Multiparticle-multihole configuration mixing within the neutron-proton interacting boson model

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The method of configuration mixing within the neutron-proton interacting boson model has been expanded to consider the simultaneous mixing of several multiparticle-multihole configurations, obtained by exciting pairs of protons and/or neutrons across major shell gaps. The determination of parameters to be employed for each configuration is discussed, along with methods for choosing the multiparticle-multihole excitation energies. As a test, the method is applied to the nucleus ^{192}Hg.

I. INTRODUCTION

Low-lying multiparticle-multihole configurations are well-known features in nuclear structure, occurring all the way from light-mass to heavy-mass nuclei. Work by Zamick and co-workers [1,2] has once again called attention to this phenomenon in light-medium-mass nuclei, where, for example, it has played an important role in describing low-lying excited 0^+ states in even-even nuclei. Iachello [3] has emphasized its possible role in heavy-mass nuclei, particularly regarding superdeformed bands. Also, recent calculations by Kaup and Barrett [4] using a schematic model have indicated that nuclear shape coexistence may favor multiparticle-multihole excitations over two-particle–two-hole excitations.

In keeping with a recent presentation by Zimick [1] calling for a unified approach to this phenomenon and the schematic-model results of Kaup and Barrett [4], we present in this paper an extension of the neutron-proton interacting boson model (also known as the IBM-2), which consistently treats the ground-state band configuration and several excited multiparticle-multihole (np-mh) configurations within the same formalism. The basic approach is one of expanding the two-configuration-mixing method of Duval and Barrett [5] within the IBM-2 to several configurations, where each configuration represents a different np-mh state. The formalism is described in Sec. II and applied, as an example, to the nucleus ^{192}Hg in Sec. III. Conclusions are given in Sec. IV.

II. CONFIGURATION-MIXING FORMALISM

The purpose of this paper is to present a procedure by which configuration mixing within the IBM-2 can be systematically extended from two configurations to a large number of multiparticle-multihole (np-mh) configurations within the same formalism.

The basic IBM-2 [6–8] consists of an active model space of s ($J=0$) and d ($J=2$) proton and neutron bosons, where the number of bosons corresponds to the number of valence nucleon pairs, counted from the nearest closed major shell. Interactions among these valence bosons are assumed to be responsible for producing the low-energy properties of medium-heavy-mass nuclei. The standard IBM-2 Hamiltonian is of the form

$$H=\epsilon(\hat{n}_{d_\pi}+\hat{n}_{d_\nu})+\kappa Q_\pi\cdot Q_\nu+V_{\pi\pi}+V_{\nu\nu}+M_{\pi\nu}\ , \quad (1)$$

where ϵ is the excitation energy of a d boson, $\hat{n}_d$ is the number operator for d bosons, κ is the strength of the quadrupole-quadrupole interaction between proton and neutron bosons, $V_{\rho\rho}$ is the residual between alike bosons ($\rho=\pi$ or ν), and $M_{\pi\nu}$ is a Majorana term that separates configurations of different neutron-proton symmetry and, in particular, insures that the low-lying configurations are mainly symmetric. The quadrupole operator is given by

$$Q_\rho=(s^\dagger\tilde{d}+d^\dagger s)^{(2)}_\rho+\chi_\rho(d^\dagger\tilde{d})^{(2)}_\rho\ , \quad (2)$$

where $\rho=\pi$ or ν, and $s^\dagger$, s, $d^\dagger$, and $\tilde{d}$ are spherical tensor operators that create and annihilate s and d bosons, respectively. The alike boson interaction is of the form

$$V_{\rho\rho}=\sum_{L=0,2,4}\tfrac{1}{2}(2L+1)^{1/2}C_{L_\rho}\times[(d^\dagger d^\dagger)^{(L)}(\tilde{d}\tilde{d})^{(L)}]^{(0)}_\rho\ , \quad (3)$$

while the Majorana term is given by

$$M_{\pi\nu}=\xi_2(s^\dagger_\nu d^\dagger_\pi-d^\dagger_\nu s^\dagger_\pi)^{(2)}\cdot(s_\nu\tilde{d}_\pi-\tilde{d}_\nu s_\pi)^{(2)}+\sum_{k=1,3}\xi_k(d^\dagger_\nu d^\dagger_\pi)^{(k)}\cdot(\tilde{d}_\nu\tilde{d}_\pi)^{(k)}\ . \quad (4)$$

For a given number of valence protons and neutrons and some appropriate values for the parameters, the IBM-2 Hamiltonian (1) produces a nuclear spectrum, which generally has a vibrational [U(5)-like], a rotational [SU(3)-like], or a gamma-soft [O(6)-like] structure [6–8]. Within the IBM-2 formalism, one obtains nuclear shape coexistence by exciting pairs of alike nucleons across the major-shell gap, so as to increase the "effective number" of valence nucleons and, thereby, of "bosons."

