\lambda\rangle = e_{\lambda}\mathcal{G}_{\lambda'\lambda}F(p'q';pq) + e_{\lambda}\sum_{\varepsilon_{1}} \{A[p(\varepsilon_{1})q(\varepsilon_{1});p'q']\mathcal{G}X\}_{\lambda\lambda'} + e_{\lambda}\sum_{\varepsilon_{1}} \{\mathcal{G}X(\varepsilon_{1})A[p(\varepsilon_{1})q(\varepsilon_{1});p'q'] + X(\varepsilon_{1})A[p(\varepsilon_{1})q(\varepsilon_{1});p'q']\mathcal{G}\}_{\lambda'\lambda} - \sum_{\tau,\varepsilon_{1},\varepsilon_{2}} e_{\tau}[\mathcal{G}X(\varepsilon_{1})]_{ij}[X(\varepsilon_{2})]_{\lambda'}\mathcal{B}_{ij\lambda'}[p(\varepsilon_{1},\varepsilon_{2}),q(\varepsilon_{1},\varepsilon_{2});p'q'],$$

$$(B4)$$

where the matrix  $\mathcal{G}$  is defined through

$$\mathcal{G}_{ij} = \langle i | r^2 Y_{22} | j \rangle (u_i u_j - v_i v_j). \tag{B5}$$

In Eqs. (B1) and (B4), the quantity  $e_{\tau}$  is an effective charge. Usually one takes  $e_p = e(1 + \epsilon)$  and  $e_n = e\epsilon$ , where  $\epsilon$  is a parameter which depends on the number of active levels introduced in the single-particle field. Finally,  $e_{\lambda}$  is the effective charge of the same kind of particles as  $\lambda$ .

## APPENDIX C: MATRIX ELEMENTS FOR THE PAIRING HAMILTONIAN $H^P$

Hereafter, we give the matrix elements for the parts  $H_{40}$ ,  $H_{31}$  and the usual contributions  $H_{22}$  and  $H'_{22}$ . The elements of  $H_{04}$  and  $H_{13}$  may easily be deduced from those of  $H_{40}$  and  $H_{31}$  by conjugation:

$$\langle p'q'\lambda' | H_{40}^{P} | pq\lambda \rangle = G_{\lambda} \sum_{i} f(\lambda',i) B_{i\tau\bar{\lambda}'\lambda}(pq;p'q') + \frac{1}{2} \delta_{\lambda\lambda'} \sum_{i,j,\tau} G_{\tau} f(i,j) B_{i\tau\bar{j}\bar{j}}(pq;p'q') - \frac{1}{2} \sum_{i,j,\tau} G_{\tau} f(i,j) \sum_{\varepsilon_{1},\ell} [X(\varepsilon_{1})]_{\lambda'\ell} D_{i\tau\bar{j}\bar{j}\lambda\ell}[p(\varepsilon_{1}),q(\varepsilon_{1});p'q'],$$
(C1)

where

$$f(i,j) = u_i^2 v_j^2 + u_j^2 v_i^2 = f(j,i),$$

 $G_{\tau}$  is the pairing force parameter for particles of kind  $\tau$  and  $G_{\lambda}$  is that of the same kind of particles than  $\lambda$ , *i* and *j* run over all single-particle states with positive  $\Omega$ , whereas the orbital  $\ell$  may have any  $\Omega$ ;

$$\langle p'q'\lambda'|H_{31}^{p}|pq\lambda\rangle = G_{\lambda}\mathcal{U}_{\lambda}\mathcal{V}_{\lambda'}A_{\overline{\lambda'}\lambda}(pq;p'q') - G_{\lambda}(\mathcal{U}_{\lambda} + \mathcal{U}_{\lambda'})\sum_{i} \mathcal{V}_{i}\sum_{\ell,\varepsilon_{1}} [X(\varepsilon_{1})]_{\lambda'}\mathscr{B}_{i\tau\lambda}\mathscr{A}[p(\varepsilon_{1})q(\varepsilon_{1});p'q']$$

