Calculations of many-particle–many-hole deformed state energies: Near degeneracies, deformation condensates

D. C. Zheng, D. Berdichevsky, and L. Zamick
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855
(Received 8 January 1988)

In deformed Hartree-Fock calculations with Skyrme interactions we observe a near degeneracy of the mean energies of many-particle–many-hole deformed intrinsic states. For example, in ^{40}Ca the np-nh states with $n=2$, 3, 4, 5, 6, 7, and 8 are nearly degenerate. The deformation parameter β increases steadily from $n=2$ to 8. The intrinsic state energy of the 8p-8h state is lower than that of the 4p-4h state for the interactions used here—SK III, SK IV, and SK VI. The calculations are also performed with the Skyrme III interaction for the even-even calcium and titanium isotopes. For ^{44}Ti there is a near degeneracy of 6p-2h and 8p-4h. For the $N>Z$ isotopes above, the two protons excitation lies lowest. Whereas the intrinsic state energies are much higher than the observed energies of the lowest-lying deformed states, the results when projection of $J=0^+$ states is carried out and pairing effects are taken into account, are encouraging.

INTRODUCTION

Low-lying highly deformed many-particle–many-hole states are a vital ingredient of the nucleus spectroscopy of light-medium mass nuclei, and their role in the spectroscopy of heavy nuclei is just beginning to be appreciated.

We feel that a reexamination of this problem is appropriate at this time, despite the fact that there have been many theoretical and experimental contributions to this subject for several decades. We wish to see if we can rigorously calculate the energies of these deformed states starting with a model which was initially devised for other purpose—mainly to fit ground-state properties of all nuclei in the periodic table. This is the Skyrme-Hartree-Fock model,[1] originally applied by Vautherin and Brink[2] to spherical nuclei, but then found to be easily extended to fit ground-state bands of deformed nuclei as well.

Early contributions to our understanding of the deformed states were made by Morinaga,[3] Talmi and Unna,[4] Engeland,[5] Brown and Green,[6,7] and Gerace and Green.[8] It was shown, for example, that the first excited 0^+ states in ^{16}O and ^{40}Ca, these being $J=0^+$, $T=0$ states at 6.05 and 3.05 MeV, respectively, were dominantly 4p-4h highly deformed states, albeit with some admixture of 0p-0h and 2p-2h. The arguments put forth to support the picture of a low-lying deformed state involved the use of Nilsson diagrams.[9]

In ^{40}Ca Gerace and Green[10] went even further. They suggested that an 8p-8h configuration, even more deformed than the 4p-4h, was necessary to explain the presence at 5.21 MeV of the second 0^+ state. A few years later, in a calculation which used the Strutinsky method,[11] Metag *et al.*[12] plotted the energy as a function of deformation and found that over and above the spherical minimum there was a second pronounced prolate minimum. They found that the deformation at this minimum was more in accord with an 8p-8h configuration rather than 4p-4h.

Extensive experimental work looking for 8p-8h states was carried out by Middelton *et al.*[13] via the ^{32}S(^{12}C,α)^{40}Ca reaction. Their results, broadly speaking, supported the picture of Gerace and Green.[10] In later publications, Fortune *et al.*[14,15] assigned as dominant configurations of the $J=0^+$ states: 0 MeV, 0p-0h; 3.35 MeV, 4p-4h; 5.21 MeV, 8p-8h; 7.30 MeV, 2p-2h; 8.28 MeV, also 2p-2h; and 8.42 MeV, 2p-2h or 4p-4h.

Getting back to theoretical contributions, the work on np-1h configurations by Bansal and French[16] was generalized to many-particle–many-hole states by Zamick[17] resulting in simple predictions for the energies of these states. Arima, Horiuchi, and Sebe[18] invoked a weak coupling model to predict the energies of the deformed states. Zuker, Buck, and McGrory[19] explained deformed states in ^{16}O in terms of four nucleons relative to a ^{12}C core. Ellis and Engeland[20] used SU(3) wave functions for the particles and for the holes.

Hartree-Fock calculations of the energies of the highly deformed states in ^{16}O were first performed by Ripka and Bassichis[21] and by Kelson.[22] Stephenson and Banerjee[23] and Das Gupta and de Takacsy[24] made a case for a triaxial solution for the 4p-4h state in ^{16}O. Hartree-Fock calculations with interactions constrained to give correct ground-state properties of nuclei were performed by Boeker.[25]

In more recent times Liu and Zamick[26] showed that one could get low-lying "4p-4h" states in ^{4}He and ^{16}O with Skyrme-like interactions. Auverlot *et al.*[27] also showed that in ^{16}O the 4p-4h configuration came low. They made the important point that because of the spin-orbit interaction the lowest solution for 4p-4h had axial symmetry, in contrast to previous calculations which yielded a triaxial solution.

