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DEFORMED NUCLEAR STATE AS A QUASIPARTICLE-PAIR CONDENSATE

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ABSTRACT

The deformed nuclear states, obtained in terms of the Hartree-Fock plus BCS method with the Skyrme SIII interaction, are approximated by condensates of the low-angular-momentum quasiparticle and particle pairs. The optimal pairs are determined by the variation after truncation method. The influence of the truncation on the deformation energy and the importence of the core-polarization effects are investigated.

1. INTRODUCTION

The deformed mean field method[1)] is a well-established approach which takes into account the multipole correlations in nuclei. It can be viewed as an efficient way to include a large number of different configurations in the spherical shell-model calculations, and has been proved to provide for an understanding of a variety of properties of medium heavy and heavy nuclei. The quadrupole collective states in such nuclei have also been interpreted in terms of the U(6) dynamic symmetry[2,3)] which is supposed to arise from the dominant role of pairs of valence *particles* (or holes past midshell) coupled to angular momentum $J=0$ and $J=2$, as introduced in the Interacting Boson Model[2)] (IBM), or of pairs of *quasiparticles* coupled to $J=2$, as proposed in the Quadrupole Phonon Model[3)] (QPM). Both models aim at defining a suitable significant reduction of the spherical shell-model space by picking coherent mixtures of supposedly most important configurations. Serving for similar purpose as the deformed mean field method, the IBM and the QPM can in principle be tested by analyzing which configurations are present in

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the deformed nuclear states, and such analysis is the goal of the present contribution.

Numerous studies have already been devoted to the microscopic analysis of the IBM (for a review see the article by Iachello and Talmi[4]) and the contribution of B.R.Barrett in these proceedings). A method to put the microscopic test of the IBM and the QPM on an equal footing has been proposed in our previous study.[5])

Similarly as in Ref. 5, we analyze here the axially deformed states of ^{128}Ba obtained by the constrained Hartree-Fock (HF) method[6,7]) with the Skyrme SIII interaction[8]) and the pairing correlations included by the BCS method. The quadrupole moment $\hat{Q} = \sum_{i=1}^{A}(2z_i^2 - x_i^2 - y_i^2)$ is used as the constraining operator. Our choice of ^{128}Ba as a testing ground for the IBM and the QPM is motivated by a relatively small calculated ground-state hexadecapole moment of this nucleus, which simplifies the discussion of the quadrupole excitations. The HF+BCS method is chosen here because it is a variational method, for which a quality of the wave function can be quantitatively judged from the value of the variational energy. Another advatage of this approach consists in its explicite use of the core states, which allows us to estimate the role of the core-polarization effects.

2. METHOD OF ANALYSIS

Our method of analysis is based on the Thouless theorem,[1]) by which the independent quasiparticle state $|\Psi\rangle$, as resulting from the HF+BCS method, can be expressed in terms of another arbitrary independent quasiparticle state $|\Psi_{\rm ref}\rangle$, which we will call the reference state, and a quasiparticle-pair creation operator $\hat{Z}^+$, i.e.

$$|\Psi\rangle = \langle\Psi_{\rm ref}|\Psi\rangle \exp\left\{\hat{Z}^+\right\}|\Psi_{\rm ref}\rangle \quad , \tag{1}$$

where

$$\hat{Z}^+ = \frac{1}{2}\sum_{\mu\nu} Z^+_{\mu\nu}\alpha^+_\mu\alpha^+_\nu \quad , \tag{2}$$

$\alpha_\mu|\Psi_{\rm ref}\rangle = 0$, and $Z_{\mu\nu}$ is a complex antisymmetric matrix. In view of this theorem, the deformed state $|\Psi\rangle$ can be considered as a condensate of the coherent quasiparticle pairs $\hat{Z}^+$ added to the reference state $|\Psi_{\rm ref}\rangle$.

