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Deformed nuclear state as a quasiparticle-pair condensate

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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. It is shown that the quasiparticle pairs, which are essentially the particle-hole nuclear excitations, provide for a better approximation than the valence particle pairs. In both cases, the inclusion of $J=0$, 2, and 4 components is necessary to reproduce the Hartree-Fock plus BCS equilibrium deformation and deformation energy.

A description of the nuclear quadrupole states in terms of the U(6) symmetry has recently been a matter of considerable interest. Two hypotheses have been put forward to provide for a microscopic foundation of the symmetry. The interacting boson model (IBM) of Arima and Iachello[1] is based on the assumption that the quadrupole collective states can be built out of the pairs of valence *particles* (or holes past midshell) coupled to angular momentum $J=0$ and $J=2$. In the quadrupole phonon model (QPM) of Janssen, Jolos, and Dönau[2] (also called the truncated quadrupole model) the same is assumed about the pairs of *quasiparticles* coupled to $J=2$. A number of studies have recently been devoted to a discussion of the former hypothesis.[3-14] It is the aim of the present paper to put both of them on an equal footing and to check their compatibility with a mean-field description of the deformed nuclear ground state.

Let $|\Psi\rangle$ denote a deformed independent quasiparticle state, i.e., the vacuum of the quasiparticle annihilation operators $\beta_\mu,\beta_\mu|\Psi\rangle=0$. In view of the Thouless theorem,[15] the state $|\Psi\rangle$ can be expressed in terms of another independent quasiparticle state $|\Psi_{\rm ref}\rangle$, which we will call the reference state, and a quasiparticle-pair creation operator $\hat{Z}^\dagger$, i.e.,

$$|\Psi\rangle=\langle\Psi_{\rm ref}|\Psi\rangle\exp\{\hat{Z}^\dagger\}|\Psi_{\rm ref}\rangle\ , \tag{1}$$

where

$$\hat{Z}^\dagger=\tfrac{1}{2}\sum_{\mu\nu}Z^\dagger_{\mu\nu}\alpha^\dagger_\mu\alpha^\dagger_\nu\ , \tag{2}$$

$\alpha_\mu|\Psi_{\rm ref}\rangle=0$, and $Z_{\mu\nu}$ is a complex antisymmetric matrix. Any independent quasiparticle state can be used as the reference state, apart from the requirement that it should not be orthogonal to $|\Psi\rangle$. The quasiparticle-pair creation operator corresponding to the chosen reference state can be determined from the coefficients of the Bogolyubov transformation connecting the quasiparticle operators β_μ and α_μ (Ref. 15). The Thouless theorem, Eq. (1), allows us to consider the deformed state as a condensate of quasiparticle pairs $\hat{Z}^\dagger$ added to the chosen reference state $|\Psi_{\rm ref}\rangle$.

The pair operator $\hat{Z}^\dagger$ can be presented as a sum of different angular-momentum components:

$$\hat{Z}^\dagger=\sum_{J=0,2,4,\ldots}x_J\hat{Z}^\dagger_J\ , \tag{3}$$

where the quasiparticle-pair operators $\hat{Z}^\dagger_J$ transform under spatial rotations as the rank-J spherical tensors and the expansion coefficients x_J are fixed by the normalization condition $2\langle\Psi_{\rm ref}|\hat{Z}_J\hat{Z}^\dagger_J|\Psi_{\rm ref}\rangle=1$. Since we assume here the axial and the parity symmetry of the state $|\Psi\rangle$, the sum in Eq. (3) is restricted to even values of J and the magnetic quantum numbers (not shown explicitly) are equal to 0 for every pair $\hat{Z}^\dagger_J$. For different reference states $|\Psi_{\rm ref}\rangle$, one may obtain different multipole compositions of the quasiparticle pair $\hat{Z}^\dagger$.