Liu, Jaqaman, and Zamick[28] extended the work in ^{4}He to 2p-2h and found a surprising near degeneracy of the 4p-4h and various 2p-2h configurations. This near degeneracy provides an important *motivation* for the present work. We wish to examine here whether this is an accident, peculiar only to ^{4}He or if it is a more widespread phenomenon. It should be added that in a completely different calculation using the symplectic shell model, Carvalho, Vassanji, and Rowe[29] also noted a near degeneracy of 4p-4h and 2p-2h configurations in ^{4}He (in their notation (2)[22] and (4)[4]).

POSITIVE AND NEGATIVE PARITY INTRINSIC STATES TREATED TOGETHER

In this section we consider the closed shell nuclei ^{4}He, ^{16}O, and ^{40}Ca. We perform constrained deformed Hartree-Fock calculations for the lowest energies of np-nh states, using a program originally written by Vautherin,[30] and modified by Brack,[31] and Sprung and Vallieres.[32] For each case we list the intrinsic state energies and the deformation parameter β. The latter is defined as

$$0.16\beta^2+\beta=\beta_0 ,$$

$$(\text{or } \beta=[\sqrt{(1+0.64\beta_0)}-1]/0.32) ,$$

where β_0, the quantity actually listed in the code is given by

$$\beta_0=\sqrt{(\pi/5)}Q_0(\pi)/[ZR^2_{\text{rms}}(\pi)] ,$$

where $Q_0(\pi)$ is the intrinsic quadrupole moment of the protons and $R_{\text{rms}}(\pi)$ is the root-mean-square radius of the protons.

We will consider both even numbers of holes (even n) corresponding to positive parity excitations, and odd numbers of holes corresponding to negative parity excitations. The reason for considering these states together will become clear from the results which will soon be shown.

We perform calculations with the Skyrme interactions SK III, SK IV, and SK VI. This enables us to carry out our study with a wide range of effective masses: $m^*/m=0.95$, 0.76, and 0.47 for SK VI, SK III, and SK IV, respectively. The Skyrme parameters are given in a work by Beiner *et al.*[33]

For the case where there are an odd number of nucleons, be they neutrons or protons, there are two degenerate states for the odd nucleon. These are $|k\rangle$ and the time-reversed partner $|\bar{k}\rangle$. The program used here maintains axial symmetry at all times. This is achieved by forcing the occupancy of each of the above two states to be 0.5.

We define the intrinsic state ϕ_0 as the single Slater determinant which emerges from our fixed configuration Hartree-Fock calculation. This state may be regarded as a wave packet formed by admixing several states, each with a different total angular momentum. The intrinsic state energy is equal to $\langle\phi_0 H\phi_0\rangle$ where H is the Skyrme Hamiltonian. For ^{4}He, ^{16}O, and ^{40}Ca the results are given in Tables I, II, and III, respectively.

For $n=2$ we include two types of excitations, one in which a neutron and a proton are excited (a), and the other two protons excited (b). (To form states of good isospin, one must take linear combinations of these two configurations as well as a state in which two neutrons are excited.) For $n\geq 3$ we restricted ourselves to configurations in which the numbers of excited protons and neutrons are as close to each other as possible. Thus, for $n=3$ we excite two protons and a neutron, for $n=5$ three protons and two neutrons, and for $n=7$ four protons and three neutrons.

The most striking observation to be made from examining the Tables I, II, and III is that there is a near degeneracy of several np-nh states, with no distinction as to whether n is even or odd. For example, in ^{40}Ca when the SK III interaction is used, the np-nh states for $n=2\rightarrow 8$ have energies of -331.8 [case (a)], -330.8 [case (b)], -329.0, -329.2, -327.8, -327.8, -328.2, and -329.9 MeV, respectively. The ground state ($n=0$) is at -341.3 MeV and the 1p-1h excitation at -335.8 MeV.

Thus, it costs about 5.5 MeV to excite the 1p-1h state and an additional 4.0 MeV to form the 2p-2h state. But from then on, it seems to cost no energy to excite additional particle-hole states up to $n=8$ (beyond $n=8$ the degeneracy gets badly broken). We seem to have formed a partial condensate. Meanwhile, the deformation steadily increases as n increases. From $n=0$ to 8 for SK III the values of β are 0, 0.05, 0.13, 0.22, 0.32, 0.38, 0.44, 0.50, and 0.55, respectively. Beyond $n=8$, though, the energies of the np-nh states increase rapidly.

TABLE I. Intrinsic state energies and deformation parameters of np-nh deformed states in ^{4}He, using the deformed Hartree-Fock approach, with various Skyrme interactions and nine major oscillator shells included.

	SK VI		SK III		SK IV	
m^*/m	0.95		0.76		0.47	
Configuration	E (MeV)	β	E (MeV)	β	E (MeV)	β
0p-0h	−26.3	0	−26.5	0	−26.8	0
1p-1h	−14.1	0.16	−12.3	0.20	−8.99	0.28
2p-2h[a]	−4.12	0.58	−2.04	0.62	1.38	0.67
2p-2h[b]	−1.57	0.96	−0.31	0.95	1.89	0.87
3p-3h	−1.21	1.07	−0.20	1.08	1.79	1.05
4p-4h	−1.22	1.10	−0.19	1.10	1.89	1.07

[a] $\pi\nu-\pi^{-1}\nu^{-1}$.
[b] $\pi^2-\pi^{-2}$.