$$+ G_{\lambda}\mathcal{V}_{\lambda'}\sum_{m,n,\varepsilon_{1}} \mathcal{U}_{m}[X(\varepsilon_{1})]_{mn}B_{mn\overline{\lambda'}\lambda}[p(\varepsilon_{1})q(\varepsilon_{1});p'q']$$

$$- G_{\lambda}\sum_{i} \mathcal{V}_{i}\sum_{\ell,\varepsilon_{1}} \mathcal{U}_{k}[X(\varepsilon_{1})]_{\lambda'}\mathscr{B}_{i\tau\lambda}\mathscr{A}[p(\varepsilon_{1})q(\varepsilon_{1});p'q']$$

$$- \sum_{\ell,\varepsilon_{1}} [X(\varepsilon_{1})]_{\lambda'}\mathscr{E}_{k,m,\varepsilon_{2}} [X(\varepsilon_{2})]_{km}\mathcal{U}_{k}\sum_{i,\tau} G_{\tau}\mathcal{V}_{i}D_{i\tau km\lambda}\mathscr{A}[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'],$$

$$(C2)$$

where  $U_i = u_i v_i$  and  $V_i = u_i^2 - v_i^2$ , with the same convention for *i* as in  $H_{40}^P$ ;

$$\langle p'q'\lambda'|H_{22}^{p}|pq\lambda\rangle = G_{\lambda}g(\lambda,\lambda')\sum_{\varepsilon_{1}} \{X(\varepsilon_{1})A[p(\varepsilon_{1})q(\varepsilon_{1});p'q']\}_{\lambda\overline{\lambda}'}^{-} - G_{\lambda}\sum_{i,j} g(i,j)\sum_{\ell,\varepsilon_{1},\varepsilon_{2}} \{[X(\varepsilon_{1})]_{i\lambda'}[X(\varepsilon_{2})]_{i\ell'} - [X(\varepsilon_{1})]_{i\tau\lambda'}[X(\varepsilon_{2})]_{i\ell'}\}B_{j\overline{j}\lambda\ell}[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'] + G_{\lambda}\sum_{i} g(\lambda',i)\sum_{\ell,\varepsilon_{1}} [X(\varepsilon_{1})]_{i\ell'}\sum_{\ell',\varepsilon_{2}} [X(\varepsilon_{2})]_{\overline{\iota}\ell'}B_{\overline{\lambda}'\lambda\ell\ell'}[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'] + G_{\lambda}\sum_{i} g(\lambda,i)\sum_{\ell,\varepsilon_{1}} [X(\varepsilon_{1})]_{\lambda'}\sum_{\ell',\varepsilon_{2}} [X(\varepsilon_{2})]_{\lambda'\ell'}B_{i\overline{\iota}\ell\ell'}[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'] + \delta_{\lambda\lambda'}\sum_{i,j,\tau} G_{\tau}g(i,j)\sum_{\ell,\varepsilon_{1}} [X(\varepsilon_{1})]_{i\ell'}\sum_{\ell',\varepsilon_{2}} [X(\varepsilon_{2})]_{\overline{\iota}\ell'}B_{j\overline{j}\ell\ell'}[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'] + \sum_{i,j,\tau} G_{\tau}g(i,j)\sum_{\ell,\varepsilon_{1}} [X(\varepsilon_{1})]_{i\ell'}\sum_{m,\varepsilon_{2}} [X(\varepsilon_{2})]_{\overline{\iota}m}\sum_{n,\varepsilon_{3}} [X(\varepsilon_{3})]_{\lambda'n}D_{j}J_{j\ell'mn\lambda}[p(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3})q(\varepsilon_{1},\varepsilon_{2},\varepsilon_{3});p'q'],$$
(C3)