Since for the deformed state the rotational invariance is broken, the pair $\hat{Z}^+$ contains in general various angular-momentum components, and can be presented as the sum:

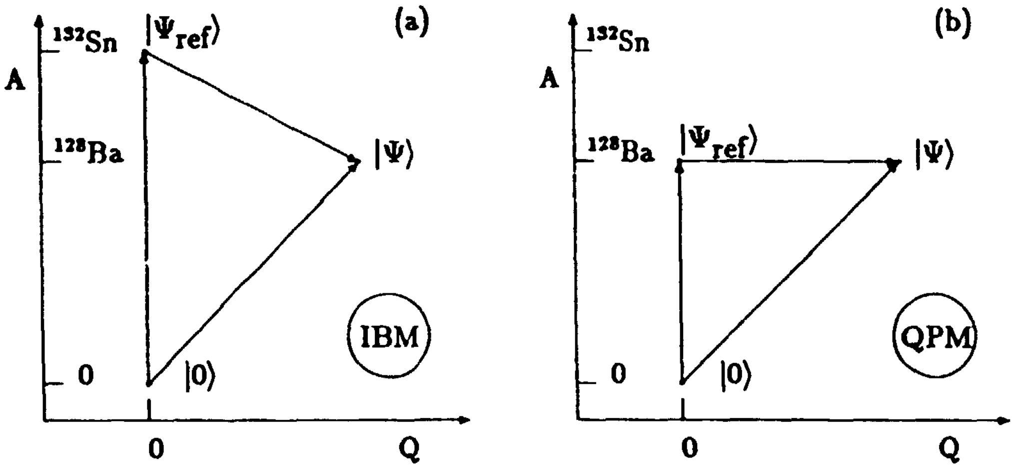

Fig. 1: Schematic illustration of the choice of the reference states (a) for the IBM and (b) for the QPM.

$$\hat{Z}^+ = \sum_{J=0,2,4,\ldots} x_J \hat{Z}_J^+ \quad , \tag{3}$$

where $\hat{Z}_J^+$ transforms under spatial rotations as the rank-J spherical tensor. The normalization constants x_J are fixed by requiring that $2\langle\Psi_{\rm ref}|\hat{Z}_J\hat{Z}_J^+|\Psi_{\rm ref}\rangle = 1$.

Depending on the choice of the reference state, the multipole composition of the pair $\hat{Z}^+$ can be very different. In order to study the assumptions of the IBM and the QPM, we will discuss here the choice of two reference states, as dictated by these two models. In Fig. 1 we schematically present the principal idea of such choice. The arrows in the Figure represent the Bogolyubov transformations, which transform one vacuum state into another one. The true vacuum $|0\rangle$ can be transformad into the deformed state $|\Psi\rangle$ of ^{128}Ba or into the spherical reference state $|\Psi_{\rm ref}\rangle$. For the QPM, the reference state is the state of ^{128}Ba obtained by imposing its spherical symmetry, while for the IBM, it is the spherical state of the nearest closed-shell nucleus, i.e. of ^{132}Sn. Both reference states, wich we will call the QPM core and the IBM core, respectively, are determined by the same HF+BCS method which is used to determine the deformed states $|\Psi\rangle$.

The Thouless theorem applied to $|\Psi\rangle$ and $|\Psi_{\rm ref}\rangle$ allows us to express them as

$$|\Psi\rangle = \langle 0|\Psi\rangle \exp\left\{\hat{C}^+\right\}|0\rangle \quad , \tag{4}$$

$$|\Psi_{\rm ref}\rangle = \langle 0|\Psi_{\rm ref}\rangle \exp\left\{\hat{R}^+\right\}|0\rangle \quad , \tag{5}$$

where $\hat{C}^+$ and $\hat{R}^+$ read in terms of the antisymmetric matrices $C_{\mu\nu}$ and $R_{\mu\nu}$ as

$$\hat{C}^+ = \frac{1}{2}\sum_{\mu\nu} C^+_{\mu\nu} a^+_\mu a^+_\nu \quad , \tag{6}$$

$$\hat{R}^+ = \frac{1}{2}\sum_{\mu\nu} R^+_{\mu\nu} a^+_\mu a^+_\nu \quad , \tag{7}$$

and a^+_μ are the creation operators of true particles.