TABLE II. Intrinsic state energies and deformation parameters of np-nh deformed states in ^{16}O for various Skyrme interactions and 11 major oscillator shells included.

	SK VI		SK III		SK IV	
Configuration	E (MeV)	β	E (MeV)	β	E (MeV)	β
0p-0h	−127.6	0	−128.0	0	−128.4	0
1p-1h	−121.5	0.07	−120.4	0.08	−117.5	0.10
2p-2h[a]	−116.5	0.27	−114.8	0.28	−109.5	0.31
2p-2h[b]	−115.1	0.22	−112.9	0.24	−108.2	0.30
3p-3h	−114.2	0.44	−111.4	0.46	−106.0	0.49
4p-4h	−115.1	0.60	−112.5	0.63	−108.5	0.65
6p-6h	−97.0	0.71	−96.3	0.73	−89.8	0.76
8p-8h	−88.6	0.81	−85.6	0.82	−78.6	0.82

[a] $\pi\nu - \pi^{-1}\nu^{-1}$.
[b] $\pi^2 - \pi^{-2}$.

This work shows that, to properly describe deformed states, one has to take all the nearly degenerate configurations into account on an equal footing. Thus, to properly describe the ground and low-lying positive parity excitations of ^{40}Ca, one should include 0p-0h, 2p-2h, 4p-4h, 6p-6h, and 8p-8h in a matrix diagonalization, and for negative parity states the 1p-1h, 3p-3h, 5p-5h, and 7p-7h excitations. There is no justification in leaving any of these out.

The admixture of all these states may provide an additional mechanism for lowering the energy of the first excited 0^+ state. There has always been a problem of getting this state low enough in a convincing fashion.

DEPENDENCE OF THE INTRINSIC STATE ENERGIES ON EFFECTIVE MASS

We note a strong dependence of the excitation energies of the intrinsic deformed states on effective mass. For SK VI with $m^*/m=0.95$, the excitation energy of the 4p-4h intrinsic state in ^{40}Ca is equal to 9.4 MeV; for SK III with $m^*/m=0.76$, the value is 12.1 MeV and for SK IV with $m^*/m=0.47$, the value is 17.1 MeV. Recall that the single-particle energy differences are inversely proportional to the effective mass, for example in the oscillator model the energy difference $\hbar\omega$ gets changed to $\hbar\omega/(m^*/m)$, we now see that the 4p-4h excitation energies also *increase* with decreasing effective mass, just like the single-particle energies.

The effective mass in the Skyrme interaction[1,2] involves a certain combination of the velocity dependent terms t_1 and t_2:

$$(m/m^*)-1=(\tfrac{1}{16})(3t_1+5t_2)\rho(2m/\hbar^2)\ .$$

There may also be a dependence on the other combination of parameters like the surface term proportional to $(9t_1-5t_2)\,|$.[33] This will be studied at a later date.

We next consider the 8p-8h excitation energies. For SK VI, SK III, and SK IV these are, respectively, 8.0, 11.4, and 15.3 MeV. These energies are even lower than the 4p-4h energies.

The phenomenology of deformed states due to Brown and Green[6,7] and Gerace and Green[8,10] would seem to indicate that the 4p-4h intrinsic state energy is lower than that of 8p-8h, and this could present a problem for the Skyrme interactions. This requires further study.

TABLE III. Intrinsic state energies and deformation parameters of np-nh deformed states in ^{40}Ca for various Skyrme interactions and 11 major oscillator shells included.

	SK VI		SK III		SK IV	
Configuration	E (MeV)	β	E (MeV)	β	E (MeV)	β
0p-0h	−339.8	0	−341.3	0	−341.2	0
1p-1h	−335.8	0.05	−335.8	0.05	−333.1	0.05
2p-2h[a]	−332.9	0.12	−331.8	0.13	−326.9	0.13
2p-2h[b]	−331.8	0.11	−330.8	0.12	−326.2	0.13
3p-3h	−330.2	0.21	−329.0	0.22	−323.3	0.23
4p-4h	−330.4	0.31	−329.2	0.32	−324.1	0.34
5p-5h	−329.0	0.37	−327.8	0.38	−321.9	0.39
6p-6h	−329.7	0.43	−327.8	0.44	−321.5	0.45
7p-7h	−329.6	0.49	−328.2	0.50	−322.8	0.51
8p-8h	−331.8	0.54	−329.9	0.55	−325.9	0.56
12p-12h	−301.1	0.50	−290.6	0.51	−267.7	0.52
16p-16h	−252.2	0.44	−235.3	0.46	−202.0	0.48

[a] $\pi\nu - \pi^{-1}\nu^{-1}$.
[b] $\pi^2 - \pi^{-2}$.

