

Superdeformed many-particle–many-hole states in $N = Z$ nuclei: Beyond the 8p-8h state in ^{40}Ca

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Using a fixed configuration deformed Hartree-Fock method, we examine possible candidates for shape isomer states in several $N = Z$ nuclei ^{40}Ca , ^{44}Ti , ^{48}Cr , ^{52}Fe , and ^{56}Ni . We treat larger deformations than we did before and thus have to excite more particles and include more major shells. We have two criteria for a stable shape isomer. We find that in all the cases considered there exist stable, highly deformed states which satisfy both the conditions. One example is the 12-particle–12-hole states in ^{40}Ca with $\beta_0 = 0.965$. We consider the possibility of associating some of these shape isomers with molecular resonances obtained in heavy ion reactions such as $^{24}\text{Mg} + ^{24}\text{Mg}$ ($^{48}\text{Cr}^*$) or $^{28}\text{Si} + ^{28}\text{Si}$ ($^{56}\text{Ni}^*$).

I. INTRODUCTION

In previous works^{1,2} we searched for highly deformed many-particle–many-hole (mp-nh) states in nuclei and examined their properties, some of which could be associated with shape isomers. We used the method of fixed configuration deformed Hartree-Fock (HF) approach with a Skyrme interaction SK3. Some of the states we obtained could be associated with shape isomers. In the present work we extend our search to even larger deformations, seeing if we can find newer shape isomers. This by itself is quite an interesting project. However we will go further, in a more speculative vein and try to see if the highly deformed intrinsic states that we obtain can be associated with quasimolecular resonances which have recently been found in heavy ion collisions.

Concerning our previous works, several interesting results were obtained. For example, in ^{40}Ca we found a near degeneracy of the intrinsic state energies of several n -particle, n -hole states (np-nh). In more detail, with the SK3 interaction, the intrinsic state energies of np-nh states from $n = 1$ to 8 were respectively 5.4, 9.5, 12.4, 12.2, 13.6, 13.6, 13.2, and 11.4 MeV. Amusingly the 8p-8h intrinsic state energy came out somewhat lower than that of the 4p-4h state. However, a combination of projection and pairing led to a reversal of this ordering. Another interesting feature was that the deformation parameter β_0 was approximately linear in n for $n = 0 \rightarrow 3$ and for $n = 4 \rightarrow 8$. From $n = 0$ to $n = 8$ the values of β_0 that we obtained were respectively 0, 0.05, 0.13, 0.22, 0.33, 0.40, 0.47, 0.53, and 0.60. Such a linearity was predicted by Bertsch.³

We also obtained low-lying states in other nuclei, e.g., in ^{44}Ti , a 6p-2h state with $\beta_0 = 0.29$ at an intrinsic excitation energy of 6.0 MeV, and an 8p-4h state with $\beta_0 = 0.41$ at even lower intrinsic excitation energy 5.6 MeV. In ^{56}Ni we reported² 2p-2h, 3p-3h, and 4p-4h states with intrinsic excitation energies of 6.99, 7.99, and 6.87 MeV and with respective deformation parameters 0.21, 0.29, and 0.36.

In the all above calculations, except for ^{56}Ni , the holes were in states which in the spherical limit were in the $0d$ -

$1s$ shell and the particles in the $0f$ - $1p$ shell. In ^{56}Ni , the holes were in the orbits which in the spherical limit correspond to the $0f_{7/2}$ shell and the particles in higher states of the $0f$ - $1p$ shell. In this work, as we go to larger deformations we find that more nucleons have to be excited and that more major shells have to be taken into account.

In the oscillator model a superdeformed state has the ratio of frequencies $q = \omega_{\perp}/\omega_z$ equal to an integer greater than 1 with the most common case being $q = \omega_{\perp}/\omega_z = 2$. Bohr and Mottelson⁴ introduced a deformation parameter δ_{osc} defined by

$$\delta_{\text{osc}} = \frac{3(\omega_{\perp} - \omega_z)}{2\omega_{\perp} + \omega_z} = \frac{3(q - 1)}{2q + 1}. \quad (1.1)$$