Let the Bogolyubov transformation leading from $|0\rangle$ to $|\Psi_{\rm ref}\rangle$ be given by

$$\alpha^+_\mu = \sum_\nu \left(A_{\nu\mu} a^+_\nu + B_{\nu\mu} a_\nu \right) \quad . \tag{8}$$

The matrix R, which determines the reference state $|\Psi_{\rm ref}\rangle$, Eq. (5), is then equal[1] to

$$R = BA^{-1} \quad . \tag{9}$$

The Bogolyubov transformation leading from $|0\rangle$ to $|\Psi\rangle$ is equal to the product of the transformation leading from $|0\rangle$ to $|\Psi_{\rm ref}\rangle$ and of the one leading from $|\Psi_{\rm ref}\rangle$ to $|\Psi\rangle$. Calculating this product explicitly one obtains that

$$Z = A^T(C - R)(1 + R^+C)^{-1}(A^+)^{-1} \quad . \tag{10}$$

When $|\Psi_{\rm ref}\rangle$ is chosen according to the QPM, both $|\Psi\rangle$ and $|\Psi_{\rm ref}\rangle$ correspond to the same nucleus, and hence the scalar (J=0) part of the C matrix is not far from the R matrix (which has only the scalar part). In this case, formula (10) suggests a strong cancelation of the scalar parts, which leads to the dominance of the J=2 term in the $\hat{Z}^+$ pair of the QPM. On the other hand, the $\hat{Z}^+$ pair of the IBM contains both J=0 and J=2 terms as the dominant ones. The numerical determination of the x_J amplitudes confirmes such simple approximate argumentation. The detailed results[5] show that at the equilibrium deformation of $Q \simeq 800 fm^2$ the J=0 and J=2 pairs of the IBM have similar magnitude and that the J=4 pair is an order of magnitude smaller. Every next multipole component is still one order of magnitude smaller. For the QPM, the J=2 component is the dominant one, and the J=0 and J=4 components are smaller by an order of magnitude.

In order to derive the explicite formula connecting the matrices Z and Z', corresponding to two different reference states $|\Psi_{\rm ref}\rangle$ and $|\Psi'_{\rm ref}\rangle$, respectively, one can use the same method as the one which was used to derive Eq. (10). Comparing the Bogolyubov transformation $|\Psi_{\rm ref}\rangle \longrightarrow |\Psi\rangle$ with the product of the two Bogolyubov transformations $|\Psi_{\rm ref}\rangle \longrightarrow |\Psi'_{\rm ref}\rangle \longrightarrow |\Psi\rangle$ one obtains

$$Z' = A'^T(Z - R')(1 + R'^+ Z)^{-1}(A'^+)^{-1} \quad , \tag{11}$$

where $R' = B'A'^{-1}$ is the matrix determining the reference state $|\Psi'_{\rm ref}\rangle$ in terms of the reference state $|\Psi_{\rm ref}\rangle$, and A' and B' are the corresponding coefficients of the Bogolyubov transformation.

The relation between Z and Z' is highly non-linear, and no obvious connection can be made between the multipole components of these two matrices. Therefore, the proof of the identicity of the IBM and the QPM given in Ref. 9 cannot be extended to the case when the generalized seniority scheme holds only approximately.

3. VARIATION AFTER TRUNCATION

By truncating multipole expansion (3), one obtains the quasiparticle pair which through the Thouless theorem, Eq. (1), determines the truncated nuclear state. Since the truncated state still has the independent-quasiparticle nature, one can easily calculate its HF+BCS energy, and compare it with the untruncated result. Results of such approach, which can be called the variation before truncation, have been discussed in Ref. 5. Here we concentrate on the variation after truncation, which consists in freely adjusting the low-angular-momentum pairs so as to minimize the HF+BCS energy for a given quadrupole moment.