SPECIAL COMMENTS ON ^{4}He

Considering ^{4}He on the same footing as ^{16}O and ^{40}Ca may appear questionable to many. After all, it is a very light nucleus. Whereas in ^{40}Ca a 4p-4h excitation may be regarded as the excitation of an α particle, in ^{4}He it obviously consists of breaking up an α particle. Furthermore, the 4p-4h excitation in ^{4}He, if exists, is near or in the continuum for four nucleon breakup.

It is not our intent here to defend the calculation in ^{4}He, but rather, to point out that it was in this nucleus that the near degeneracy of the various np-nh configuration was first noticed by Liu, Zamick, and Jaqaman.[28] The behavior in this nucleus gave the present authors the clue that the calculated near degeneracy of various np-nh excitations might be a more widespread phenomenon as indeed it is. It occurs in ^{16}O and ^{40}Ca.

In Table I it should be pointed out that the $J=0$, $T=0$ 1p-1h state is a spurious state, and so will not appear in the physical spectrum.

DEFORMED STATES IN CALCIUM AND TITANIUM ISOTOPES

In this section we will consider deformed states in other calcium isotopes ^{42}Ca, ^{44}Ca, ^{46}Ca, and ^{48}Ca, as well as some titanium isotopes ^{44}Ti, ^{46}Ti, ^{48}Ti, and ^{50}Ti. We shall only use SK III in this section and consider only positive parity states. One can expect the similar results for other Skyrme interactions.

The results for the calcium isotopes are given in Table IV. We can follow the trend with increasing neutron numbers. We will first focus on the lowest-energy excitation which in all cases consists of two protons being excited from the "sd" to the "fp" shell. The energies of these excitations for $A=42$, 44, 46, and 48 are 5.8, 3.9, 5.6, and 10.5 MeV, respectively. It should be added that in ^{40}Ca the energy of a two proton excitation is about 10 MeV. For ^{42}Ca, ^{44}Ca, and ^{46}Ca the calculated excitation energies are quite low. There are known low-lying 0^+ excited states in the calcium isotopes e.g., at 1.837 MeV in ^{42}Ca, at 1.883 MeV in ^{44}Ca, and at 2.42 MeV in ^{46}Ca. Allowing for the fact that projection will lower the $J=0$ state energy relative to that of the intrinsic state, it is not unreasonable to associate the first excited states of these nuclei with the two proton excitation. The first excited 0^+ state in ^{48}Ca is at 4.28 MeV and this might be a dominantly $(fp)^8$ configuration. If we look at more complicated configurations in ^{42}Ca we note a near degeneracy of a 6p-4h and 8p-6h state. The intrinsic state excitation energies are 7.9 and 7.7 MeV, respectively. They are reasonably close to the 4p-2h state so that all three of these states could be mixed strongly via a residual interaction.

In ^{44}Ca the 8p-4h state $\pi^4\nu^4-\pi^{-4}$ is 7.7 MeV above the ground state, and then there are two nearly degenerate states, another 8p-4h state $\pi^2\nu^6-\pi^{-2}\nu^{-2}$ and a 10p-6h state $\pi^4\nu^6-\pi^{-4}\nu^{-2}$ which are both near 11 MeV above the ground state.

In Table V the results are presented for the titanium isotopes. For ^{44}Ti we have the interesting result of a near degeneracy of the first excited state with the 6p-2h and 8p-4h configurations which have intrinsic state energies of 6.0 and 5.6 MeV, respectively. In more detail the configurations are $\pi^4\nu^2-\pi^{-2}$ and $\pi^4\nu^4-\pi^{-2}\nu^{-2}$. The 0_2^+ state has been identified as an 8p-4h state by Fortune *et al.*[14,15] in agreement with a theoretical estimate of Arima, Gillet, and Ginocchio.[34]

In ^{46}Ti, ^{48}Ti, and ^{50}Ti, however, the two proton excitation is the lowest. The respective energies are 3.9, 4.5, and 9.3 MeV. For these the results are somewhat similar to the calcium isotopes. Experimentally the first excited states in ^{44}Ti, ^{46}Ti, ^{48}Ti, and ^{50}Ti are at 1.904, 2.611, 2.997, and 3.870 MeV.

In a complete shell model diagonalization of ^{44}Ti in the $(fp)^4$ space the first excited state comes at about 7 MeV. Thus, the 1.904 state is undoubtedly a deformed state. However, as mentioned previously, we get a near degeneracy of the 6p-2h and 8p-4h intrinsic states.

Shell model diagonalizations in the $(fp)^n$ space give the first excited state in ^{46}Ti at 5.5 MeV and in ^{48}Ti at 4.34 MeV (in these calculations one particle was allowed to be excited from the $f_{7/2}$ shell). These energies are somewhat higher than the observed energies but not so much higher that we can say unequivocally that the states in

TABLE IV. Intrinsic state energies and deformation parameters of excited states in the calcium isotopes with the SK III interaction and 11 major oscillator shells included.