The deformation parameter β_0 in this work is defined by

$$\beta_0 = \sqrt{\pi/5} \frac{Q_0}{A \langle r^2 \rangle}, \quad (1.2)$$

where Q_0 is the intrinsic mass quadrupole moment and $\langle r^2 \rangle$ the mean-square radius. The relations between β_0 and q or δ_{osc} are⁵

$$\beta_0 = 2\sqrt{\pi/5} \frac{q^2 - 1}{q^2 + 2}, \quad (1.3)$$

$$\beta_0 = \frac{2}{3}\sqrt{\pi/5} \delta_{\text{osc}} \left[\frac{6 - \delta_{\text{osc}}}{3 - 2\delta_{\text{osc}} + \delta_{\text{osc}}^2} \right] \\ \approx 1.057 \delta_{\text{osc}} \left[1 + \frac{\delta_{\text{osc}}}{2} - \frac{\delta_{\text{osc}}^3}{6} + \dots \right], \quad (1.4)$$

With $q = 2$ we find that $\delta_{\text{osc}} = 0.60$ and $\beta_0 = 0.79$. For small deformations, $q \approx 1 + \delta_{\text{osc}} \approx 1 + 0.946\beta_0$.

Note that in the case of ^{40}Ca , the value of δ_{osc} which is close to 0.6 is for the 8p-8h state ($\beta_0 = 0.60, \delta_{\text{osc}} = 0.48$). However, we obtain many other deformed bands which are of interest such as the 4p-4h band which has almost one-half the value of δ_{osc} than the 8p-8h state.

In the fixed configuration axial deformed HF approach, the deformed single-particle levels are labeled by

the quantum numbers Ω^π where Ω is the projection of the total angular momentum along the axis of symmetry and π is the parity. We expand the wave function in oscillators

$$\psi(\Omega^\pi) = \sum_{N=0}^{N_{\max}} C_{Nn_z\Lambda} |Nn_z\Lambda\Omega^\pi\rangle. \quad (1.5)$$

Besides the parameters for the interaction, the program has some other input parameters. The most important ones are N_{\max} , the maximum numbers of oscillator shells that are chosen to expand in; a size parameter $1/b_0 = \sqrt{\hbar/m\omega}(fm^{-1})$; a quadrupole parameter $q_{\text{in}} = \omega_1/\omega_z$ and the number of iterations.

We include 13 major shells (i.e., $N_{\max} = 13$). The size parameter b_0 is determined by

$$\frac{\hbar^2}{mb_0^2} = \frac{45}{A^{1/3}} - \frac{25}{A^{2/3}}. \quad (1.6)$$

In order to have a reasonable input for the quadrupole parameter q_{in} , we do the calculations in two steps. We first make a guess at q_{in} . As long as this q_{in} value is not too far away from the reasonable one, the calculation will converge with an output deformation parameter β_0 with which we may obtain a new q_{in} through Eq. (1.3) for the second step calculation. From this procedure, we also find that some output quantities (e.g., the intrinsic state energy E^{in} , the deformation β_0 etc.) are not very sensitive to q_{in} but some others (e.g., the moment of inertia \mathcal{J}) are.

It should be made clear that the nomenclature mp-nh is with respect to a *spherical* basis. In the fixed configuration approach we can construct, say a 4p-4h state in ^{40}Ca by removing four nucleons from the last occupied level $\Omega_{n_l}^\pi = \frac{3}{2}0d_{3/2}^+$ (where and hereafter the subscript nl_j indicates the spherical limit correspondence of the orbit Ω^π) and putting them into the orbit $\frac{1}{2}0f_{7/2}^-$. In the spherical limit the proton single-particle splitting $\Delta\epsilon_p$ for these two orbits is positive (+5.47 MeV with $\frac{3}{2}0d_{3/2}^+$ lower). However, the system is free to deform. The deformed state with lowest energy will be such that $\Delta\epsilon_p$ is negative (-0.74 MeV with $\frac{1}{2}0f_{7/2}^-$ lower). Again, the orbit with lower energy is occupied and the one with higher energy empty. From this point of view we are still putting the nucleons in the lowest single-particle states.