The minimization can be done in the following way. The HF+BCS energy E can be considered as a function of either the Z or the C matrix, Eqs. (1) and (4). Its gradient with respect to the C matrix, $(\nabla_C E)_{\mu\nu} = \partial E/\partial C_{\mu\nu}$, reads

$$\begin{aligned} \nabla_C E &= (1-\rho)(h-\lambda)\kappa + \kappa(h^* - \lambda)(1-\rho^*) \\ &\quad + \kappa\Delta^*\kappa + (1-\rho^*)\Delta(1-\rho) \quad , \end{aligned} \tag{12}$$

where h and Δ are the usual mean field and the pairing field, and ρ and κ are the density matrix and the pairing tensor (defined as in Ref. 1). In the BCS approximation, which we use here, the only non-vanishing elements of the Δ matrix are the ones between the time-reversed states, and they are all equal one to another. The condition for the minimum, $\nabla_C E = 0$, leads to the well-known BCS expressions for the occupation probabilities.

The gradient of the energy with respect to the Z matrix can be found as

$$\nabla_Z E = A^+(1 + R^+C)\nabla_C E(1 + CR^+)A^* \quad , \tag{13}$$

and of course it vanishes whenever the gradient $\nabla_C E$ vanishes. In order to find the minimum of energy with respect to the quasiparticle matrix Z truncated to some angular momenta, on has to solve the equation $\nabla_Z E = 0$ *truncated* to the

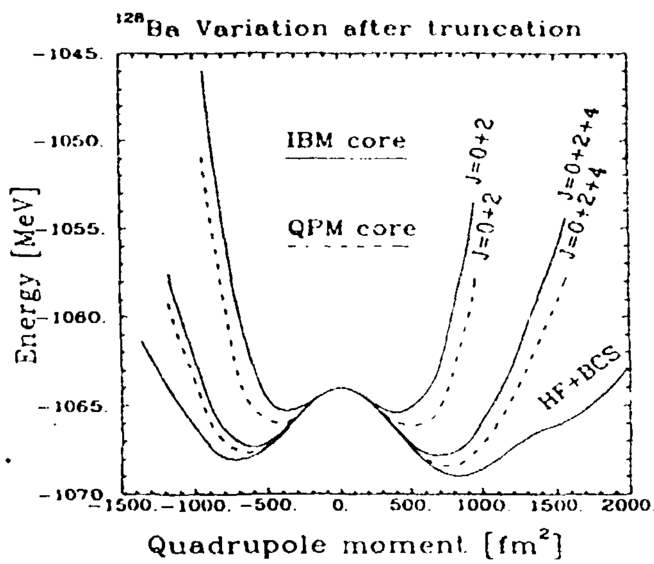

Fig. 2: Energies obtained by the variation after truncation of the quasiparticle pairs to $J = 0+2$ and to $J = 0+2+4$ compared to the untruncated HF+BCS results as a function of the quadrupole moment.

same angular momenta. A practical method of approaching the minimum (the projected gradient method[1]) consists in correcting the truncated matrix Z with the truncated gradient multiplied by a suitable small coefficient. This method is numericaly much more time consuming, roughly by an order of magnitude, than the usuall methods used to solve the HF equations, However, it is the only one known in the case when the variational space is restricted to a much smaller subspace.

The gradients with respect to the two matrices Z and Z', corresponding to two different reference states, are related by

$$\nabla_{Z'}E = A'^{+}(1 + R'^{+}Z)\nabla_Z E(1 + ZR'^{+})A'^{*} \quad , \tag{14}$$

with the notation as in Eq. (11). Again it is seen, that as soon as the Z matrix differs from a scalar one, the truncated condition $\nabla_Z E = 0$ and the truncated condition $\nabla_{Z'} E = 0$ are not identical, and therefore may yield different solutions.

The results of our variation after truncation for ^{128}Ba are presented in Fig. 2. As seen from the results shown in this Figure, the energies obtained for the QPM core are for a given truncation lower than those for the IBM core. In the variational sense, the QPM core is therefore better suited for a description of the deformation in terms of the low-angular-momentum fermion pairs. However, the differences are not very dramatic, and moreover, the truncation to $J = 0 + 2$ gives for both cores the deformation-energy curve very different from the one of the HF+BCS method. Truncation to $J = 0 + 2 + 4$ allows for a fair description of the equilibrium deformation, while a large discrepancy still persists for larger deformations.

