Many-particle many-hole states near the magic number 20: deformed and superdeformed states

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Abstract

Many-particle many-hole states near the magic number 20 have been investigated in the relativistic mean field formalism using the fixed configuration method. Neutron particle-hole states in neutron-rich nuclei with $N \sim 20$, i.e. $^{30,32,34}$Mg, and $^{28,30}$Ne are studied to find out the ground state configuration. The ground state of $^{32}$Ne, Mg as well as possibly $^{34}$Mg comes out actually as particle-hole states. Proton-neutron excitation across the shell gap at 20 in nuclei with $N = Z$, i.e. $^{32}$S, $^{36}$Ar, $^{40}$Ca and $^{44}$Ti is investigated as possible origins of superdeformed configuration. Observed superdeformed bands in $^{36}$Ar and $^{40}$Ca can be described as many-particle many-hole states.

1 Introduction

One of the most interesting topics in recent years in the study of low energy structure of light nuclei is the existence of highly deformed states in near-closed shell nuclei at relatively low excitation energy. Superdeformed (SD) bands have been observed in light $N = Z$ nuclei $^{36}$Ar\cite{1,2} and $^{40}$Ca\cite{3,4} as well as in $^{38}$Ar\cite{5} with the band heads situated around 5 MeV excitation energy. Studies on $^{32}$Mg and the neighbouring neutron rich nuclei with $N \sim 20$ showed very large B(E2) values for the $2_+^+ \rightarrow 0_+^+$ transition indicating a large quadrupole deformation $\beta_2$. The existence of highly deformed solutions near the magic number 20 is now understood to be a result of many-particle many-hole excitation across the shell gap.
From the spherical shell model perspective, particles are promoted from the \( sd \) shell to the \( f_{7/2} \) orbital across the shell gap at \( N, Z = 20 \). When the prolate deformation is large, the oblate deformation driving last orbitals of the \( sd \) shell are higher in energy than the low \( \Omega \) orbitals coming from the \( f_{7/2} \) orbital. Thus a state may be formed with a large prolate deformation at a relatively low excitation energy by filling up the single particle levels from below.

In neutron rich nuclei around \( ^{32}\text{Mg} \), a pair of neutrons may be excited across the \( N = 20 \) shell gap resulting in the \( 2\hbar \omega \) configurations. In \( Z = 10 - 12 \) and \( N = 19 - 22 \) nuclei, recent shell model calculations \cite{10,11,12,13} predict these \( 2\hbar \omega \) states to lie energetically below the normal \( 0\hbar \omega \) states. In the Nilsson model picture, the shell gap vanishes at large deformation for neutrons. This so called 'island of inversion' where the \( 2\hbar \omega \) states lie below the normal states have been extensively investigated both theoretically and experimentally. Different mean field calculations \cite{14,15,16,17} differ in their predictions for the ground state configurations of different nuclei in this region. There is considerable disagreement among the different calculations regarding the boundary of the island of inversion. Another area where the calculations do not agree is whether the neutron and proton distributions are identical in these nuclei. Pritychenko \textit{et al.} have measured the transition probabilities \( B(E2; 0^+_1 \rightarrow 2^+_1) \) in the nuclei \( ^{26,28}\text{Ne} \) and \( ^{30,32,34}\text{Mg} \) to study the role of these intruder configurations in an effort to determine the boundary. They conclude that the ground state of the nuclei \( ^{26}\text{Ne} \) and \( ^{30}\text{Mg} \) are well understood in terms of normal \( 0\hbar \omega \) configurations. On the other hand Chisté \textit{et al.} have performed inelastic scattering experiment to measure the charge and mass deformation of \( ^{30,32}\text{Mg} \). They conclude that both the isotopes show similar type of structure involving \( 2\hbar \omega \) configurations and there is no significant difference between the proton and the neutron distributions.