where

$$(i,j) = u_i^2 u_j^2 + v_i^2 v_j^2 = g(j,i),$$

g

$$\langle p'q'\lambda' | H_{22}^{[p]} | pq\lambda \rangle = 2G_{\lambda} \delta_{\lambda\lambda'} \mathcal{U}_{\lambda} \sum_{\epsilon,\epsilon_{1}} \mathcal{U}_{\epsilon} \{X(\epsilon_{1})A[p(\epsilon_{1})q(\epsilon_{1});p'q']\}_{\ell\ell'} - 2G_{\lambda} \mathcal{U}_{\lambda} \mathcal{U}_{\lambda'} \sum_{\epsilon_{1}} \{X(\epsilon_{1})A[p(\epsilon_{1})q(\epsilon_{1});p'q']\}_{\lambda'\lambda}$$

$$- 2G_{\lambda} [\mathcal{U}_{\lambda} + \mathcal{U}_{\lambda'}] \sum_{\epsilon_{1}} \{X(\epsilon_{1})\mathcal{U}A[p(\epsilon_{1})q(\epsilon_{1});p'q']\}_{\ell\ell'}$$

$$+ \delta_{\lambda\lambda'} \sum_{\ell',\tau} G \mathcal{U}_{\epsilon} \{X(\epsilon_{1})\mathcal{U}A[p(\epsilon_{1})q(\epsilon_{1});p'q']\}_{\ell\ell'}$$

$$+ \sum_{\ell',\epsilon_{1}} [X(\epsilon_{1})]_{\lambda'} \sum_{m,n,\tau} G_{\tau} \sum_{\epsilon_{2}} \mathcal{U}_{m} \mathcal{U}_{n} [X(\epsilon_{2})]_{mn} B_{mn\lambda'} [p(\epsilon_{1},\epsilon_{2})q(\epsilon_{1},\epsilon_{2});p'q']$$

$$+ 2G_{\lambda} \sum_{\ell',\epsilon_{1}} \mathcal{U}_{\epsilon} [X(\epsilon_{1})]_{\lambda'} \sum_{m,n,\epsilon_{2}} \mathcal{U}_{m} [X(\epsilon_{2})]_{mn} B_{mn\lambda'} [p(\epsilon_{1},\epsilon_{2})q(\epsilon_{1},\epsilon_{2});p'q']$$

$$+ 2G_{\lambda} [\mathcal{U}_{\lambda} + \mathcal{U}_{\lambda'}] \sum_{\epsilon_{1}} [X(\epsilon_{1})]_{\lambda'} \sum_{m,n,\epsilon_{2}} \mathcal{U}_{m} [X(\epsilon_{2})]_{mn} B_{mn\lambda'} [p(\epsilon_{1},\epsilon_{2})q(\epsilon_{1},\epsilon_{2});p'q']$$

$$- \delta_{\lambda\lambda'} \sum_{\tau} G_{\tau} \sum_{k,\ell',\epsilon_{1}} \mathcal{U}_{k} [X(\epsilon_{1})]_{k'} \sum_{m,n,\epsilon_{2}} \mathcal{U}_{m} [X(\epsilon_{2})]_{mn} B_{k\ell'mn} [p(\epsilon_{1},\epsilon_{2})q(\epsilon_{1},\epsilon_{2});p'q']$$

$$+ \sum_{\ell,\epsilon_{1}} [X(\epsilon_{1})]_{\lambda'} \sum_{\tau} G_{\tau} \sum_{m,n,\epsilon_{2}} \mathcal{U}_{m} [X(\epsilon_{2})]_{mn} \sum_{r,s,\epsilon_{3}} \mathcal{U}_{k} [X(\epsilon_{3})]_{rs}$$

$$\times D_{mnrs\lambda'} [p(\epsilon_{1},\epsilon_{2},\epsilon_{3})q(\epsilon_{1},\epsilon_{2},\epsilon_{3});p'q'].$$