When analyzing the structure of deformed states of a given nucleus we will consider here two reference states, related respectively to the IBM and the QPM, namely, (i) the spherical ground state of the closed-shell nucleus nearest to the given one, and (ii) the state of the given nucleus obtained with the imposed spherical symmetry. The two reference states will be referred to as the IMB core and the QPM core, respectively. For the IBM core, the quasiparticle pair $\hat{Z}^\dagger$ is mainly composed of pairs of valence particles (or holes past midshell), while for the QPM core, it is predominantly constituted of particle-hole excitations.

In the present study,[16] we have carried out the analysis of deformed states of ^{128}Ba. In order to determine the deformed states $|\Psi\rangle$, we use the constrained Hartree-Fock (HF) method with the Skyrme interaction SIII.[17] The pairing correlations are included by means of the BCS approximation with constant gap parameters[18] determined from the experimental odd-even mass differences[19] ($\Delta_n=1.41$ MeV and $\Delta_p=1.38$ MeV). The quadrupole moment $\hat{Q}=\sum_{i=1}^{A}(2z_i^2-x_i^2-y_i^2)$ is used as the constraining operator. The reference states are also determined by the HF+BCS method and are equal (i) to the (unpaired) solution for the ground state of the doubly magic nucleus ^{132}Sn (IBM core) and (ii) to the solution for ^{128}Ba obtained by imposing the spherical symmetry when solving the HF+BCS equation (QPM core). The HF equation is solved by expanding the single-particle wave functions in the spherical oscillator basis up to the $N_0=12$ oscillator shell.

As opposed to the studies done so far,[3-14] we neither assume in our HF+BCS calculations any inert core nor restrict the calculations to a limited number of valence shell-model states. The core-polarization effects are thus explicitly included in our approach. The use of the Skyrme force instead of a schematic quadrupole-quadrupole interaction ensures the present state-of-the-art description of the deformed nucleus.

For the deformed states of ^{128}Ba obtained by the HF+BCS method, we have determined the multipole components of the quasiparticle pairs $\hat{Z}^\dagger$ with respect to the IBM and QPM cores. The resulting squared expansion coefficients, x_J^2 for $J=0,2,\ldots,10$, are plotted in Figs. 1(a) and 1(b) for the IBM and QPM cores, respectively, as functions of the HF quadrupole moment $Q_{\rm HF}=\langle\Psi|\hat{Q}|\Psi\rangle$. In both cases, the multipole expansions are very well convergent. For the IBM core, the $J=0$ (S) and $J=2$ (D) components dominate the quasiparticle pair $\hat{Z}^\dagger$, as it is assumed by the IBM. At the equilibrium deformation of $Q_{\rm HF}=800$ fm^2 the components with $J>2$ are roughly an order of magnitude smaller for every higher value of J. For the QPM core, the $J=2$ ($\mathcal{D}$) component is the dominating one, while the $J=0$ and $J=4$ components are both an order of magnitude smaller (at the equilibrium deformation). The other components are again an order of magnitude smaller for every higher value of J.