The SD band \cite{3,4} in \( ^{40}\text{Ca} \) is based on the \( J^x = 0^+ \) state at 5.21 MeV. In \( ^{40}\text{Ca} \), low lying states with large collectivity have been explained in terms of neutron-proton excitation across the shell gap at \( N, Z = 20 \). Fortune \textit{et al.} \cite{18,19} have suggested the dominant configurations of the \( J^x = 0^+ \) states at 0 MeV, 3.35 MeV and 5.21 MeV to be \( 0p - 0h \), \( 4p - 4h \) and \( 8p - 8h \), respectively. A full shell model calculation involving both the \( sd \) shell and the \( fp \) shell is still beyond the present day capabilities. A recent truncated shell model calculation \cite{20} has confirmed that the SD band in \( ^{40}\text{Ca} \) is indeed based on \( 8p - 8h \) configuration. Cranked Hartree-Fock-BCS method has been applied by Bender \textit{et al.} to study the ND and SD states in \( ^{32,36,38}\text{Ar} \) and \( ^{40}\text{Ca} \). In Ref. \cite{3} cranked relativistic mean field theory without pairing was applied to study the highly deformed states in \( ^{40}\text{Ca} \). Zheng \textit{et al.} \cite{22,23} have performed fixed configuration deformed Hartree-Fock calculation to study the deformed states in a number of nuclei including \( ^{40}\text{Ca} \) and \( ^{44}\text{Ti} \). The origin of the SD band is predicted to be an \( 8p - 8h \) configuration in all the theoretical investigations. Configuration dependent cranked Nilsson-Strutinsky and truncated shell model calculations were performed \cite{1} in highly deformed states in \( ^{36}\text{Ar} \). All calculations agree that in \( ^{36}\text{Ar} \), these states are expected to be based on \( 4p - 8h \) configuration coming from the excitation
of two protons and two neutrons across the shell gap.

The aim of the present work is to study these large deformation multiparticle-hole states. We have applied the fixed configuration deformed mean field approach, a method applied earlier in this mass region by Zheng et al. [22, 23] using a Skyrme Hartree Fock model. We propose to use the same method using deformed Relativistic Mean Field (RMF) approach. This approach has been very successful in describing various features of nuclear structure. Ground state properties like binding energy, deformation, magnetic moment, isotopic shift and nuclear radius has been calculated with considerable accuracy [24]. It has also succeeded in describing excited states like normal deformed (ND) and SD bands, giant dipole resonances, etc. One of the prominent successes of RMF is the reproduction of the spin-orbit splitting naturally. It has been observed in [22] that the spin-orbit interaction plays a major role in the calculation for the excited states. The RMF approach naturally accommodates a correct spin-orbit interaction and thus, is expected to give a good description of the multiparticle-hole states. We have not come across any RMF calculation using the fixed configuration approach.

2 Calculation

Relativistic Mean Field theory is well known and has been described in detail elsewhere [24]. We have employed the force NL3 [25] which was obtained by fitting the binding energy, charge radii and neutron radii of a number of spherical singly and doubly closed nuclei. This was explicitly designed for treatment of variation in isospin and has proved to be very useful in describing the ground state properties throughout the periodic table. Some of the nuclei studied in the present work, e.g. $^{32,34}$Mg and $^{36}$Ne are away from the stability valley and should be well described using the force NL3. We assume axial symmetry and reflection symmetry and work using deformed harmonic oscillator basis. The method of calculation described in Refs. [26, 27] has been followed. Throughout this work, 12 Fermion and Boson shells have been used for the calculation. The quadrupole charge deformation parameter $\beta_C$ is obtained from the intrinsic charge quadrupole moment $Q_0$ using the prescription

$$Q_0 = \sqrt{\frac{16\pi}{5}} \frac{3}{4\pi} Z R_0^2 \beta_C$$  \hspace{1cm} (1)

where $R_0 = 1.2A^{1/3}$, $A$ being the mass number. The mass deformation parameter $\beta_A$ can be similarly defined.

