PHYSICAL REVIEW C VOLUME 16, NUMBER 4 OCTOBER 1977

Multiphonon $K^\pi = 0^+$ states in even-even deformed nuclei. I. Calculation of the norms

B. Silvestre-Brac and R. Piepenbring
Institut des Sciences Nucléaires, B. P. 257, 38044 Grenoble-Cédex, France
(Received 1 June 1977)

The exact norms of the multiphonon states built upon a $K^\pi = 0^+$ collective deformed phonon are derived. Comparison with various approximations are carefully analyzed and the role of the Pauli principle is emphasized.

[NUCLEAR STRUCTURE Norms of multiphonon $K^\pi = 0^+$ states in deformed nuclei. Exact and approximate expressions.]

The explanation of anharmonicities of nuclear vibrations is a very exciting and challenging problem. A rather large amount of work has been devoted to such a program in spherical nuclei but little has been done in the case of deformed nuclei. Among all the techniques available for the treatment of anharmonicities in the spectrum of even even deformed nuclei, the boson expansion of fermion pairs is one of the best suited. Nevertheless, one is faced with difficulties concerning the convergence of the expansion. Kleber[1] showed that one way to get over this problem is to deal with an expansion expressed at the very beginning in terms of collective bosons; the price one has to pay is the calculation of the norm of the states with many phonons. Numerical computations using such a method were carried out by Lie and Holzwarth.[2] An approximate recursion formula for the norm was derived in the work of Holzwarth, Janssen, and Jolos,[3] and, very recently, Iwasaki, Sakata, and Takada[4] proposed an exact recursion formula for the multiphonon norms. However, a numerical calculation becomes more and more laborious when the number of phonons increases. For the quadrupole vibrations of intrinsic states in even even deformed nuclei the problem is somewhat simpler, since no coupling to good angular momentum is needed. In the present paper we restrict ourselves to 0^+ states built upon a single collective phonon consisting of two quasiparticles coupled to $K^\pi = 0^+$. By a simple generalization of Holzwarth's method[3] we derive exact and approximate expressions for the norm of the many-phonon states. A numerical application is made in the case of a simple model in order to compare various approximations and to emphasize the role of the Pauli principle. More realistic calculations may be performed by the same procedure.

We consider a set of fermion quasiparticles $\alpha_\mu^\dagger$ (μ labels the projection of j on the axis of symmetry of the nucleus and all other quantum numbers necessary to specify uniquely the state) whose vacuum is denoted $|0\rangle$ and which obeys the well-known anticommutation rules

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

Let us define now an arbitrary transformation which transforms the elementary excitation fermion pairs $\alpha_\mu^\dagger \alpha_\nu^\dagger$ into new phonons

$$Q^+(i) = \sum_{\mu,\nu}^{<} X_{\mu\nu}(i) \alpha_\mu^\dagger \alpha_\nu^\dagger$$

(coupled to $K^\pi = 0^+$) under the condition that among the set of $Q^+(i)|0\rangle$ one state $Q^+|0\rangle$ presents some degree of collectivity. $\sum^<$ indicates that some order is specified for the indices μ, ν to avoid the double counting due to the property $\alpha_\mu^\dagger \alpha_\nu^\dagger = -\alpha_\nu^\dagger \alpha_\mu^\dagger$. The X matrix may, for instance, be chosen as the solution of a Tamm-Dancoff problem, but this is not a necessary condition for what follows. Henceforth we consider only the collective operator Q^+ and thus suppress the index i in the corresponding matrix. Moreover, we suppose without any loss of generality that X is a real matrix. Because of its definition $X_{\mu\nu}$ has a sense only for a certain order of indices $\{\mu, \nu\}$; we formally put $X_{\nu\mu} = -X_{\mu\nu}$ so that $Q^+ = \frac{1}{2}\sum_{\mu\nu} X_{\mu\nu} \alpha_\mu^\dagger \alpha_\nu^\dagger$ without any restriction of the indices.

We shall need the successive powers of the matrix X defined in the usual way

$$(X^n)_{\mu\nu} = \sum_{\{\rho_i\}} X_{\mu\rho_1} X_{\rho_1\rho_2} \cdots X_{\rho_{n-2}\rho_{n-1}} X_{\rho_{n-1}\nu} . \tag{2}$$

If the state $Q^+|0\rangle$ is assumed to be normalized one has

$$\mathrm{Tr}(X^2) = -2 . \tag{3}$$

The problem we want to solve is the calculation of the norm of the multiphonon state $(Q^+)^n|0\rangle$, or in other words,

$$N_n^{-2} = \langle 0 | Q^n (Q^+)^n | 0 \rangle . \tag{4}$$

Owing to the Pauli principle, it is a cumbersome task to get this quantity in a closed form; actually, direct application of Wick's theorem would resolve such a problem but its use seems very prohibitive in the case of large n. It is more elegant and numerically essential, to have a recursion formula for the norm N_n.