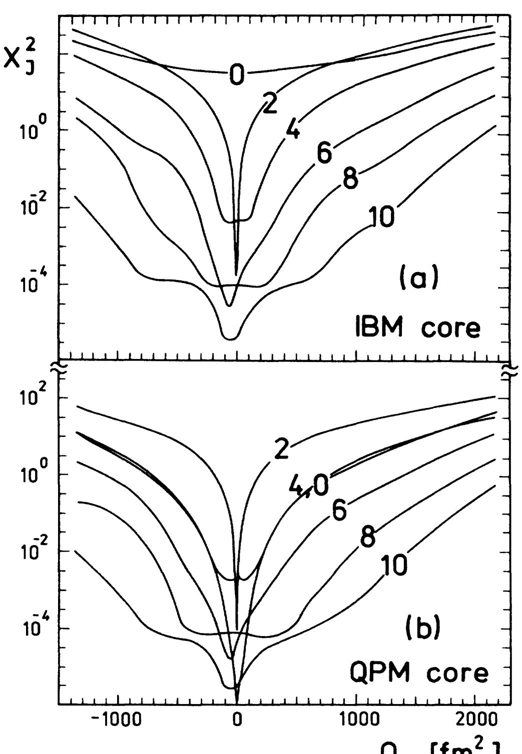

FIG. 1. Squared amplitudes x_J^2 of various multipole components, Eq. (3), of the pair creation operators $\hat{Z}^\dagger$ obtained for the HF+BCS deformed states of ^{128}Ba with respect to (a) the IBM core and to (b) the QPM core. The values of the angular momenta J are indicated at every line.

The dominance of the $J=0$ and $J=2$ components (the S-D dominance) has already been observed for the IBM core by several authors[6-11] in somewhat more schematic models. The microscopic manifestation of the dominance of the $J=2$ component for the QPM core (the $\mathcal{D}$ dominance) has not been reported previously.

The S-D dominance or the $\mathcal{D}$ dominance cannot be considered as an immediate justification for the IBM or the QPM, respectively, in their efforts to describe deformed nuclear states. That is so because the independent quasiparticle state of a deformed nucleus, Eq. (1), is a condensate of *many* quasiparticle pairs, and hence the Pauli principle may change the relative importance of the dominant and the small components. In order to estimate the significance of the small components one should study the properties of the truncated states, i.e., the states which one obtains in terms of Eq. (1) from the truncated multipole expansion, Eq. (3), of the quasiparticle pairs.

The truncation can be performed in two ways. Either one can simply set the high-J expansion coefficients x_J, Eq. (3), of the HF+BCS pair equal to zero, which is the truncation after variation, or one can first truncate the multipole expansion of Eq. (3) and then perform the variation with respect to the kept multipole pairs, which is the variation after truncation. In the latter method, one allows the kept components to properly readjust themselves and to take over, at least partly, the role of the removed components. In the present study, we have performed both types of calculations. The projected-gradient method[15] has been used to find the variation-after-truncation solutions.

Let us first discuss the results of the truncation after variation. Our calculations show that the quadrupole moment $\tilde{Q}$ of the truncated state is for both cores, the IBM and the QPM core, equal to the quadrupole moment $Q_{\rm HF}$ (within a few percent), provided that the $J=0$, 2, and 4 components are kept in the quasiparticle pair. However, if one keeps only the dominant components, the disagreement between $\tilde{Q}$ and $Q_{\rm HF}$ amounts at the equilibrium deformation to 6% (11%) for the IBM (QPM) core, and reaches 17% (37%) at the maximal deformation studied here ($Q_{\rm HF}=2200$ fm^2). When only the dominant components are kept, the mean particle number $\tilde{N}$ of the truncated state differs by -0.13 ($+0.87$) (at the equilibrium deformation) from the exact value of $N_{\rm HF}=128$, and by 10(13) at $Q_{\rm HF}=2200$ fm^2.

These results illustrate the wound given by the truncation to the HF+BCS state. One should remember, however, that the quadrupole moment and the proton and neutron numbers are the constrained quantities and should be considered as independent variables in terms of which one investigates the total energy of the system. Since we are using a constrained variational theory, the quality of the truncated state should be judged from the difference between the energy $\tilde{E}$ of the truncated state and the energy $E_{\rm HF}$ of the HF+BCS state *at the same quadrupole moment and particle numbers*. This kind of comparison would require the determination of the HF+BCS solutions for particle numbers slightly departing from those of ^{128}Ba, as such are the particle numbers of the truncated states. Instead, we have decided to use an approximate treatment and simply scale the energy of the truncated state as $\tilde{E}'=128(\tilde{E}/\tilde{N})$. The scaled energies are plotted for various truncations in Fig. 2 as functions of $\tilde{Q}$ (thin solid and dashed lines for the IBM and the QPM cores, respectively) and compared with the HF+BCS energy $E_{\rm HF}$ plotted as function of $Q_{\rm HF}$ (thick line).