4. CORE POLARIZATION

In the HF+BCS method with the Skyrme interaction one uses all the single-particle states, starting from 'he bottom of the nuclear well, when constructing the one-body density for the deformed state $|\bar{\Psi}\rangle$. Hence, no effective charges are necessary to determine the electric multipole moments, to which the core states contribute significantly. The quasiparticle pair $\hat{Z}^+$, Eq. (2), is in general composed of all single-particle orbits. In order to quantitatively estimate the role of different orbits in building up the nuclear deformation, let us split the set of the single-particle states of the reference state into three following classes according to their single-particle energies. For ^{128}Ba the major valence shell consists of states between the magic numbers 50 and 82, both for neutrons and for protons. Therefore, we will call the 50 lowest single-particle states the hole (h) states, next 32 the valence (v) states and all the other the particle (p) states. The single-paricle indeks μ will be denoted by h, v or p depending on which value it assumes. One should note that this definition explicitely refers to the single-paricle energies of the reference state, and in what follows we use the IBM core ore the QPM core when discussing the IBM or the QPM pairs, respectively.

The magnitude of the valence-valence (VV) component of the pair $\hat{Z}_J^\dagger$ can be defined as $y_J^{VV} = \sum_{vv'} |Z_{Jvv'}|^2$, and that of its valence-hole (VH) component as $y_J^{VH} = 2\sum_{vh} |Z_{Jvh}|^2$, where the factor 2 accounts for the asymmetry of the Z_J matrix. Similarly, one can define all the other components: PP, HH, PV and PH. The sum of the six y_J values is equal to x_J, Eq. (3), and the importance of a given component is quantitatively described by the fraction y_J/x_J.

We have calculated such fractions for the J=0 and J=2 pairs resulting from the variation after truncation for both considered cores. It turns out that the J=0 pair for the IBM core is perfectly (up to 95%) concentrated in the valence-valence space. The fractions y_J/x_J for the neutron J=2 pairs are presented in Fig. 3. It can be seen that the valence-valence (VV) component amounts at Q=0 to 90%(80%) of the J=2 pair for the IBM(QPM). However, this component decreases rather rapidly with increasing deformation, and the sum of the other components (of which the PV component is the largest one) reaches at the equilibrium deformation

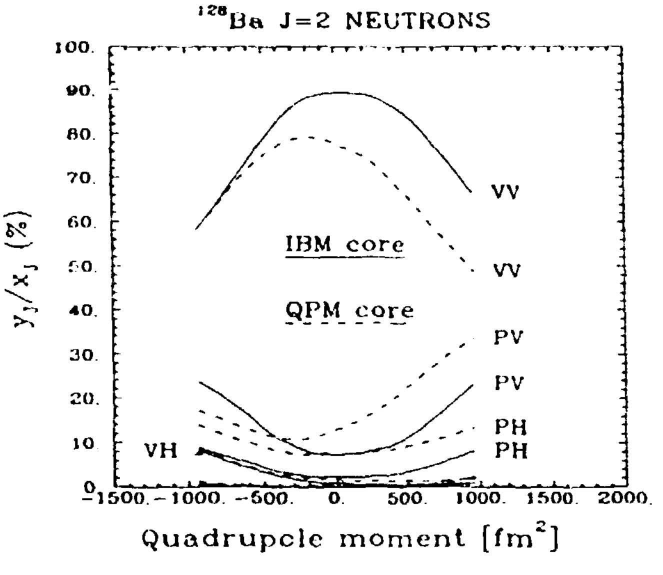

Fig. 3: Fractions y_J/x_J (as defined in the text) for the J=2 pairs and different components related to the particle, valence and hole single-particle states, presented in percent as function of the quadrupole moment.

as much as 30%(50%). For proton pairs and both cores, the VV component decreases to 50% at the equilibrium deformation, and the VH component is the second important one. These numbers show that the core polarization (i.e. the influence of the hole states) and the vacuum polarization (i.e. the influence of the particle states) are fairly important for the buildup of the nuclear deformation. In accordance with the position of the neutron and proton Fermi energy in the valence shell, the core polarization is more important for protons, while the vacuum polarization is more important for neutrons.