$$(C4)$$

# APPENDIX D: MATRIX ELEMENTS FOR THE QUADRUPOLE HAMILTONIAN $H^{\mathcal{Q}}$

Similarly to the pairing Hamiltonian, only the contributions of  $H_{40}$ ,  $H_{31}$ ,  $H_{22}$ , and  $H'_{22}$  are given:

$$4 \langle p'q'\lambda' | H_{40}^{0} | pq\lambda \rangle = 2\chi \sum_{i,j,\ell,\tau} \left[ (F_{1})_{\lambda'\ell} (F_{2})_{ij}^{\tau} + (F_{1})_{ij}^{\tau} (F_{2})_{\lambda'\ell} \right] B_{ij\lambda\ell} (pq;p'q') + \chi \delta_{\lambda\lambda'} \sum_{i,j,\tau} (F_{1})_{ij}^{\tau} \sum_{k,\ell,\tau'} (F_{2})_{k\ell}^{\tau'} B_{ijk\ell} (pq;p'q') + \chi \sum_{i,j,\tau} (F_{1})_{ij}^{\tau} \sum_{k,\ell,\tau'} (F_{2})_{k\ell}^{\tau'} \sum_{\varepsilon_{1},m} [X(\varepsilon_{1})]_{\lambda'm} D_{ijk\ell\lambda m} [p(\varepsilon_{1}),q(\varepsilon_{1});p'q'].$$
(D1)

In this equation, and hereafter,  $F_1 = \mathcal{F}$ , defined in (B2) and

$$(F_2)_{ij} = \langle i | r^2 Y_{2-2} | \overline{j} \rangle (u_i v_j + u_j v_i).$$

For  $H_{31}^Q$  one has

$$2\langle p'q'\lambda'|H_{31}^{Q}|pq\lambda\rangle = -2\chi\sum_{e} \left[\mathcal{F}(e)A(pq;p'q')\mathcal{G}(\bar{e})\right]_{\lambda'\lambda} + \chi\sum_{e} \operatorname{Tr}[\mathcal{F}(e)A(pq;p'q')][\mathcal{G}(\bar{e})]_{\lambda'\lambda} -\chi\sum_{e}\sum_{i,j,\tau} \left[\mathcal{F}(e)\right]_{ij}^{\tau}\sum_{\mathcal{F}_{e_{1}}} \left[\left[\mathcal{G}(\bar{e})X(\varepsilon_{1})\right]_{\ell\lambda'} - \left[\mathcal{G}(\bar{e})X(\varepsilon_{1})\right]_{\lambda'/}^{\lambda'}\right]B_{ij\lambda'}\left[p(\varepsilon_{1})q(\varepsilon_{1});p'q'\right] -\chi\delta_{\lambda\lambda'}\sum_{e}\sum_{i,j,\tau} \left[\mathcal{F}(e)\right]_{ij}^{\tau}\sum_{k,\ell,\tau',\varepsilon_{1}} \left[\mathcal{G}(\bar{e})X(\varepsilon_{1})\right]_{k'}^{\tau'}B_{ijk'}\left[p(\varepsilon_{1})q(\varepsilon_{1});p'q'\right] +\chi\sum_{e}\sum_{i,j,\tau} \left[\mathcal{F}(e)\right]_{ij}^{\tau}\sum_{k} \left[\mathcal{G}(\bar{e})_{k\lambda}\sum_{\ell,\varepsilon_{1}} \left[X(\varepsilon_{1})\right]_{\lambda'/}B_{ijk'}\left[p(\varepsilon_{1})q(\varepsilon_{1});p'q'\right] +2\chi\sum_{e,\ell} \left[\mathcal{F}(e)\right]_{\lambda'\ell}\sum_{i,j,\tau,\varepsilon_{1}} \left[\mathcal{G}(\bar{e})X(\varepsilon_{1})\right]_{ij}^{\tau'}B_{ij\lambda'}\left[p(\varepsilon_{1})q(\varepsilon_{1});p'q'\right] +\chi\sum_{e}\sum_{i,j,\tau} \left[\mathcal{F}(e)\right]_{ij}^{\tau}\sum_{k,\ell,\tau',\varepsilon_{1}} \left[\mathcal{G}(\bar{e})X(\varepsilon_{1})\right]_{k'\ell}^{\tau'}\sum_{m,\varepsilon_{2}} \left[X(\varepsilon_{2})\right]_{\lambda'm}D_{ijk\ell\lambda m}\left[p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q'\right],$$
(D2)