Generalizing Holwarth's method, we define the following operators:

$$R_1 = [[Q, Q^+], Q^+], \quad R_{2p} = [Q, [Q, R_{2p-1}]] \tag{5}$$

and

$$R_{2p+1} = [[R_{2p}, Q^+], Q^+] .$$

It is only a matter of algebra to show that

$$R_{2p} = 2^{2p-1} \sum_{\mu\nu} (X^{4p+1})_{\mu\nu} \alpha_\nu \alpha_\mu ,$$
$$R_{2p+1} = 2^{2p} \sum_{\mu\nu} (X^{4p+3})_{\mu\nu} \alpha_\mu^\dagger \alpha_\nu^\dagger . \tag{6}$$

It is easy to check the following properties:

$$\langle 0 | R_{2p+1} U | 0 \rangle = 0 = \langle 0 | U R_{2p} | 0 \rangle \tag{7}$$

for any operator U,

$$[R_{2p+1}, Q^+] = 0 = [Q, R_{2p}] , \tag{8}$$

$$\langle 0 | Q R_{2p+1} | 0 \rangle = -2^{2p} \operatorname{Tr}(X^{4p+4}) ,$$
$$\langle 0 | R_{2p} Q^+ | 0 \rangle = -2^{2p-1} \operatorname{Tr}(X^{4p+2}) . \tag{9}$$

Let us proceed now to the derivation of the norm with the help of the previous quantities:

$$N_n^{-2} = \langle 0 | Q^n (Q^+)^n | 0 \rangle = \sum_{i=0}^{n-1} L_i(n) , \tag{10}$$

where

$$L_i(n) = \langle Q^{n-1} (Q^+)^{n-i-1} [Q, Q^+] (Q^+)^i \rangle$$
$$= L_{i-1}(n) + A_1(n) , \tag{11}$$

with

$$A_1(n) = \langle Q^{n-1} R_1 (Q^+)^{n-2} \rangle . \tag{12}$$

Let us note that $L_0(n) = \langle Q^{n-1} (Q^+)^{n-1} [Q, Q^+] \rangle = \langle Q^{n-1} (Q^+)^{n-1} \rangle = N_{n-1}^{-2}$. Eliminating the L_i quantities from (10), we get

$$N_n^{-2} = C_n^1 N_{n-1}^{-2} + C_n^2 A_1(n) . \tag{13}$$

[The C_n^p are the usual combinatory quantities $C_n^p = n!/p!(n-p)!$.] We now define the mean values

$$A_{2p+1}(n) = \langle Q^{n-2p-1} R_{2p+1} (Q^+)^{n-2p-2} \rangle ,$$
$$A_{2p}(n) = \langle Q^{n-2p-1} R_{2p} (Q^+)^{n-2p} \rangle . \tag{14}$$

Proceeding exactly in the same way as above, the following equality can be shown:

$$A_k(n) = -2^{k-1} C_{n-k}^1 \operatorname{Tr}(X^{2k+2}) N_{n-k-1}^{-2} + C_{n-k}^2 A_{k+1}(n) . \tag{15}$$

This ends with

$$A_{n-1}(n) = -2^{n-2} \operatorname{Tr}(X^{2n}) . \tag{16}$$

A first expression for the norm is thus provided by the two recursion formulas (13) and (15) with the initial condition (16). A more convenient form of this recursion is obtained by removing the $A_k(n)$ quantities from these equations. This is achieved by introducing a new quantity $\mathfrak{N}_n$ related to the norm by

$$\mathfrak{N}_n = (n! N_n)^{-2} , \tag{17}$$

leading to the relation

$$n\mathfrak{N}_n = \mathfrak{N}_{n-1} - \frac{1}{2} \sum_{l=1}^{n-1} \operatorname{Tr}(X^{2l+2}) \mathfrak{N}_{n-l-1} , \tag{18}$$

where $\mathfrak{N}_0 \equiv 1$ by definition.

The second term of the right-hand side of relation (18) is the exchange term measuring the difference with the norm of a pure boson. We remind that result (18) is nothing else than Wick's theorem written in a more convenient way.