The fixed configuration calculation is essentially very simple. The states studied in the present calculation are particle-hole states only in the sense of the spherical shell model. As already explained, at large deformation, the levels coming from the higher $fp$ shell cross the upper levels of the $sd$ shell giving rise to the configuration of these states. The level sequence obtained from Nilsson-like diagrams are used to construct solutions with large deformation. For example, in Fig. 1, the single particle neutron orbitals in $^{40}$Ca are plotted as a function of the quadrupole
deformation parameter $\beta_C$. Single particle proton orbitals also show a similar kind of structure. The orbits are identified by the asymptotic quantum number $\Omega^\pi [Nn \Lambda]$ at large deformation and by $L_J$ at zero deformation. For $N=20$, there are two crossings. The first one is around $\beta_C = 0.3$ between the $3/2^+ [202]$ orbit and the $1/2^- [330]$ orbit. The second crossing is at $\beta_C \sim 0.6$ between the $1/2^+ [200]$ orbit and $3/2^- [321]$ orbit. In the fixed configuration approach, to obtain the $4p - 4h$ solution, the $3/2^+ [202]$ orbits are kept empty and the $1/2^- [330]$ orbits are kept filled for both types of nucleons. The relativistic Hartree equations are then solved iteratively to obtain the binding energy and the deformation self-consistently. The resulting solution is expected to have a deformation beyond 0.3. Similarly, the $8p - 8h$ solution obtained by further keeping the $1/2^+ [200]$ orbits empty and the $3/2^- [321]$ orbits filled are expected to have a deformation beyond 0.6. The Hartree-BCS equations are then self-consistently solved to obtain the lowest energy solution. The solutions obtained in this way are of course intrinsic solutions, i.e. they contain contributions from all possible $J$ values in the band. We are principally interested in the $J^\pi = 0^+$ state, i.e. the band head of the $K=0$ bands. To obtain the energy of the $0^+$ state we have used the cranking model formula

$$E(0^+) = E_{in} - \frac{<J^2_\perp>}{2I_{cr}}$$

where the moment of inertia $I_{cr}$ is calculated using the cranking model formula \[28\] and $J^2 = J^2_x + J^2_y$. Here, $E_{in}$ refers to the energy of the intrinsic solution. This is a very important correction as at a large deformation, it can be quite large while being zero for spherical configurations. For example, angular momentum projection in HF calculation in the superdeformed minimum of $^{40}\text{Ca}$ lowers the bandhead by 4 MeV \[21\].

Pairing has been included in our calculation in the form of BCS method in the constant gap approach. We have taken both the proton and the neutron gaps to be equal to 1.0 MeV except for the closed shell configurations. In the light nuclei studied, the pairing energy is quite small. We have verified that our essential conclusions remain unaltered for reasonable variation of the gap parameters.

3 Results

We first present our results for neutron excitation across the $N = 20$ shell gap in a number of neutron rich nuclei near $^{32}\text{Mg}$. Next we discuss the proton-neutron excitation across the shell gap $N = Z = 20$ in the $N = Z$ nuclei, $^{32}\text{S}$, $^{36}\text{Ar}$, $^{40}\text{Ca}$ and $^{44}\text{Ti}$. We present the results of our calculation in Table I. Here $E(0^+)$ refers to the energy of the $0^+$ state belonging to the particular configuration and $\beta_C$ and $\beta_A$ refer to charge and mass quadrupole deformation parameters, respectively.