The original shape coexistence calculations of Duval

and Barrett [5] considered the Hg isotopes, which have only one-proton-boson hole, since $Z=80$ for Hg. Because the nuclear deformation is driven by the $Q_\pi \cdot Q_\nu$ term in the IBM-2 Hamiltonian (1) and its strength is proportional to $N_\pi N_\nu$, the nuclear spectrum looks vibrational or U(5)-like for $N_\pi=1$ and arbitrary values of N_ν, while it becomes more rotational or SU(3)-like for larger values of N_π as N_ν increases. ($N_\rho=$ the number of bosons of type ρ, where $\rho=\pi$ or ν.)

The method of Duval and Barrett (hereafter referred to as DB) considers the lowest possible excitation, that of one proton pair across the major-shell gap, as shown in Fig. 1 for the Hg isotopes. This leads to a 2p-4h proton configuration (i.e., one-proton-particle boson and two-proton-hole bosons), which is treated as being "effectively" three-proton-hole bosons. However, the schematic-model calculations of Kaup and Barrett [4] indicate that multiparticle-multihole excitations are energetically favored. In fact, in the Kaup-Barrett model it is the maximum allowed excitation, namely, the half filling of the empty shell above the gap, that leads to the deformed configuration of lowest energy. This result prompted these authors to call for more realistic calculations to test their finding.

The extension of the basic DB method is straightforward, namely, to consider excitations of more pairs of protons across the major-shell gap, leading successively to (4p-6h), (6p-8h), etc., configurations or, equivalently, "effective" five, seven, etc., boson configurations. The IBM-2 calculations for increasing effective boson number are performed in the usual manner with appropriate changes in the parameters based on their empirically determined variations with N_π.

The more difficult problem is to mix these multiparticle-multihole configurations. In the DB approach, only two configurations (i.e., $N_\pi=1$ and $N_\pi=3$) are considered for a given value of N_ν. A general mixing interaction of the following form is employed for connecting the two configurations in their effective boson spaces:

$$V_{\rm mix}=\alpha(s_\pi^\dagger s_\pi^\dagger+s_\pi s_\pi)^{(0)}+\beta(d_\pi^\dagger d_\pi^\dagger+\tilde{d}_\pi\tilde{d}_\pi)^{(0)} . \quad (5)$$

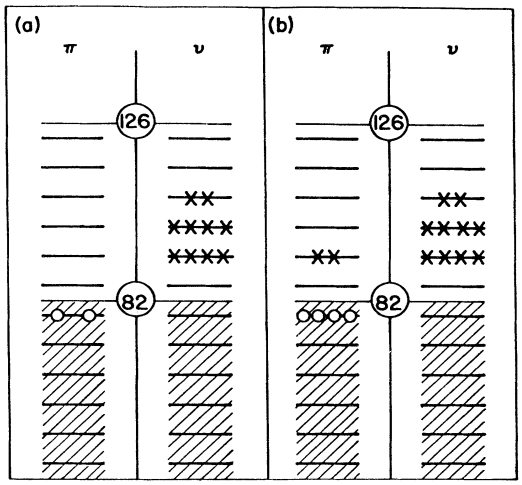

FIG. 1. (a) The single-particle proton and neutron configurations for the even-even Hg isotopes. (b) The single-particle proton and neutron configurations for the even-even Hg isotopes when a proton pair has been excited across the 82 shell gap.

The generalization of this interaction to include the mixing of several configurations, all with different boson number (i.e., N_π, $N_\pi+2$, $N_\pi+4$, etc.), would be extremely difficult and complicated. For simplicity, we assume that only neighboring configurations couple strongly and neglect any coupling between configurations that differ by more than two protons boson (or two neutron bosons). That is, $N_\pi=1$ couples with $N_\pi=3$, and $N_\pi=3$ with $N_\pi=5$, etc., but $N_\pi=1$ does *not* couple with $N_\pi=5$ (all such mixing matrix elements are *assumed* to be zero), etc.