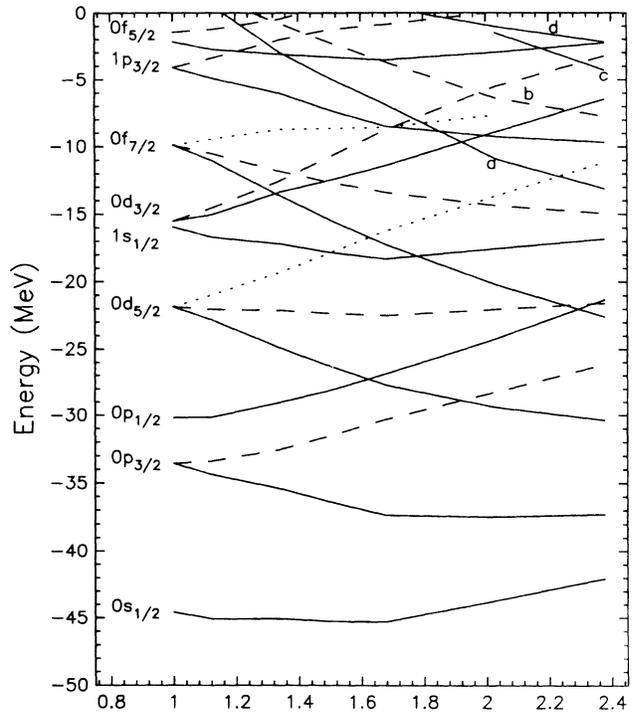
II. MOTIVATION OF THIS WORK AND n -HOLE STATE CONFIGURATIONS

The object of this work is to extend the search for highly deformed prolate shape isomers to larger deformations in several $N=Z$ nuclei— ^{40}Ca , ^{44}Ti , ^{48}Cr , ^{52}Fe , and ^{56}Ni . Recent experiments by Betts *et al.*,⁶ Zurmühle *et al.*,⁷ and Wuosmaa *et al.*⁸ provide one motivation for such a study. They performed $^{24}\text{Mg} + ^{24}\text{Mg}$, $^{24}\text{Mg} + ^{28}\text{Si}$, $^{28}\text{Si} + ^{28}\text{Si}$ elastic and inelastic scattering and observed a number of narrow resonances at bombarding energies of approximately twice the Coulomb barrier, carrying very high angular momentum ($34\hbar \sim 42\hbar$). Similar resonances have not been seen in other nearby systems such as $^{28}\text{Si} + ^{30}\text{Si}$, $^{30}\text{Si} + ^{30}\text{Si}$, $^{32}\text{S} + ^{32}\text{S}$ and $^{40}\text{Ca} + ^{40}\text{Ca}$. In

this work we ask if these “molecular resonances” can be thought of as members of rotational bands, which are associated with excited intrinsic states, indeed shape isomers, that we can find in our fixed configuration Hartree-Fock method.

We perform HF fixed configuration calculations using an axial symmetric code. Good candidates for shape isomer states are assumed to satisfy the following criteria: (a) the calculation converges (the intrinsic state energy E^{in} , and quadrupole moment Q_0 , etc., become stable) as we increase the number of iterations; (b) a substantial energy gap $\Delta\epsilon$ exists between unoccupied and occupied states.

As in previous work,^{1,2} we use the level sequence found in Nilsson diagrams to guide our search for prolately deformed states. To this end we show in Fig. 1 the energies of neutron orbits as a function of q in the HF calculation for ^{40}Ca . The results are similar but not identical to those of Nilsson because the HF calculations are not restricted to $\Delta N=0$. The quantity q is determined by the output deformation parameter β_0 through Eq. (1.3). The solid, dashed, and dotted lines represent respectively the



q

FIG. 1. The neutron orbits for prolate deformation in the Hartree-Fock calculation for ^{40}Ca . In this figure we show the energies of neutron orbits as a function of q , the deformation parameter which is defined by Eq. (1.3). The solid, dashed, and dotted lines represent the orbits with $\Omega = \frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$, respectively (for both the positive and negative parity states). A few lines in the upper right corner are the following: $a \sim \frac{1}{2}0g_{9/2}^+$, $b \sim \frac{3}{2}0g_{9/2}^+$, $c \sim \frac{1}{2}0h_{11/2}^-$, and $d \sim \frac{1}{2}0g_{7/2}^+$. The orbits with $\Omega \geq \frac{7}{2}$ are not shown.