As seen in the results shown in Fig. 2, the truncation of all but the dominant components gives a poor agreement with the HF+BCS energy for both cores considered here. The results for the QPM core and the $\mathcal{D}$ pairs are better than those for the IBM core and the $S+D$ pairs. However, in both cases the deformation energy and the equilibrium deformation are both substantially smaller than the corresponding HF+BCS values. Addition of the consecutive components with higher multipolarities gradually improves the results. One observes that (i) the energies corresponding to the QPM core are for a given truncation always lower than those for the IBM core, (ii) in order to reproduce the equilibrium deformation one has to include more multipole components for the IBM core (up to $J=6$) than for the QPM core (up to $J=4$), and (iii) high multipolarities must be taken into account to reproduce the HF+BCS energy in the whole range of the studied deformations.

Let us now discuss the results of the variation-after-truncation calculations, which we have performed for several selected values of the quadrupole moment. The mean proton and neutron numbers are now properly adjusted, and the scaling of energy, which we used for the truncated HF+BCS pairs, is not needed any more.

The energies obtained for the optimal pairs are presented in Fig. 2 for the truncation to $J=0$ and 2 (squares) and to $J=0$, 2, and 4 (circles), and for both cores, the IBM core (full symbols) and the QPM core (open symbols). For the QPM core, the $J=0$ component plays an important role in reproducing the pairing properties of the deformed state, and therefore, we have not performed the variation-after-truncation calculations for the $J=2$ pair alone. The results show that (i) the energies corresponding to the QPM core are for a given truncation and quadrupole moment still lower than those for the IBM core, (ii) the energies obtained for the optimal pairs are for the QPM core close to those for the truncated HF+BCS pairs, while for the IBM core the former are substantially

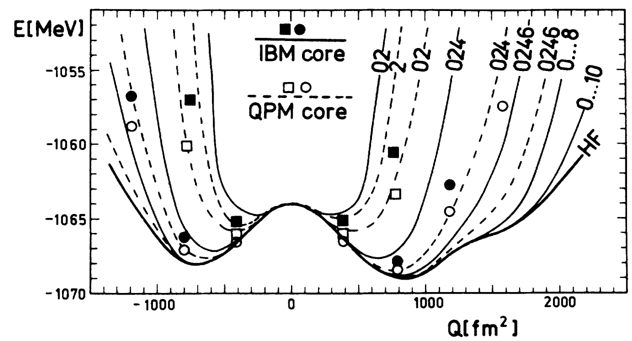

FIG. 2. Energies of the truncated states (thin lines and isolated symbols) as compared to the energies of the HF+BCS states (thick line) presented for ^{128}Ba as functions of the corresponding quadrupole moments. The solid thin lines and the full symbols correspond to the multipole pairs defined with respect to the IBM core, while the dashed thin lines and open symbols correspond to those for the QPM core. The thin solid and dashed lines correspond to the truncation after variation. The angular momenta kept in the multipole expansion are for a given truncation indicated at every line. The isolated symbols correspond to the variation after truncation to $J=0$ and 2 (squares) and to $J=0$, 2, and 4 (circles).

lower than the latter, and (iii) for both cores, the $J=4$ component has to be included in order to obtain the correct equilibrium deformation.

In summary, we have shown to what extent the deformed nuclear state, as given by the HF+BCS method with the Skyrme SIII interaction and with the core-polarization effects included, can be approximated by a condensate of small-J multipole components of the coherent fermion pairs. We have found that the quality of the approximation is better for the quasiparticle pairs introduced in the quadrupole phonon model[2] than for the particle pairs introduced in the interacting boson model.[1] The dominant multipole components ($J=2$ for the QPM and $J=0$ and 2 for the IBM) are not sufficient to reproduce the HF+BCS equilibrium deformation and deformation energy. The agreement becomes fairly good when one includes in both cases the $J=0$, 2, and 4 components.

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