Nucleus	Configuration	E (MeV)	β
^{42}Ca	ν^2 (ground)	−359.7	0.05
	$\pi^2\nu^2-\pi^{-2}$	−353.9	0.24
	$\pi^2\nu^4-\pi^{-2}\nu^{-2}$	−351.8	0.36
	$\pi^4\nu^4-\pi^{-4}\nu^{-2}$	−352.0	0.48
^{44}Ca	ν^4 (ground)	−379.6	0.09
	$\pi^2\nu^4-\pi^{-2}$	−375.7	0.29
	$\pi^4\nu^4-\pi^{-4}$	−371.9	0.40
	$\pi^2\nu^6-\pi^{-2}\nu^{-2}$	−368.7	0.34
	$\pi^4\nu^6-\pi^{-4}\nu^{-2}$	−368.8	0.45
^{46}Ca	ν^6 (ground)	−398.6	0.08
	$\pi^2\nu^6-\pi^{-2}$	−393.0	0.26
	$\pi^4\nu^6-\pi^{-4}$	−389.0	0.38
^{48}Ca	ν^8 (ground)	−417.1	0.01
	$\pi^2\nu^8-\pi^{-2}$	−406.6	0.17

TABLE V. Intrinsic state energies and deformation parameters of excited states in the titanium isotopes with the SK III interaction and 11 major oscillator shells included.

Nucleus	Configuration	E (MeV)	β
^{44}Ti	$\pi^2\nu^2$ (ground)	−370.8	0.17
	$\pi^4\nu^2-\pi^{-2}$	−364.8	0.29
	$\pi^4\nu^4-\pi^{-2}\nu^{-2}$	−365.2	0.41
^{46}Ti	$\pi^2\nu^4$ (ground)	−395.1	0.21
	$\pi^4\nu^4-\pi^{-2}$	−391.2	0.33
^{48}Ti	$\pi^2\nu^6$ (ground)	−416.3	0.19
	$\pi^4\nu^6-\pi^{-2}$	−411.8	0.30
^{50}Ti	$\pi^2\nu^8$ (ground)	−436.1	0.09
	$\pi^4\nu^8-\pi^{-2}$	−426.8	0.22

^{46}Ti and ^{48}Ti are deformed states. However, it is quite possible that they are, or at least that these states are mixtures of $(fp)^n$ and deformed states, especially two proton excitation states.

Lawson[35] was the first one to suggest that the 0_2^+ state at 3.00 MeV in ^{48}Ti was indeed a deformed state. The calculations done here support this. However, this 0^+ state decays strongly to the 2_1^+ state with a $B(E2)$ of 17 W.u. (Weisskof unit). [It should be remembered though that $B(E2)$ $0^+ \rightarrow 2^+$ is five times bigger than the reverse process $B(E2)$ $2^+ \rightarrow 0^+$.] A pure $(fp)^{10}(sd)_\pi^{-2}$ state could not decay to a pure $(fp)^8$ state. At this time the issue is unresolved. Perhaps the deformed and $(fp)^8$ configurations are strongly admixed via a residual interaction.

PROJECTION AND PAIRING

We have thus far calculated the intrinsic state energies. In order to make comparison with experiment it is necessary to project out states of good angular momentum. It is also well known that pairing correlations can be important for the many-particle–many-hole states, even though they are not expected to contribute significantly to the closed shell ground state.

In this work we limit ourselves to $J=0^+$ states. In the context of projected Hartree-Fock theory, Villars[36] derived a formula for the energy of the $J=0$ projected state:

$$E(0^+)=\langle \phi_0 H \phi_0 \rangle - \langle \phi_0 H J_\perp^2 \phi_0 \rangle_L / \langle J_\perp^2 \rangle ,$$

where $J_\perp^2 = J_x^2 + J_y^2$ with $J_x = \Sigma j_x(i)$ and ϕ_0 is the relevant np-nh state, i.e., the state which is the Slater determinant emerging from a Hartree-Fock calculation with the Hamiltonian H. The "Villars intrinsic state" $\tilde{\phi}_0$ is the solution of the Hamiltonian of nonrotational motion $\tilde{H}$, which is given by (see page 17 of Ref. 36) $\tilde{H} = H - J^2/(2I)$ with I the moment of inertia. The state $\tilde{\phi}_0$ should not be confused with the state that we call ϕ_0.