orbits with $\Omega = \frac{1}{2}, \frac{3}{2},$ and $\frac{5}{2}$ (for both the positive and negative parity states). To aid the reader we classify the orbits by their quantum numbers as we approach the spherical limit nl_j . It should be emphasized, however, that we are usually working at a large deformation where the actual wave function is a weighted sum over states with different $n, l,$ and j . For the 4p-4h state in ^{40}Ca , as mentioned previously, four nucleons were removed from the orbit $\frac{3}{2}0d_{3/2}^+$ and put in the orbit $\frac{1}{2}0f_{7/2}^-$. The system would then be sufficiently deformed that the occupied orbits are all lower than the unoccupied ones, corresponding to the deformation region $q = 1.24 \sim 1.44$ in Fig. 1. For the 8p-8h state, another four nucleons were taken away from $\frac{1}{2}0d_{3/2}^+$ and put in $\frac{3}{2}0f_{7/2}^-$, resulting in a larger deformation. It should be pointed out that a stable configuration could only be formed by carefully choosing the right orbits which nucleons are removed from and put in. For doing this, Fig. 1 is very helpful.

For mp-nh states in ^{40}Ca , ^{44}Ti , and ^{48}Cr , we form the “holes” by removing nucleons from the orbits $\frac{3}{2}0d_{3/2}^+, \frac{1}{2}0d_{3/2}^+,$ and $\frac{5}{2}0d_{5/2}^+$, depending on the number of holes. We form the “particles” by filling nucleons into the orbits $\frac{1}{2}0f_{7/2}^-, \frac{3}{2}0f_{7/2}^-, \frac{1}{2}0g_{9/2}^+,$ and $\frac{1}{2}1p_{3/2}^-$, depending on the number of particles. Therefore, for example, the 8p-8h state in ^{40}Ca has configuration

$$\left(\frac{3}{2}0d_{3/2}^+ \frac{1}{2}0d_{3/2}^+\right)^{-8} \left(\frac{1}{2}0f_{7/2}^- \frac{3}{2}0f_{7/2}^-\right)^8.$$

The 16p-12h state in ^{44}Ti has configuration

$$\left(\frac{3}{2}0d_{3/2}^+ \frac{1}{2}0d_{3/2}^+ \frac{5}{2}0d_{5/2}^+\right)^{-12} \left(\frac{1}{2}0f_{7/2}^- \frac{3}{2}0f_{7/2}^- \frac{1}{2}0g_{9/2}^+ \frac{1}{2}1p_{3/2}^-\right)^{16},$$

and the 16p-8h state in ^{48}Cr has configuration

$$\left(\frac{3}{2}0d_{3/2}^+ \frac{1}{2}0d_{3/2}^+\right)^{-8} \left(\frac{1}{2}0f_{7/2}^- \frac{3}{2}0f_{7/2}^- \frac{1}{2}0g_{9/2}^+ \frac{1}{2}1p_{3/2}^-\right)^{16}.$$

For ^{52}Fe and ^{56}Ni , the “holes orbits” are $\frac{7}{2}0f_{7/2}^-, \frac{5}{2}0f_{7/2}^-,$ $\frac{3}{2}0d_{3/2}^+, \frac{1}{2}0d_{3/2}^+,$ and $\frac{5}{2}0d_{5/2}^+$. The “particles orbits” are $\frac{1}{2}1p_{3/2}^-, \frac{1}{2}0g_{9/2}^+, \frac{3}{2}0g_{9/2}^+, \frac{1}{2}0h_{11/2}^-,$ and $\frac{1}{2}0g_{7/2}^-$.

III. RESULTS

We require the energy gap between the lowest unoccupied and the highest occupied proton orbits $\Delta\epsilon_p$ be greater than 1.5 MeV. We then find the following stable, superdeformed states in the nuclei considered: 8-hole and 12-hole states in ^{40}Ca , 8-hole states in ^{44}Ti and in ^{48}Cr , 16-hole states in ^{52}Fe and in ^{56}Ni . The results for the ground and the above stable n -hole states are shown in Tables I and II together with some other states with $\Delta\epsilon_p$ positive but less than 1.5 MeV.

In Tables I and II, we give for the ground states, the intrinsic energy E_g^{in} and the projected 0^+ state energy $E_g^{\text{pr}}(0^+)$ (for ^{40}Ca and ^{56}Ni they are the same).