A separate IBM-2 calculation is done for each value of N_π, using the computer code NPBOS [9] and results for the various configurations are then combined. The mixing Hamiltonian matrix has the form

$$H_{\rm mix}=\begin{bmatrix} (\lambda_1) & [V_{\rm mix}(1,2)] & (0) & (0) & \cdots \\ [V_{\rm mix}(1,2)] & (\lambda_2+\Delta_1) & [V_{\rm mix}(2,3)] & (0) & \cdots \\ (0) & [V_{\rm mix}(2,3)] & (\lambda_3+\Delta_2) & [V_{\rm mix}(3,4)] & \cdots \\ (0) & (0) & [V_{\rm mix}(3,4)] & (\lambda_4+\Delta_3) & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} , \quad (6)$$

where λ_1 is the diagonal matrix of the IBM-2 (NPBOS) eigenvalues for the normal configuration (or some subset thereof), the λ_i contain the IBM-2 eigenvalues for the excited configurations, $[V_{\rm mix}(i,j)]$ is defined by (5), and the Δ_i are the relevant pair-excitation energies. Diagonalization of this matrix for each value of the angular momentum leads to the eigenenergies and eigenvectors of the mixed configurations.

In addition to the strength parameters α and β in (5), the mixing calculation requires Δ_1, Δ_2, etc., which represent the energies needed to excite the pair(s) across the gap. The simplest choice for multiple-pair excitations would be to take multiples of Δ_1: Δ_1 for 2p-2h, $2\Delta_1$ for 4p-4h, $3\Delta_1$ for 6p-6h, etc., but this would not be realistic because the nucleus deforms with increasing particle-hole excitations leading, in general, to a smaller shell gap and, hence, a lower excitation energy for the next pair of nucleons. Heyde *et al.* [10] have studied this change in Δ in some detail but have not considered the problem for multiple-pair excitations and the mixing of several configurations. We will use a simple scaling argument, based on the Nilsson model, to estimate the changes in the (np-mh) excitation energy with increasing N_π. This is discussed in more detail in Sec. III.

III. APPLICATION AND RESULTS

Because of our previous studies of configuration mixing in the mercury isotopes [5,11] and because of Iachello's suggestion [3] that the mixing of multiparticle-multihole configurations in the IBM might be a useful approach to investigating superdeformed bands in nuclei such as ^{192}Hg, we have chosen ^{192}Hg as a test for our multiconfiguration mixing approach in the IBM-2.

In the present investigations we are primarily interested in exploring the model and are not principally interested in obtaining agreement with experimental data. We mainly want to see how the results change when (1) the number of (np-mh) configurations in the calculations is varied, and (2) different choices and/or assumptions are made for the multipair excitation energies Δ_i.

Regarding the first point, we consider two cases: (1) $N_\pi=1$, 3, 5, and 7, and $N_\nu=7$ (four configurations); (2) $N_\pi=1$, 3, 5, 7, and 9, and $N_\nu=7$ (five configurations). In this way we can study the effects of varying the number of proton pairs excited. For convenience, the configurations are referred to as 1π (normal configuration), 3π (2p-4h), 5π (4p-6h), etc. We note that approximating the higher excited configurations by $(n+m)/2$ proton-boson holes is a great oversimplification, because the particles and holes are in different major shells and because the "structure of the bosons" will change as more and more nucleons are excited across the major-shell gap. However, we take this assumption as a first approximation for testing the model, before attempting a more complicated description.

On the second point, we consider two cases: (1) $\Delta_n=n\Delta_1$, i.e., equally spaced two-particle excitation energies, and (2) $\Delta_n<n\Delta_1$, for $n>1$. The latter is consistent with the expectation that the energy needed to excite the second, third, etc., pair of nucleons should be less than the energy needed to excite the first pair, because the nucleus has become deformed in the process.

For the second case, we *estimate* the energies Δ_n (the energy to excite n pairs) relative to Δ_1 from the Nilsson diagram for protons, $50\le Z\le 82$ [12]. For simplicity, we consider only differences in single-particle (or quasiparticle) energies and ignore pairing and other effects.