The nucleus $^{32}\text{Mg}$ has $N = 20$ and $Z = 12$. In general, a ground state calculation without particle-hole excitation predicts the ground state to be spherical. This has been observed in earlier relativistic calculations also \[12\] \[17\]. In particular, although the deformation of a number of
light nuclei was calculated \cite{17, 29} with some degree of accuracy in the relativistic hybrid derivative coupling model, the ground state of $^{32}$Mg is still found to be spherical in this model. In the present calculation, we find that the spherical minimum has a binding energy 250.97 MeV. Next we study the $2p - 2h$ neutron excitation across the magic number 20. This corresponds to two holes in the $\nu 3/2^+ [202]$ state and two particles in the $\nu 1/2^- [330]$ state. The intrinsic solution has the binding energy 248.93 MeV. After the correction due to angular momentum, the binding energy of the deformed $2p2h$ 0$^+$ state comes out to be 252.50 MeV. Thus the $\nu^2 - \nu^{-2}$ state becomes the actual ground state. The experimentally measured binding energy is 249.69 MeV \cite{30}. The charge and the mass quadrupole deformation parameters come out to be 0.457 and 0.492, respectively. The different experimental measurements on charge deformation parameters give the observed values $\beta C = 0.512 \pm 0.044$ \cite{9} in intermediate energy Coulomb excitation and $\beta C = 0.61 \pm 0.04$ from inelastic scattering experiment \cite{8}. From the results of another Coulomb excitation study \cite{7}, a slightly lower value of $\beta C = 0.438 \pm 0.046$ can be derived. Thus the experimentally measured values are reasonably close to the theoretical result. The proton and the neutron distributions come out to be similar. This is in agreement with the measurements of Chisté et al. \cite{8} who have found no hint of any large decoupling between the proton and the neutron distribution. Our result also agrees with shell model calculations \cite{11, 13} as well as HFB results \cite{15}. In contrast, another HFB calculation \cite{14} predict the ground state to be spherical, i.e. of normal configuration. We have also examined the $\nu^4 - \nu^{-4}$ excitation but could not obtain any converged self-consistent solution.

We have studied a few nearby even-even nuclei in the present formalism to find out the boundary of the island of inversion. In $^{30}$Mg, the ground state turns out to be a $0h\omega$ state with no $p - h$ excitation. The binding energy of the ground state is calculated to be 243.66 MeV. The experimentally measured binding energy is 241.63 MeV \cite{30}. The $\nu^2 - \nu^{-4}$ state is obtained by exciting two neutrons from the $\nu 1/2^+ [200]$ orbital to the $\nu 1/2^- [330]$ orbital across the $N = 20$ gap. The binding energy of the $2p4h$ $0^+$ state comes out to be 242.17 MeV, approximately 1.5 MeV above the ground state. The calculated charge and mass deformation values are 0.522 and 0.601, respectively. Inelastic scattering gives the experimental value $\beta C = 0.52 \pm 0.04$ \cite{8}. Coulomb excitation experiment gives a somewhat lower value $\beta C = 0.43 \pm 0.19$ \cite{7}. As already mentioned, Pritychenko et al. \cite{7} have suggested that the ground state of $^{30}$Mg to be a $0h\omega$ state while Chisté et al. \cite{8} have concluded it to be a $2h\omega$ state. The energy systematics observed in our calculation seem to support the former alternative although a configuration mixing calculation is required to reach a definite conclusion.

In $^{34}$Mg, the two solutions corresponding to the $0h\omega$ and $2h\omega$ configurations come out to be very close in energy. The latter configurations has two holes in the $\nu 3/2^+ [202]$ orbital and two particles in the $\nu 1/2^- [330]$ and $\nu 3/2^- [321]$ orbitals each. The $0h\omega$ state has binding energy 260.48 MeV and the charge (mass) deformation values 0.345 (0.327). The binding energy for the $2h\omega$ state is 260.42 MeV and the $\beta C$ and $\beta A$ values are 0.511 and 0.562, respectively. Coulomb excitation experiment provides
a upper bound for the charge deformation $\beta_C < 0.599$ [17]. The experimental ground state binding energy is 256.59 MeV [30]. A more accurate treatment, particularly of the pairing correlation, may show that the $2h\omega$ configuration is actually the ground state.

In $^{30}$Ne, the $0h\omega$ solution turns out to be spherical with the binding energy 215.93 MeV. The $2h\omega$ $0^+$ state has the binding energy 216.62 MeV, making it the ground state. The experimental binding energy is 256.59 MeV [30]. A more accurate treatment, particularly of the pairing correlation, may show that the $2h\omega$ configuration is actually the ground state.