The physical quantities are the traces of the powers of matrix X. The time needed to compute those expressions increases rapidly with the power of the matrix and the necessity to look for approximate relations occurs naturally. We define an approximate expression of order p by the following prescriptions:

$$R_{p-1} \text{ scatters in all the states,}$$
$$R_p \text{ scatters only in collective states.} \tag{19}$$

Repeating exactly the same kind of calculations, the pth approximation $\mathfrak{N}_n^{(p)}$ of the norm looks like

$$n\mathfrak{N}_n^{(p)} = \mathfrak{N}_{n-1}^{(p)} - \frac{1}{2} \sum_{l=1}^{p-1} \operatorname{Tr}(X^{2l+2}) \mathfrak{N}_{n-l-1}^{(p)} - \tfrac{1}{2}(n-p) \times \operatorname{Tr}(X^{2p+2}) \mathfrak{N}_{n-p}^{(p)} . \tag{20}$$

We note that the pth approximation gives exactly $N_1, N_2, \ldots, N_{p+1}$. The most difficult trace we have to calculate in that case is $\operatorname{Tr}(X^{2p+2})$. The approximate expression of Holzwarth *et al.*[3] just corresponds to our first approximation.

Comparing relations (20) and (18), it is seen that in the pth approximation the long time-consuming terms

$$\sum_{l=p}^{n-1} \operatorname{Tr}(X^{2l+2}) \mathfrak{N}_{n-l-1}$$

are replaced by $(n-p) \operatorname{Tr}(X^{2p+2}) \mathfrak{N}_{n-p}^{(p)}$ (and also the exact norms are replaced by the approximate ones). The violation of Pauli principle is caused by that replacement.

These general considerations are applied to a simple model consisting of $2m$ particles in $2m$ pairwise degenerate levels. The distance between

two consecutive levels is assumed to be a constant $2D$ and the particles interact by a pure monopole pairing force. Moreover, it is assumed that the j_z projection Ω_μ of all the single particle states are different. All these conditions give to the model a number of symmetries which enable us to make exact calculations very rapidly. Nevertheless, it is complete enough to provide general features valid also for more realistic cases. An usual Bogoliubov-Valatin transformation is performed to take care of the pairing modes and the X matrix is obtained by solving the Tamm-Dancoff secular equation and keeping only the most collective root. The nonconservation of the number of particles introduces some spurious states which may be important for dynamical aspects. But, as far as the kinematical constraints are concerned, they are quite unessential. The important features of the Pauli principle which arise in the exchange term of relation (18) are mainly sensitive to the collectivity of the state which is a decreasing function of the ratio D/Δ (where Δ is the gap parameter).

In our simple case, only "diagonal" matrix elements $X_{\nu\nu} = -X_{\bar{\nu}\bar{\nu}}$ exist and hence the set of physical quantities $\{\mathrm{Tr}(X^{2p}), p = 2 \text{ to } n\}$ is an alternating series whose general term is decreasing with the collectivity of the state. To allow a comparison with earlier work we plot in the table and figure the variable defined by Holzwarth *et al.*[3]:

$$(\mathfrak{N}_n)_H = (N_n^B)^2/N_n^2 = n!\,\mathfrak{N}_n, \tag{21}$$

which measures the deviation of the fermion state $(Q^+)^n|0\rangle$ from a pure boson one $(B^+)^n|0\rangle$.

In the figure the degree of validity of the first-order approximation is visualized as the function of the collectivity. When the number of phonons increases, the first-order approximation deviates more and more sensitively from the exact norm. However, when the collectivity of the phonon Q^+ is strong enough (e.g., $D/\Delta = 0.04$), the first-order approximation is extremely good. This is not surprising since the origin of the approximation is based essentially on the fact that R_1 scatters in collective states only and this is more and more efficient when the collectivity increases. One also notes that the effects of the exchange term in relation (18) diminish with increasing collectivity.

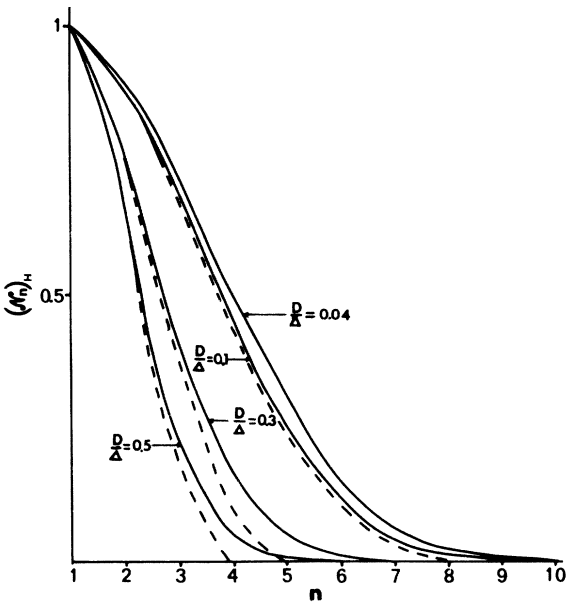

FIG. 1. Comparison of exact (solid lines) and first-order approximation (dashed lines) of the ratio $(\mathfrak{N}_n)_H$ defined by relation (21) for different collectivities of the Tamm-Dancoff solution. For $D/\Delta = 0.04$ the $(\mathfrak{N}_n)_H$ differ by less than 10% and the corresponding plots cannot be distinguished.