We then give, for the superdeformed states, the intrinsic energy E^{in} , the deformation parameter β_0 , the energy gap $\Delta\epsilon_p$ for proton orbits, the squared angular momentum $J_1^2 = J_x^2 + J_y^2$ in the direction perpendicular to the symmetry axis z and the intrinsic moment of inertia \mathcal{J}_{cr} of the cranking model. Also listed in the tables are $E^{\text{pr}}(0^+), E^{\text{pr}}(20^+)$ and $E^{\text{pr}}(40^+)$, the energies of the selected angular momentum states projected from the intrinsic, superdeformed n -hole bands.

We now discuss the case of ^{40}Ca in detail. The intrinsic energy of the 12-hole state is -317.18 MeV with the deformation $\beta_0 = 0.9647$. The intrinsic moment of inertia \mathcal{J}_{cr} is 12.79 MeV $^{-1}$, and J_1^2 is 146.3 . Using the formula

$$E^{\text{pr}}(0^+) = E^{\text{in}} - \frac{\langle J_1^2 \rangle}{2\mathcal{J}_{\text{cr}}}, \quad (3.1)$$

we find the projected 0^+ state from this 12-hole band has the energy -322.90 MeV. This is 18.70 MeV above the intrinsic ground state ($E_g^{\text{in}} = -341.60$ MeV). The state with angular momentum J^π in the rotational band built on this intrinsic state has the energy

$$E^{\text{pr}}(J^+) = E^{\text{pr}}(0^+) + \frac{J(J+1)}{2\mathcal{J}_{\text{cr}}}. \quad (3.2)$$

We find that $E^{\text{pr}}(20^+) = -306.48$ MeV, this is 35.12

TABLE I. The Hartree-Fock calculations of the ground states and the superdeformed n -hole states in ^{40}Ca , ^{44}Ti , and ^{48}Cr . In this table, the energy is in unit MeV. β_0 is the deformation, $\Delta\epsilon_p$ is the energy gap between the lowest unoccupied orbit and the highest occupied orbit, \mathcal{J}_{cr} is the moment of inertia in cranking model. The energies for selected J^+ states projected from the intrinsic n -hole state are also shown with respect to the energy of the projected 0^+ ground state, i.e., $E^{\text{pr}}(J^+)^* = E^{\text{pr}}(J^+) - E_g^{\text{pr}}(0^+)$.

Nucleus	^{40}Ca		^{44}Ti		^{48}Cr
	8 hole	12 hole	8 hole	12 hole	8 hole
E_g^{in}					
$E_g^{\text{pr}}(0^+)$					
β_0	0.599	0.965	0.813	0.985	0.847
$\Delta\epsilon_p$	2.08	2.04	2.27	0.28	2.31
J_1^2	57.92	146.3	113.4	175.7	132.0
\mathcal{J}_{cr}	6.722	12.79	11.45	15.23	13.43
E^{in}	-330.21	-317.18	-355.40	-346.76	-387.50
$E^{\text{pr}}(0^+)$	-334.52	-322.90	-360.35	-352.53	-392.42
$E^{\text{pr}}(0^+)^*$	7.08	18.70	12.04	19.86	18.99
$E^{\text{pr}}(20^+)^*$	38.32	35.12	30.38	33.64	34.63
$E^{\text{pr}}(40^+)^*$	129.07	82.82	83.65	73.70	80.05

TABLE II. The Hartree-Fock calculations of the ground states and the superdeformed n -hole states in ^{52}Fe and ^{56}Ni . See Table I for detail.

Nucleus	^{52}Fe			^{56}Ni	
E_g^{in}		−445.00		−482.29	
$E_g^{\text{pr}}(0^+)$		−448.70		−482.29	
n hole	8 hole	12 hole	16 hole	16 hole	20 hole
β_0	0.713	0.913	1.144	1.053	1.218
$\Delta\epsilon_p$	0.74	0.86	1.93	3.34	1.10
J_{\perp}^2	162.3	181.9	365.3	271.9	464.1
\mathcal{J}_{cr}	18.56	15.72	26.02	20.86	33.02
E^{in}	−420.08	−416.56	−406.00	−444.16	−430.66
$E^{\text{pr}}(0^+)$	−424.45	−422.34	−413.02	−450.68	−437.68
$E^{\text{pr}}(0^+)^*$	24.25	26.35	35.67	31.61	44.60
$E^{\text{pr}}(20^+)^*$	35.56	39.71	43.74	41.67	50.96
$E^{\text{pr}}(40^+)^*$	68.43	78.52	67.19	70.92	69.43