In the projected Hartree-Fock approximation the moment of inertia in the Villars formalism[36] is given by

$$\hbar^2/2I_{PHF} = \langle \phi_0 H J_\perp^2 \phi_0 \rangle_L / \langle J_\perp^2 \rangle^2 .$$

For more information we refer the reader to a recent review by Moya de Guerra.[37]

In this work however, we use the cranking model:

$$E_{J=0} - E^{\rm intr} = -\hbar^2 \langle J_\perp^2 \rangle / 2I_{\rm cr} ,$$

where the moment of inertia $I_{\rm cr}$ is calculated using the cranking formula[38–40]

$$I_{\rm cr} = \Sigma'_{kl} \, | \langle k \, | j_+ | \, l \rangle^2 / (E_k + E_l)(u_k v_l - u_l v_k)^2 + \tfrac{1}{2} \Sigma''_{kl} \, | \langle k \, | j_+ | \, \bar{l} \rangle \, |^2 / (E_k + E_l)(u_k v_l - u_l v_k)^2 ,$$

where Σ' corresponds to a sum over all Hartree-Fock orbitals with a J_z component $k>0$ while Σ'' runs only over those orbits having $k=\frac{1}{2}$. In the above the E_k are the quasiparticle energies given by $E_k = [(\epsilon_k - \lambda)^2 + \Delta^2]^{1/2}$, with ϵ_k the single-particle Hartree-Fock eigenvalues. The quantity v_k^2 is the probability that a state is occupied:

$$v_k^2 = 1 - u_k^2 = \tfrac{1}{2}[1 - (\epsilon_k - \lambda)/E_k] ,$$

and where Δ, the pairing gap, is given by $\Delta = G \Sigma_k u_k v_k$ with G the strength of the pairing interaction.

Note that we can obtain $\langle J_\perp^2 \rangle$ by using the preceding expression without the energy denominators. By setting $u=1$ for states above the Fermi surface and $u=0$ for states below, we obtain the results for the projection without pairing.

In Table VI we present the results for the excitations of selected $J=0^+$ states, where the interaction SK III was used to generate the intrinsic state. We see that both the pairing correlations and the projection lower the energies of the $J=0^+$ states and bring the results into remarkable good agreement with experiment.

We see from this table that the stronger the deformation the more one gains in energy from projection. On the other hand, as a compensation one gains less energy from pairing. This is evident in comparing the results for 4p-4h and 8p-8h in ^{40}Ca. For nonclosed shell nuclei, e.g., ^{42}Ca, one must remember that not only the deformed state but also the ground state gains binding energy from pairing. Thus, in ^{42}Ca the *excitation energy* is raised because of pairing.

TABLE VI. The excitation energies of selected $J=0^+$ many-particle–many-hole states, where the SK III interaction is used, and where pairing correlations and projection have been taken into account and 11 major oscillator shells are included.

Nucleus	Configuration	Energy gain pairing (MeV)	Energy gain projection (MeV)	Final excitation energy (MeV)
^{4}He	4p-4h		−7.0	19.7
^{16}O	4p-4h	−1.1	−5.5	8.9
^{40}Ca	4p-4h	−3.0	−3.8	5.3
	8p-8h	−0.5	−4.3	6.6
^{42}Ca	2*p*	−4.0		
	4p-2h	−3.5	−3.1	3.2
^{44}Ca	4*p*	−2.8		
	6p-2h	−2.2	−2.3	2.2

DEPENDENCE OF THE RESULTS ON THE INPUT PARAMETERS

The axially symmetric deformed oscillator basis states are well discussed by Vautherin.[30] Some input parameters in the program are N_0, B_0, and Q such that (N_0+1) is equal to the number of major shells, and in terms of the harmonic oscillator frequencies $\omega_\perp$ and ω_z and $\omega_0=(\omega_\perp^2\omega_z)^{1/3}$, we have $B_0=(m\omega_0/\hbar)^{1/2}$ and $Q=\omega_\perp/\omega_z$. Note that B_0 is the reciprocal of the oscillator length parameter b_0, and that as a crude approximation $Q\approx(1+\beta_0)$ where β_0 is the deformation parameter described in the text.

Obviously we will obtain better results, i.e., obtain greater binding energies, if we increase the number of major shells (N_0+1) and if we choose the input parameters B_0 and Q so as to produce as close as possible the correct radius and quadrupole moment of the nucleus in question. In order to determine Q we run the code twice for each configuration. In the first run a guess was made for Q, then the program yielded an output deformation β_0. In the next run the value of Q was taken to be $(1+\beta_0)$.

In Table VII we show the dependence on N_0 of the energy for the ground state, 4p-4h state, and 8p-8h state in ^{40}Ca. An important point to notice is that the difference in energies of the np-nh and 0p-0h states converge faster than the absolute energies. For example, in going from $(N_0+1)=11$ to 13, the absolute change in energy of 0p-0h state is -0.36 MeV; but the excitation energy of 4p-4h state changes from 12.07 to 12.15 MeV and that of 8p-8h from 11.36 to 11.35 MeV.

In Table VIII we show the dependence on B_0. Note that for 4p-4h and 8p-8h the middle value $B_0=0.54$ (fm^{-1}), which is used for Table III, yields a lower energy than the two other values $B_0=0.50$ and 0.60. For the ground state the best result is obtained for the largest value, $B_0=0.60$. This is not surprising because Liu *et al.*[26,28] have previously shown using the deformed oscillator model that the value of the oscillator length parameter $b=(b_xb_yb_z)^{1/3}$ is larger for the 4p-4h state than the corresponding length parameter b_0 for the ground state.