where the sum over e runs from 1 to 2, and  $\overline{e}=3-e$ ;  $\mathcal{F}(e)=F_e$ ;  $\mathcal{G}(e)=G_e$ ;  $G_1=\mathcal{G}$  defined in (B5) and

$$(G_2)_{ij} = \langle i | r^2 Y_{2-2} | j \rangle (u_i u_j - v_i v_j).$$

For the two parts  $H_{22}^Q$  and  $H_{22}^{\prime Q}$  one gets

$$\begin{split} 4 \langle p' q' \lambda' | H_{22}^{Q} | pq \lambda \rangle &= -4 \chi \sum_{e,e_1} \left\{ F(e) X(\varepsilon_1) A[p(\varepsilon_1)q(\varepsilon_1); p' q'] F(e) \right\}_{\lambda\lambda'} + 2 \chi \sum_{e,e_1} \operatorname{Tr} \{F(e) A[p(\varepsilon_1)q(\varepsilon_1); p' q'] \} [F(e) X(\varepsilon_1)] \\ &\times \{F(e) A[p(\varepsilon_1)q(\varepsilon_1); p' q'] \}_{\lambda'\lambda} + 2 \chi \sum_{e,e_1} \operatorname{Tr} \{F(e) A[p(\varepsilon_1)q(\varepsilon_1); p' q'] \} [F(e) X(\varepsilon_1)]_{\lambda\lambda'} \\ &- \chi \delta_{\lambda\lambda'} \sum_{e,e_1} \operatorname{Tr} \{F(e) A[p(\varepsilon_1)q(\varepsilon_1); p' q'] \} \operatorname{Tr} [F(e) X(\varepsilon_1)] \\ &- \chi \sum_{e,e_1} \operatorname{Tr} \{F(e) X(\varepsilon_1) \} \sum_{i,j,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_2} [X(\varepsilon_2)]_{\lambda'} \mathcal{A}_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ 2 \chi \sum_{e,e_1,i,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_1,e_2} [X(\varepsilon_1)F(e) X(\varepsilon_2)]_{\lambda'} \mathcal{A}_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ 2 \chi \sum_{e,e_1,i,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_1} [F(e) X(\varepsilon_1)]_{\lambda'} \sum_{\ell',e_2} [X(\varepsilon_2)]_{\lambda'} \mathcal{A}_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ 2 \chi \sum_{e,i,i,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_1} [F(e) X(\varepsilon_1)]_{\lambda'} \sum_{\ell',e_2} [X(\varepsilon_2)]_{\lambda'} \mathcal{A}_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ 2 \chi \sum_{e,i,j,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_1} [F(e) X(\varepsilon_1)]_{\lambda'} \sum_{\ell',e_2} [X(\varepsilon_2)]_{\lambda'} \mathcal{A}_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ 2 \chi \sum_{e,i,j,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_1} [F(e) X(\varepsilon_1)]_{\lambda'} \sum_{\ell',e_2} [X(\varepsilon_2)]_{\lambda'} \mathcal{A}_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ \chi \sum_{e,i,j,\tau} [F(e)]_{ij}^{\tau} \sum_{\ell',e_1,e_2,\tau'} [X(\varepsilon_1)F(e) X(\varepsilon_2)]_{\lambda'}^{\tau'} B_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ \chi \sum_{e,i,j,\tau} [F(e)]_{ij} \sum_{k,\ell',e_1,e_2,\tau'} [X(\varepsilon_1)F(e) X(\varepsilon_2)]_{k'}^{\tau'} B_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ \chi \sum_{e,i,j,\tau} [F(e)]_{ij} \sum_{k,\ell',e_1,e_2,\tau'} [X(\varepsilon_1)F(e) X(\varepsilon_2)]_{k'}^{\tau'} B_{ij\lambda'} [p(\varepsilon_1,\varepsilon_2)q(\varepsilon_1,\varepsilon_2); p' q'] \\ &+ \chi \sum_{e,i,j,\tau} [F(e)]_{ij} \sum_{k,\ell',e_1,e_2,\tau'} [X(\varepsilon_1)F(\varepsilon_1)\xi_2]_{k'} \sum_{m,e_3} [X(\varepsilon_3)]_{\lambda'm} \\ &\times D_{ijk'\lambda m} [p(\varepsilon_1,\varepsilon_2,\varepsilon_3)q(\varepsilon_1,\varepsilon_2,\varepsilon_3); p' q'] \end{split}$$