The energy to excite the first pair of protons across the $Z=82$ shell gap is roughly twice the difference in energy of the $h_{9/2}$ and $d_{3/2}$ levels, for zero deformation, so that $E_1\approx 1\hbar\omega_0$ (from the Nilsson diagram). The nucleus, with $Z=80$, is now deformed and can be approximately described by two protons in $\frac{3}{2}^-$ [532], two holes in $\frac{3}{2}^+$[651], and two holes in $\frac{1}{2}^+$[660], with lower orbits filled. Exciting another pair of protons from $\frac{1}{2}^-$[651] to $\frac{1}{2}^-$[530] requires additional energy $E_2\approx 0.4\hbar\omega_0$ (for deformation $\epsilon\approx 0.27$), to give a 4p-6h configuration. Subsequently, exciting a pair from $\frac{9}{2}^-$[514] to $\frac{11}{2}^-$[505] requires $E_3\approx 0.6\hbar\omega_0$ and yields a 6p-8h configuration, etc. The phenomenological fits for the Hg chain [5,11] have employed the value $\Delta_1=4$ MeV to describe the pair excitation energy for the 3π configuration. If this corresponds to E_1, then we estimate the energy needed to excite two pairs of protons to be $\Delta_2=E_1+E_2\approx 6$ MeV, rounding to the nearest MeV. Similarly, $\Delta_3=E_1+E_2+E_3\approx 8$ MeV, etc.

Next, we discuss the determination of the IBM-2 Hamiltonian parameters. Finding appropriate parameters with which to describe the excited configurations is difficult because little, if any, data are available. One possible description employs parameter values that give reasonable fits to known nuclei that have the same number of valence protons and neutrons, e.g., $^{192}Hg_{112}$ ($Z=80$), $^{188}Os_{112}$ ($Z=76$), $^{168}Hf_{96}$ ($Z=72$), and $^{164}Er_{96}$ ($Z=68$), for $N_\nu=7$ and $N_\pi=1$, 3, 5, and 7, respectively. This method has been rejected because the resulting energies for the 3π configuration are much too high, relative to the deformed bands in $^{182-190}$Hg, for which data are available. This poor result is not surprising, in view of the simplistic effective boson number approximation for the particle-plus-hole situation. Instead, we have chosen to utilize previously determined ^{192}Hg parameter values for the 1π and 3π configurations, and to obtain the parameters for the other configurations either by keeping them fixed at the 3π values or by extending the trends for the 1π and 3π cases.

The parameter values of Barfield [13] are used in tact to describe both the 1π (normal) and the 3π (2p-4h) configurations. These parameters result from an overall fit with the even mercury isotopes $182\le A\le 198$, which gives a good description both for the normal vibrational-like states and for the shape-coexisting rotational-like band seen in the light nuclides $^{180-190}$Hg. This particular fit for the normal configuration is characterized by $\chi_\pi=1.0$, which was shown by Semmes *et al.* [14] to give better results for neighboring odd-A nuclei in quasiparticle-core coupling calculations than does the earlier parameter set [11] with $\chi_\pi=-0.4$. The χ_π values for the excited configurations are guided by semimicroscopic arguments [15] and are consistent with values previously employed to describe $Z=72-78$ nuclei [16–18].

The 3π value for the parameter epsilon in Eq. (1) is employed for all the excited configurations, and the values for the quadrupole-quadrupole strength κ are determined by extrapolation of the 1π and 3π values. The Majorana

TABLE I. IBM-2 Hamiltonian parameters employed in the calculations. For all configurations, $\xi_2=0.15$ MeV, $\xi_1=\xi_3=-0.30$ MeV ($FS=0.15$, $FK=0$). All parameters are in MeV, except for χ_ν and χ_π, which are dimensionless.

N_ν	N_π	ϵ	κ	χ_ν	χ_π	$C_{0\nu}$	$C_{2\nu}$	$C_{4\nu}$
7	1	0.68	−0.165	0.4	1.0	0.63	0.05	0.14
7	3	0.35	−0.145	0.4	−1.3	0.00	0.00	0.04
7	5	0.35	−0.12	0.4	−1.8	0.00	0.00	0.00
7	7	0.35	−0.10	0.4	−2.0	0.00	0.00	0.00
7	9	0.35	−0.08	0.4	−2.0	0.00	0.00	0.00

parameters in Eq. (4) and the values for χ_ν in Eq. (2) are kept the same for all configurations. The proton-proton interaction $V^{\pi\pi}$ in Eq. (1) is *not* included for any of the configurations, and the neutron-neutron interaction $V_{\nu\nu}$ is dropped for the 5π and higher configurations. The mixing strengths in Eq. (5) are held constant and taken from previous calculations [11], $\alpha=0.15$ MeV, $\beta=0.10$ MeV. The IBM-2 parameter values for the various configurations are given in Table I.