CLOSING REMARKS

The most striking feature to emerge from our Skyrme-Hartree-Fock studies of many-particle–many-hole deformed states is the occurrence of near degeneracies of mean intrinsic state energies of many of these states even though the deformations are different. In the future we should try to study more deeply why these degeneracies occur. Are they due to some dynamical symmetry of our effective interaction which we have not get uncovered?

It should be pointed out that the degeneracy becomes more exact as the calculations get better and better. For example, if we approximate the Hartree-Fock wave functions by deformed oscillator wave functions the near degeneracy is not realized as well. This is because the more deformed the state, and the more particle-holes that are involved, the more major shells are required to adequately describe such states. Thus, for example, in the deformed oscillator model the 4p-4h and 8p-8h states in ^{40}Ca would occur at much higher energies than in better calculations in which many major shells are involved. On the other hand, for the 2p-2h state the difference would not be so large.

Also, to get the degeneracy we must use the full Skyrme interaction. For example, if we set the spin-orbit interaction equal to zero the 8p-8h state in ^{40}Ca would be much higher than the 4p-4h state. The spin-orbit interaction plays an important role, along with the other parts of the Skyrme interaction, in *establishing* the degeneracy.

We have found that the odd parity excitations are nearly degenerate with even ones. It appears that we have a near condensate in the sense that for a certain range of n in ^{40}Ca we can add particle-hole excitations to the system (these can perhaps be represented as bosons) without any additional cost in energy, although the deformation of the system progressively increases.

We do not see why in a given diagonalization any of the nearly degenerate states should be excluded. For example, for even parity states in ^{40}Ca one should include 0p-0h, 2p-2h, 4p-4h, 6p-6h, and 8p-8h in a diagonalization. Perhaps an excited state in which all these configurations are strongly admixed is more aptly described as a large *amplitude vibration* rather than a state of fixed deformation.

We should also comment upon the fact that when projection and pairing are included the excitation energies of the deformed states come reasonably low in energy so as to be readily associated with low-lying excitations of the physical spectrum. The results with SK III are certainly encouraging.

In this work our objective was not to get an impressive fit to experiment, but rather, to follow the logical consequences of a predetermined model—Skyrme-Hartree-Fock. Of course there is some phenomenology involved in this model in the sense that the parameters are chosen to fit ground-state properties such as binding energies and radii. The parameters however, were never adjusted to fit

TABLE VII. The dependence of the np-nh state energies (in MeV) of ^{40}Ca on the number of major shells (N_0+1) using the SK III interaction with $B_0=0.54$ (fm^{-1}).

State	$N_0=8$	$N_0=10$	$N_0=12$
0p-0h	−340.53	−341.26	−341.60
4p-4h	−327.51	−329.19	−329.45
8p-8h	−327.92	−329.90	−330.25

TABLE VIII. The dependence of the np-nh state energies (in MeV) of ^{40}Ca on the oscillator parameter B_0 (in fm^{-1}) using the SK III interaction and with 11 major shells.

State	$B_0=0.50$	$B_0=0.54$	$B_0=0.60$
0p-0h	−340.87	−341.26	−341.42
4p-4h	−328.76	−329.19	−328.92
8p-8h	−329.34	−329.90	−329.63

the properties of many-particle–many-hole states considered here. However, it is the mark of a good model or theory to go beyond what was originally intended. In that sense the Skyrme-Hartree-Fock model is a good model.

In the near future we must focus more strongly on the deviations between the theoretical results obtained here and the combination of experiment and phenomenology espoused by Fortune and his collaborators.[13–15] They have developed a picture of deformed states which certainly hangs together very well, but which requires a simple direct interaction interpretation of multiparticle transfer reactions. They identified several many-particle—many-hole states and do not seem to require as high a degree of degeneracy as we obtain in our calculation (although the basically 4p-4h and 8p-8h states in ^{40}Ca are not that far apart). From the theoretical point of view we should consider whether nuclear correlations beyond Hartree-Fock might be important. For example, in the simpler problem of the low-lying 1p-1h octupole states found in almost all nuclei, it is known that the inclusion of a phonon exchange between the particle and the hole is a vital mechanism for preventing an octupole collapse in nuclei.[41] Perhaps this mechanism is also important when we have several particles and several holes. It would also be of interest to make connections with recent theoretical approaches such as those of Bertsch, Barranco, and Broglia[42] concerning how nuclei change shape. It would also be useful to make a closer connection to the Strutinsky methods.[11]

Let us close by noting that the calculations done here lend strong support to the highly intuitive ideas of early workers in this field, and indeed make their contributions seem all the more remarkable. Our work suggests that there may be more surprises ahead and that future confrontation between theory and experiment should prove to be very stimulating.

ACKNOWLEDGMENTS

This work is supported by a grant from the U.S. Department of Energy under Contract No. DE-FG05-86ER40299. One of us (D.B.) also acknowledges support from the nuclear experimental group via the U.S. National Science Foundation and Rutgers University, especially Allen Robbins and Noemie Koller. We thank George Bertsch and Elvira Moya de Guerra for useful comments. We are grateful to Michael Vallieres and Donald Sprung for the Hartree-Fock codes used in this work.