$$\begin{split} \langle p'q'\lambda'|H_{22}^{(Q)}[pq\lambda\rangle &= -\chi \sum_{e_{1}} \left\{ GX(\varepsilon_{1})GA[p(\varepsilon_{1})q(\varepsilon_{1});p'q'] + X(\varepsilon_{1})GA[p(\varepsilon_{1})q(\varepsilon_{1});p'q']G \right\}_{\lambda'\lambda} \\ &-\chi \sum_{e_{1}} \left\{ GX(\varepsilon_{1})A[p(\varepsilon_{1})q(\varepsilon_{1});p'q'] GX(\varepsilon_{1})G + GA[p(\varepsilon_{1})q(\varepsilon_{1});p'q']G \right\}_{\lambda'\lambda} \\ &-\chi \sum_{e_{1}} \left\{ A[p(\varepsilon_{1})q(\varepsilon_{1});p'q'] GX(\varepsilon_{1})G + GA[p(\varepsilon_{1})q(\varepsilon_{1});p'q'] GX(\varepsilon_{1}) \right\}_{\lambda\lambda'} \\ &+\chi \delta_{\lambda\lambda'} \sum_{e_{1}} \operatorname{Tr} \left\{ GX(\varepsilon_{1})GA[p(\varepsilon_{1})q(\varepsilon_{1});p'q'] \right\} \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1})G \right]_{ij}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &-\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{ij}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{ij}^{T} \sum_{\ell',e_{2}} \left[ GX(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{\ell',e_{2}} \left[ GX(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &-\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{\ell',e_{2}} \left[ X(\varepsilon_{2}) \right]_{\lambda'} B_{ij\lambda'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'}^{T} \sum_{k,\ell',\tau',\varepsilon_{2}} \left[ X(\varepsilon_{2}) \right]_{k'} B_{ijk'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'} \sum_{k,\ell',\tau',\varepsilon_{2}} \left[ X(\varepsilon_{2}) \right]_{k'',\sigma} \left[ X(\varepsilon_{2}) \right]_{\lambda'm} B_{ijk'} B_{ijk'} \left[ p(\varepsilon_{1},\varepsilon_{2})q(\varepsilon_{1},\varepsilon_{2});p'q' \right] \\ &+\chi \sum_{i,j,\tau,e_{1}} \left[ GX(\varepsilon_{1}) \right]_{i'} \sum_{k,\ell',\tau',\varepsilon_{2}} \left[ X(\varepsilon_{2}) \right]_{k'',\sigma} \left[ X(\varepsilon_{2}) \right]_{k'',\sigma} \left[ X(\varepsilon_{2}) \right]_{k'',\sigma} \left[ X(\varepsilon_{2}) \right]_{i'm} B_{ijk',\sigma} \left[ x(\varepsilon_{2},\varepsilon_{2})$$

where  $G = G_1$  and  $\overline{G}_{ij} = G_{ji}$ .

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(D4)