MeV above the ground state, and $E^{\text{pr}}(40^+) = -258.78$ MeV, 82.82 MeV above the ground state. Note that the deformation of the 12-hole state in ^{40}Ca is consistent with the Bertsch formula³ which says that β_0 is proportional to the number of holes n .

The intrinsic state energy of the 12-hole state that we obtain here (24.1 MeV) is much lower than what we would obtain if we did not allow excitations into the $N=4$ shell ($0g_{9/2}$ in the spherical limit). In a previous calculation,¹ in which we allowed only excitations into the $N=3$ shell ($0f-1p$), the intrinsic state excitation energy for 12-hole state was 50.7 MeV, essentially double the present one. On the other hand, for the 8-hole state in ^{40}Ca , it does not pay to excite nucleons into the $N=4$ shell. What is of course happening is that for very large deformation, the single-particle orbit in $N=4$ labeled by $\frac{1}{2}0g_{9/2}^+$ (the orbit a in Fig. 1) is coming below many of the $N=3$ orbits. The 8-hole deformation $\beta_0=0.60$ ($q=1.68$) is too small, but the 12-hole deformation $\beta_0=0.97$ ($q=2.38$) is large enough to benefit.

How can we reach the 12-hole state? Fortune and collaborators^{9–11} identified 4p-4h and 8p-8h states in ^{40}Ca by starting with 4 holes (^{36}Ar) and 8 holes (^{32}S) and transferring 4 particles and 8 particles, respectively, via heavy ion transfer reactions. In the same vein it might be possible to start with a 12-hole system (^{28}Si) and attempt to transfer 12 particles.

Another possibility is to try to form quasimolecular resonances by the reaction $^{20}\text{Ne} + ^{20}\text{Ne}$. The experimental ground-state energy of this nucleus is -160.65 MeV. We thus have

$$E_g^{\text{exp}}(^{20}\text{Ne} + ^{20}\text{Ne}) = -321.30 \text{ MeV}.$$

This is 1.6 MeV higher than the energy (-322.90 MeV) of the 0^+ member of the 12-hole intrinsic band in ^{40}Ca .

We note that there is a crossing between the 8-hole and 12-hole bands. As shown in Fig. 1, the 8-hole band starts at a lower energy but it rises more rapidly because of smaller moment of inertia \mathcal{J}_{cr} . The two bands cross each other at $J=17.65$

As shown in Table II, for ^{56}Ni , we find stable, superdeformed 16-hole and 20-hole states. We also try 8-hole

and 12-hole states. For both these two configurations, we find that the calculations converge but the condition (b) in Sec. II is not satisfied, i.e., the energy gap $\Delta\epsilon_p$ is either negative (there exists an unoccupied orbit which is more bound than the highest occupied one) or too small.

In general, the band with larger deformation has higher intrinsic state energy and larger moment of inertia. Therefore, one would expect to see the band crossing in other nuclei for which there are more than one superdeformed bands. Indeed in ^{44}Ti (8-hole and 12-hole bands), ^{48}Cr (4-hole and 8-hole bands) and ^{56}Ni (16-hole and 20-hole bands), there are band crossings. But surprisingly in our calculation we find that in ^{52}Fe , the 8-hole band has a larger \mathcal{J}_{cr} than in the 12-hole band and