[1]T. H. R. Skyrme, Philos. Mag. **1**, 1043 (1956); Nucl. Phys. **9**, 615 (1959).
[2]D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972).
[3]H. Morinaga, Phys. Rev. **101**, 254 (1956); Phys. Lett. **21**, 78 (1966).
[4]I. Talmi and I. Unna, Nucl. Phys. **30**, 280 (1962).
[5]T. Engeland, Nucl. Phys. **72**, 68 (1965).
[6]G. E. Brown and A. M. Green, Phys. Lett. **15**, 168 (1965).
[7]G. E. Brown and A. M. Green, Nucl. Phys. **75**, 401 (1966).
[8]W. J. Gerace and A. M. Green, Nucl. Phys. **93**, 110 (1967).
[9]S. G. Nilsson, Dan. Mat. Fys. **29**, No. 16, 1 (1955).
[10]W. J. Gerace and A. M. Green, Nucl. Phys. **A123**, 241 (1969).
[11]V. M. Strutinsky, Nucl. Phys. **A95**, 420 (1967); **A122**, 1 (1968).
[12]V. Metag, R. Repnow, P. Von Brentano, F. Dickmann, and K. Dietrich, Phys. Lett. **34B**, 257 (1971).
[13]R. Middleton, J. D. Garrett, and H. T. Fortune, Phys. Lett. **39B**, 339 (1972).
[14]H. T. Fortune, R. R. Betts, J. N. Bishop, M. N. I. Al-Jadir, and R. Middleton, Phys. Lett. **55B**, 439 (1975).
[15]H. T. Fortune, M. N. I. Al-Jadir, R. R. Betts, J. N. Bishop, and R. Middleton, Phys. Rev. C **19**, 756 (1979).
[16]R. K. Bansal and J. B. French, Phys. Lett. **11**, 145 (1964).
[17]L. Zamick, Phys. Lett. **19**, 580 (1965).
[18]A. Arima, H. Horiuchi, and T. Sebe, Phys. Lett. **24B**, 129 (1967).
[19]A. P. Zuker, B. Buck, and J. B. McGrory, Phys. Rev. Lett. **21**, 39 (1968).
[20]P. J. Ellis and T. Engeland, Nucl. Phys. **A144**, 161 (1970).
[21]W. H. Bassichis and G. Ripka, Phys. Lett. **15**, 320 (1965).
[22]I. Kelson, Phys. Lett. **16**, 143 (1965).
[23]G. J. Stephenson, Jr. and M. K. Banerjee, Phys. Lett. **24B**, 209 (1967).
[24]S. Das Gupta and N. de Takacsy, Phys. Rev. Lett. **22**, 1969 (1964).
[25]E. Boeker, Nucl. Phys. **91**, 27 (1967).
[26]H. Liu and L. Zamick, Phys. Rev. C **29**, 1040 (1984).
[27]D. Auverlot, P. Bonche, H. Flocard, and P. H. Heenen, Phys. Lett. **149B**, 6 (1984).
[28]H. Liu, L. Zamick, and H. Jaqaman, Phys. Rev. C **31**, 2251 (1985).
[29]J. Carvalho, M. Vassanji, and D. J. Rowe, Nucl. Phys. **A465**, 265 (1987).
[30]D. Vautherin, Phys. Rev. C **7**, 296 (1973).
[31]M. Brack, Phys. Lett. **71B**, 239 (1977).
[32]D. W. L. Sprung and M. Vallieres, Can. J. Phys. **59**, 177 (1981).
[33]M. Beiner, H. Flocard, N. Van Giai, and P. Quentin, Nucl. Phys. **A238**, 29 (1975).
[34]A. Arima, V. Gillet, and J. Ginocchio, Phys. Rev. Lett. **25**, 1043 (1970).
[35]R. D. Lawson, Nucl. Phys. **A173**, 17 (1971).
[36]F. Villars, in *Nuclear Physics,* Proceedings of the International School of Physics "Enrico Fermi," Course XXXVI, Varenna, 1966, edited by C. Bloch (Academic, New York, 1966).
[37]E. Moya de Guerra, Phys. Rep. C **138**, 293 (1986).
[38]S. G. Nilsson and O. Prior, Mat.-Fys. Medd. Dan Vidensk. Selsk. **32**, No. 16 (1960).
[39]O. Prior, F. Boehm, and S. G. Nilsson, Nucl. Phys. **A110**, 257 (1968).
[40]D. W. L. Sprung, S. G. Lie, M. Vallieres, and P. Quentin, Nucl. Phys. **A326**, 37 (1979).
[41]J. Blomqvist and T. T. S. Kuo, Phys. Lett. **29B**, 544 (1969).
[42]G. Bertsch, F. Barranco, and R. A. Broglia, in *Windsurfing the Fermi Sea,* edited by T. T. S. Kuo and J. Speth (Elsevier Science, New York, 1987), Vol. 1.