In the IBM, one assumes the exact confinement of the fermion pairs to the valence shell, and one derives from this assumption the number of active pairs to be equal to half of the number of valence particles (or holes). In our approach, one can directly calculate the mean number of quasiparticles necessary to transform the reference state into the deformed state. In order to find the mean number of quasiparticles occupying the valence states, one calculates the average value of the corresponding operator:

$$\hat{N}_V = \sum_v \alpha_v^\dagger \alpha_v \quad . \tag{15}$$

The total mean number of quasiparticles is equal to the sum of the average values

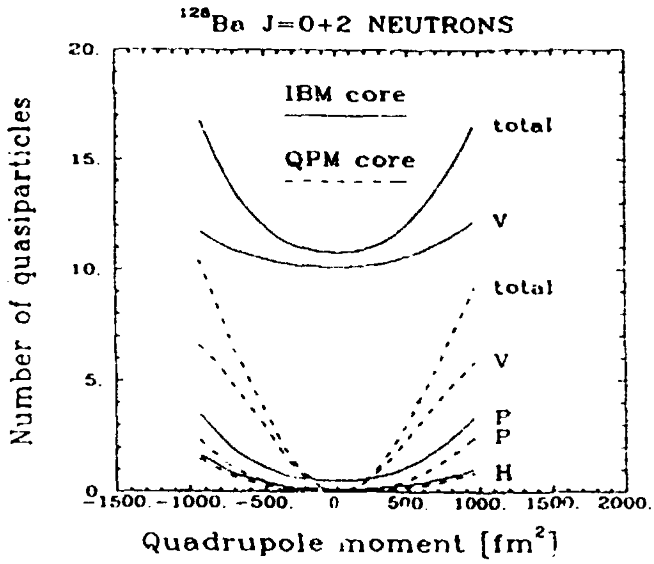

Fig. 4: Particle, valence, hole and total neutron quasiparticle numbers with respect to the IBM core and to the QPM core as a function of the quadrupole moment.

of $\hat{N}_V$, $\hat{N}_P$ and $\hat{N}_H$, with obvious definitions for the latter two operators.

In Fig. 4 we present the mean neutron quasiparticle numbers in the deformed states obtained by the variation after truncation for the IBM and the QPM. For the IBM core, the total number of quasiparticles at Q=0 is around 11, which is close to the number of neutron holes (10) necessary to transform ^{132}Sn into ^{128}Ba. The difference illustrates the fact that the self-consistent single-particle states in both nuclei are slightly different. When the deformation increases to $Q \simeq 800 fm^2$, the total number of quasiparticles increases to about 15, to which contribute two additional quasiparticles coming from the particle space, one quasiparticle from the valence space and one from the hole space. These numbers illustrate the degree of the violation of the fixed-pair-number assumption made in the IBM, and a possible necessity of the configuration mixing, introduced already in some phenomenological approches.[10,11] One should note that in the QPM the number of pairs is not assumed to be constant, and the increase the number of quasiparticles is the desired source of the increasing deformation.

5. CONCLUSIONS

Summarizing, the following conclusions can be drown from our analysis of the deformed nuclear states:

- The $J=2$ quasiparticle pairs dominate the condensate of pairs which transforms the spherical state of ^{128}Ba into the deformed one. On the other hand, the $J=0$ and $J=2$ pairs dominate the condensate which transforms the closed-shell nucleus ^{132}Sn into the same deformed state of ^{128}Ba. These two results confirm respectively the assumptions made in the Quadrupole Phonon Model[3] (QPM) and in the Interacting Boson Model[2] (IBM).

- The energies of states obtained by the variation after truncation to the $J = 0 + 2$ components are for both QPM and IBM very different from the deformed HF+BCS results. The equilibrium deformation is reproduced when the $J=4$ component is taken into account.

- The core-polarization and the vacuum-polarization effects are found to be fairly strong. Up to 50% of the quasiparticle pair must be located outside the valence shell in order to create the deformation equal to the HF+BCS equilibrium deformation.

- At the HF+BCS equilibrium deformation, the number of active fermion pairs may differ by one or two units from the value assumed by the IBM.

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