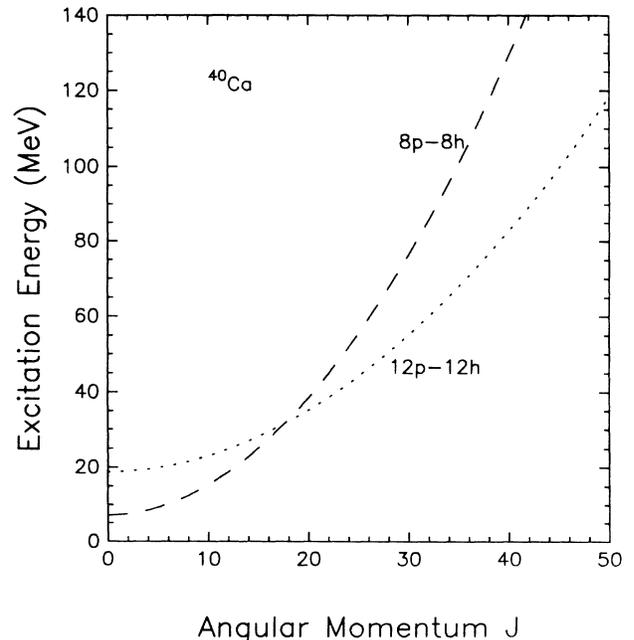


FIG. 2. The band crossing in ^{40}Ca . We show here the highly deformed 8-hole (dashed line) and 16-hole (dotted line) bands in ^{40}Ca . The band crossing occurs at $J=17.65$.

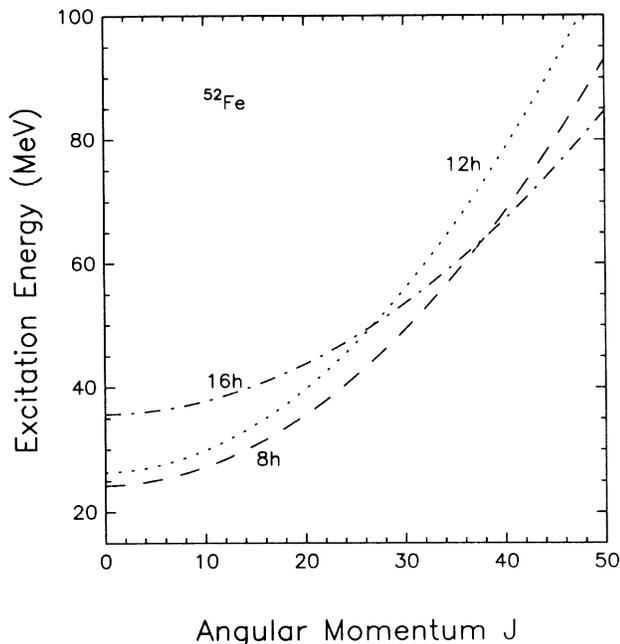


FIG. 3. The 8-hole, 12-hole, and 16-hole bands in ^{52}Fe . Note that there is no crossing between the 8-hole (dashed line) and 12-hole (dotted line) bands. But both the two bands cross with the 16-hole band (dashed-dotted line).

there is no crossing between them, although there is a crossing between 8-hole and 16-hole bands, and also between 12-hole and 16-hole bands. This is shown in Fig. 3.

For ^{48}Cr , ^{52}Fe , and ^{56}Ni , where experiments have been performed, our results are quite encouraging. The $J^\pi=36^+$ member of the 8-hole band in ^{48}Cr has the excitation energy 68.6 MeV while experimental value⁸ is about 60 MeV. In ^{56}Ni , the $J^\pi=36^+$ and 40^+ members

of the 16-hole band have energies 63.5 and 70.9 MeV respectively, very close to experimental values⁶ of 64 and 70 MeV.

The good agreement is undoubtedly fortuitous because the Skyrme Hartree-Fock method is not expected to be that precise and because we have not taken into account the variation of moment of inertia with angular momentum. An important problem is why one does not see γ decays of superdeformed states all the way down to angular momentum $J=0$. The γ cascade in a wide variety of nuclei terminates at some intermediate angular momentum well above $J=0$. An answer to this question is offered by examining Figs. 2 and 3. The state with fewer holes usually has a smaller deformation and lower intrinsic energy. But it also has a smaller moment of inertia. Hence the energy as a function of angular momentum rises faster than a band with a higher deformation. Thus there will always be some band crossings. Thus the γ decay from a superdeformed band will get diverted to the other bands.

In conclusion, our fixed configuration Hartree-Fock calculations predict that several new shape isomers should exist in the $N=Z$ nuclei considered here— ^{40}Ca , ^{44}Ti , ^{48}Cr , ^{52}Fe , and ^{56}Ni . We recommend that they be searched for by heavy ion transfer reactions or by the formation of quasimolecular resonances.

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