Although the mixing strengths α and β are held constant, the matrix elements of $V_{\rm mix}$ [Eqs. (5) and (6)] are state dependent, increasing in magnitude with increasing boson number. For example, for angular momentum $J=0$ and the IBM-2 parameter values utilized, $V_{\rm mix}(1,2)=-0.163$ MeV, $V_{\rm mix}(2,3)=0.437$ MeV, $V_{\rm mix}(3,4)=-0.638$ MeV, and $V_{\rm mix}(4,5)=-0.856$ MeV. The magnitude of these matrix elements decreases somewhat with increasing angular momentum. (The sign of the matrix elements depends on the phase convention adopted for the IBM-2 eigenfunctions and is unimportant.)

As a first trial, we consider four configurations with the successive multipair excitation energies taken to be Δ, 2Δ, and 3Δ, where $\Delta=4$ MeV is the value employed in the two-configuration-mixing calculations [11]. For simplicity, only the ground-state bands for each configuration are included in the calculation, with spin up to $20\hbar$. The results of this calculation, after mixing, are shown in Fig. 2. The experimental yrast levels [19], denoted as ×'s, are shown for reference. We note that the calculated levels for $J\geq 10$ do *not* correspond to the experimental levels shown because the latter states are known to be two-quasiparticle (2qp) in nature [19] and are outside of our model space. However, the yrast states for $J\leq 6$, which are clearly collective, are well reproduced by our model, as they should be. (Rotation-aligned bands cannot be reproduced within the IBM unless 2qp degrees of freedom are explicitly added to the model space.)

There is very little mixing among the excited bands because of the initial, large separation energies assumed between the unmixed bands. The 3π band, which crosses the 1π band between $J=8$ and 10, should not be identified with the experimental yrast states around $J\geq 10$, as previously mentioned because 2qp degrees of freedom are not included in our model space. The calculated energies of the $J=2$, 4, and 6 states in the 1π band are in good agreement with the experimental observed energies for these levels, as expected from our previous calculations [11].

From theoretical investigations [20] it is known that the "effective moment of inertia" of the ground-state band (gsb) in IBM-2 calculations is inversely proportional to the values of both ϵ and κ in Eq. (1). This effect is clearly seen in Fig. 2 where the moment of inertia is significantly smaller for the 1π band than for the other three bands because its ϵ value is almost twice as big as the ϵ value for the other bands. The moments of inertia for the excited bands are not very different, but do in-

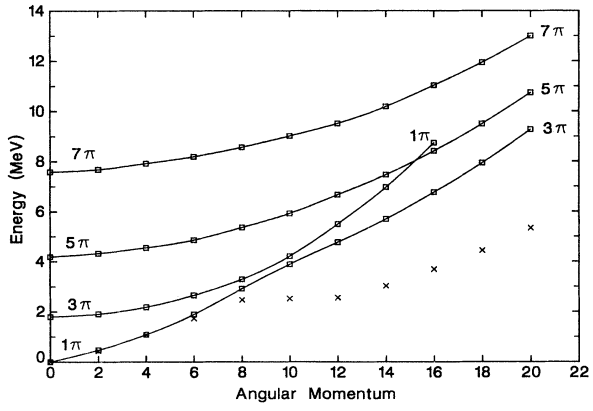

FIG. 2. Calculated energy levels after mixing for the ground-state bands of the 1π, 3π, 5π, and 7π configurations of ^{192}Hg with multipair excitation energies Δ_1 through $\Delta_3=4.0$, 8.0, and 12.0 MeV, respectively. The experimental yrast band, denoted by crosses, is shown for comparison. For $J>8$, these states are 2qp in nature and should not be reproduced by the calculations because they are outside of the model space. The data are from Ref. [19].

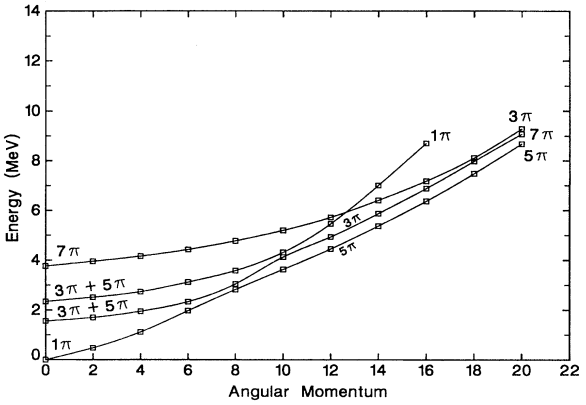

FIG. 3. Calculated energy levels after mixing for the same four configurations as in Fig. 2 (1π, 3π, 5π, and 7π), with Δ_1 through $\Delta_3=4.0$, 6.0, and 8.0 MeV, respectively.

crease with N_π, as κ decreases.