In the table we compare the exact norm with approximations up to order 5 for a model with 10 levels (so that $N_n^{-2} \equiv 0$ for $n > 10$) and for a typical average value $D/\Delta = 0.2$ Several instructive remarks may be made.

TABLE I. Exact and approximate values of ratios $(\mathfrak{N}_n)_H$ defined by relation (21) for multiphonon states $(Q^+)^n|0\rangle$ with $1 \le n \le 10$.

Numbers of phonons	Exact	Order 1	Order 2	Order 3	Order 4	Order 5
1	1	1	1	1	1	1
2	0.8274	0.8274	0.8274	0.8274	0.8274	0.8274
3	0.5562	0.5418	0.5562	0.5562	0.5562	0.5562
4	0.2979	0.2613	0.3112	0.2979	0.2979	0.2979
5	0.1244	0.8092×10^{-1}	0.1739	0.1103	0.1244	0.1244
6	0.3944×10^{-1}	0.1109×10^{-1}	0.1353	-0.2252×10^{-1}	0.5764×10^{-1}	0.3944×10^{-1}
7	0.9136×10^{-2}	-0.3943×10^{-3}	0.1480	−0.1136	0.1007	-0.1857×10^{-1}
8	0.1456×10^{-2}	0.8186×10^{-4}	0.1946	−0.1142	0.2054	−0.1562
9	0.1428×10^{-3}	-0.3115×10^{-4}	0.2965	0.6105×10^{-1}	0.2598	−0.3905
10	0.6504×10^{-5}	0.1723×10^{-4}	0.5120	0.4282	0.3204	−0.5465

The approximations of order p with odd p lead to negative values of $\mathfrak{N}^{(p)}$ which are, of course, senseless. When p is even the norm $\mathfrak{N}^{(p)}$ passes through a minimum and then diverges, which is also senseless. It is interesting to notice that the troubles appear (by trouble we mean a deviation of more than 50% from the exact result) qualitatively for a unique critical value N_c of the number of phonons whatever the order p is. (In the case of Table I, $N_c = 6$.) This result is very general, irrespective of the range of the parameters. For each set of parameters D/Δ or of the number of levels, there exists a number N_c for which all approximations with $p < N_c$ fail. If $p > N_c$ the norms are exact up to N_{p+1} but are completely wrong as early as N_{p+2} (see, for instance, order 5 in the table). The origin of such a number N_c is not yet well understood but it seems to be related to the cutoff factor of a SU(6) scheme for a boson expansion.[5] To describe physical properties in terms of boson expansions it is meaningless to deal with a space including more than N_c bosons. For low values of the number of phonons n, p odd approximations lie under the exact norm, while p even approximations lie above it. This fact is due to the previously mentioned property of the set $\{\mathrm{Tr}(X^{2p})\}$; it is an alternating series.

These alternating terms also insure the convergence of the exact norm $\sum_{l=p}^{n-1} \mathrm{Tr}(X^{2p+2})\mathfrak{N}_{n-l-1}$, while the approximate expression of it, $\frac{1}{2}(n-p)\,\mathrm{Tr}(X^{2p+2}) \times \mathfrak{N}_{n-p}$, does not converge with increasing n and leads to the troubles already mentioned.

The order of approximation to choose in realistic calculations depends on what one needs. If the phonon operator is very collective or if we need an overall approximation for the norms N_n of states with different n, the first-order approximation is certainly the best suited. But if the phonon is not very collective and if we want a good accuracy for the norms of low n values (this is the case for a boson expansion) it would be preferable to use approximations of higher order. In any case it is very important to have an estimate of the cutoff factor N_c; for instance, a comparison of $\mathfrak{N}_n^{(1)}$ and $\mathfrak{N}_n^{(2)}$ may give an idea of N_c. Lastly, a criteria of collectivity is provided by the ratio

$$\mathrm{Tr}(X^{2k+2})/\mathrm{Tr}(X^{2k}),$$

which is qualitatively (at least in our academic case) independent of k.

[1]M. Kleber, Phys. Lett. 30B, 588 (1969).
[2]S. G. Lie and G. Holzwarth, Phys. Rev. C 12, 1035 (1975).
[3]G. Holzwarth, D. Janssen, and R. V. Jolos, Nucl. Phys. A261, 1 (1976).
[4]S. Iwasaki, F. Sakata, and K. Takada, Prog. Theor. Phys. 57, 1289 (1977).
[5]D. Janssen, R. V. Jolos, and F. Dönau, Nucl. Phys. A224, 93 (1974); A. Arima and F. Iachello, Phys. Rev. Lett. 35, 1069 (1975).