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Among the $N = Z$ nuclei, we start with the doubly magic nucleus $^{40}$Ca. The binding energy of the ground state is calculated to be 341.92 MeV, in good agreement with the experimental value 342.05 MeV. The ground state is spherical. A number of $np - nh$ states has been studied in $^{40}$Ca under the SkHF formalism [22]. They observed that for $n = 2$ to 8, although $\beta$ increases linearly with $n$, the solutions are nearly degenerate in energy. The $8p - 8h$ state has been identified with the SD band whose band head lies at 5.21 MeV excitation energy. The $4p - 4h$ state has been identified with the ND band whose band head lies at 3.35 excitation energy. However for some of the Skyrme parameterizations, the $0^+$ state of the ND band was found out to lie higher than that of the SD band in contradiction with experimental results.

In the present calculation, we have concentrated on the $4p - 4h$ excitation and the $8p - 8h$ excitation. The different configurations have been discussed earlier. In our calculation also, the ND band comes up very high in energy. In contrast, the excitation energy of the $0^+$ state of the $8p - 8h$ band comes out to be 5.86 MeV. The transition quadrupole moment values also show a similar trend. The ND band quadrupole moment is calculated to be 1.14 eb, large compared to the experimental value $Q_0 = 0.74 \pm 0.14$eb [4]. However, the SD band quadrupole moment comes out to be 1.89 eb, in excellent agreement with the experimental value $Q_0 = 1.89^{+0.30}_{-0.24}$eb [3]. In contrast, the cranked RMF calculation without pairing [5] predicts $Q_0$ to be 2.0 eb.

One of the problems in getting a good description of the ND band may be the near degeneracy of the $np - nh$ states for even $n$. This degeneracy was observed in the present calculation also. A proper calculation should take into consideration the mixing between all the $0^+$ states coming from the different $np - nh$ configurations. This may provide a more accurate description.

The ground state of the nucleus $^{36}$Ar turns out actually to be oblate. This is in agreement with the number and angular momentum projected HF calculation of Bender et al. [21]. The calculated binding energy is 306.36 MeV. In comparison, the experimental value is 306.72 MeV. For the $4p - 8h$ state, we remove two protons and two neutrons from the $3/2^+$ orbit and put them in the $1/2^-$ orbit. The energy of the excited $0^+$ state

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state after correction comes out to be 300.39 MeV. The excitation energy of the band head is thus 5.97 MeV. In comparison, this energy is calculated to be 5.90 MeV in Ref. [21]. The experimental value of the band head is at 4.33 MeV. The experimental transition quadrupole moment is $1.18 \pm 0.09$ eb [2]. The calculated intrinsic quadrupole moment is 1.37 eb.

We also study two other nuclei with $N = Z$, $^{32}$S and $^{44}$Ti where the SD band has not been observed. In $^{32}$S, the experimental binding energy of the ground state is 271.78 MeV. We tried to look for solutions with 12 holes in the $3/2^+ [202]$, $1/2^+ [200]$ and $5/2^+ [202]$ orbitals and 4 particles in the $1/2^- [330]$ orbitals. The excitation energy of the solution comes out to be 6.22 MeV and the deformation to be very high, $\beta \sim 1.0$. We could not get any converged self consistent solution for only proton or neutron excitation. In $^{44}$Ti, the experimental binding energy is 375.47 MeV while the calculated value comes out to be 372.48 MeV. We have obtained an $8p - 4h$ solution with the $3/2^+ [202]$ orbitals empty and the $1/2^- [330]$ and the $3/2^- [321]$ orbitals filled. The excitation energy of the corresponding band comes out to be 3.36 MeV and the charge deformation 0.530. In Ref. [22], the excitation energy of the $8p - 4h$ band is found to be 5.6 MeV and the deformation value $\beta = 0.41$.

4 Conclusions

We have observed that the nuclei $^{32}$Mg, $^{30}$Ne, and possibly $^{34}$Mg belong to the island of inversion. As for the nuclei $^{30}$Mg and $^{28}$Ne, both nuclei with $N = 18$, the ground states are predicted to be moderately deformed $0h\omega$ states while the $2h\omega$ states have very large deformation. Measurements indicate that the ground state in these two nuclei are actually strongly deformed. The present calculation is unable to describe the ground state properties of these nuclei. In all the strongly deformed systems, we find that the proton and the neutron distributions are not decoupled, in agreement with Chisté et al. [8].