Figure 3 shows results after mixing for the same four configurations, with the multipair excitation energies $\Delta_1=4$ MeV, $\Delta_2=6$ MeV, and $\Delta_3=8$ MeV, as estimated from the Nilsson diagram. There is now considerable mixing among the excited configurations, even for spin $J=0$. Adding the $9\pi,7\nu$ configuration, with $\Delta_4=10$ MeV, lowers the energy of the 7π band somewhat, as shown in Fig. 4, and again the band associated with the most excited pairs has the largest moment of inertia.

It is reasonable to assume that neutron pairs can be excited across the $N=126$ shell gap. However, because we have no way of adequately predicting the changes in the IBM-2 parameter values when increasing both the proton and neutron boson numbers, we will not attempt the addition of excited neutron pairs to the model at this time.

As a general feature of the results, we note that increasing the number of excited pairs does increase the effective moment of inertia, so that the band with the largest number of excited pairs does possess the largest moment of inertia. On the other hand, none of the bands obtained (Figs. 2–4) has an effective moment of inertia large enough to correspond to that of a superdeformed (SD) band, as recently observed in ^{192}Hg [21,22].

The results shown have included only one state per spin for each of the configurations. Calculations with several basis states for each configuration give somewhat different values for the eigenvalues and eigenfunctions after mixing, but do not change the overall results in any substantial way.

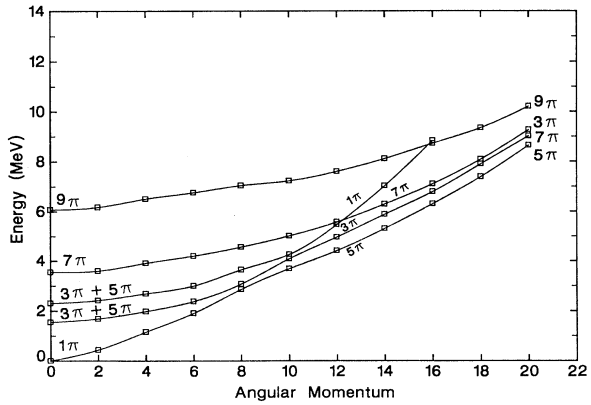

FIG. 4. Calculated energy levels after mixing for five configurations (1π, 3π, 5π, 7π, and 9π). The multipair excitation energies Δ_1 through Δ_4 are 4.0, 6.0, 8.0, and 10.0 MeV, respectively.

IV. DISCUSSION AND CONCLUSIONS

The IBM-2 configuration mixing method of Duval and Barrett [5] has been generalized from two to several configurations, each corresponding to a different (np-mh) excitation of the nucleus. This was done by assuming that only "nearest-neighbor" configurations, defined as N_π and $N_\pi+2$, etc. (or N_ν and $N_\nu+2,\ldots$), mix strongly. The generalization of the existing mixing codes from two to several configurations is straightforward, the main problem being the choice of the IBM-2 parameter values to use with each multiparticle-multihole configuration included in the calculation. It is assumed that the excitation energy of the first pair of nucleons across the shell gap is larger, in general, than the energy needed to excite subsequent pairs.

As a test, the generalized configuration method is applied to the nucleus ^{192}Hg. Up to five configurations are considered, including the normal $N_\pi=1$, $N_\nu=7$ configuration. Four excited proton configurations are included, with effective proton boson numbers of 3, 5, 7, and 9. The IBM-2 parameters for the first two configurations are taken from two-configuration-mixing calculations for ^{192}Hg. The parameters for the other configurations are estimated from trends for the first two, and from semimicroscopic considerations.

Two different assumptions for the multipair excitation energies are considered. While no significant mixing of the excited bands occurs when equally spaced excitation energies are employed for each multiparticle-multihole state, decreasing the multipair energies relative to the one-pair excitation energy results in significant mixing at low spin. For the parameters employed, the effective moment of inertia of the bands increases with the number of excited pairs. In spite of this, we obtain no results resembling a superdeformed band for the mixing of five configurations and for the present parameters, indicating that an SD band must correspond to a rather large num-

ber of proton *and* neutron pairs.

To summarize, in this study we have expanded the Duval-Barrett IBM-2 configuration-mixing approach in a straightforward manner and demonstrated the feasibility of extending the method to five or more np-mh states. Our test calculations produce encouraging trends for the effective moments of inertia of the excited bands, which should stimulate future investigations involving large numbers of excited proton and neutron pairs.

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