In $^{40}$Ca and $^{36}$Ar, the SD band seems to be reasonably described in the present formalism. Particularly, the prediction of the intrinsic quadrupole moments is in excellent agreement with experimental measurements. However, in $^{40}$Ca, the normal deformed configuration comes too high in energy. A source of error in the excitation energy of the bandhead may be the neglect of configuration mixing in the particle-hole bands. Surprisingly, we find no indication of any SD minimum in $^{32}$S.

We have included pairing through BCS approximation. The nuclei in the island of inversion have very large neutron excess and are close to the drip line. A more accurate treatment should involve the Bogoliubov approach and possible coupling to the continuum as well as particle number and angular momentum projection.

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Table 1: Theoretical results obtained in the present calculation. See text for details. Configurations denoted normal are $0\hbar\omega$ solutions.

| Nucleus | Configuration | $E_{in}$ (MeV) | $J^2/\hbar^2$ | $I_{cr}/\hbar^2$ (MeV$^{-1}$) | $E.(0^+)$ (MeV) | $\beta_C$ | $\beta_A$ |
|---------|---------------|----------------|----------------|-----------------------------|----------------|-----------|-----------|
| $^{32}$Mg | normal        | -250.97        | -250.97        | 0.000                       | 0.000           |           |           |
|         | $\nu^2 - \nu^{-2}$ | -248.93        | 33.67          | 4.73                        | 252.50          | 0.457     | 0.492     |
| $^{30}$Mg | normal        | -240.68        | 10.95          | 1.84                        | -243.66         | 0.285     | 0.230     |
|         | $\nu^2 - \nu^{-4}$ | -237.75        | 36.93          | 4.18                        | -242.17         | 0.522     | 0.601     |
| $^{34}$Mg | normal        | -257.62        | 21.53          | 3.77                        | -260.48         | 0.345     | 0.327     |
|         | $\nu^4 - \nu^{-2}$ | -255.81        | 45.20          | 4.91                        | -260.42         | 0.511     | 0.562     |
| $^{30}$Ne | normal        | -215.93        | -215.93        | 0.000                       | 0.000           |           |           |
|         | $\nu^2 - \nu^{-2}$ | -213.06        | 27.62          | 3.88                        | -216.62         | 0.444     | 0.502     |
| $^{28}$Ne | normal        | -208.61        | 5.32           | 1.35                        | -210.57         | 0.202     | 0.162     |
|         | $\nu^2 - \nu^{-4}$ | -204.72        | 29.35          | 3.58                        | -208.82         | 0.499     | 0.619     |
| $^{40}$Ca | normal        | -341.92        | -341.92        | 0.000                       | 0.000           |           |           |
|         | $\nu^2\pi^2 - \nu^{-2}\pi^{-2}$ | -328.43        | 42.70          | 5.50                        | -332.31         | 0.449     | 0.442     |
|         | $\nu^4\pi^4 - \nu^{-4}\pi^{-4}$ | -329.80        | 70.29          | 5.61                        | -336.06         | 0.743     | 0.733     |
| $^{36}$Ar | normal        | -302.59        | 12.20          | 1.62                        | -306.36         | -0.204    | -0.201    |
|         | $\nu^2\pi^2 - \nu^{-4}\pi^{-4}$ | -295.25        | 47.65          | 4.64                        | -300.39         | 0.642     | 0.632     |
| $^{32}$S | normal        | -266.12        | 10.19          | 1.43                        | -269.68         | 0.240     | 0.236     |
|         | $\nu^2\pi^2 - \nu^{-6}\pi^{-6}$ | -256.45        | 64.52          | 4.60                        | -263.46         | 1.030     | 1.017     |
| $^{44}$Ti | normal        | -370.80        | 11.03          | 3.28                        | -372.48         | 0.135     | 0.133     |
|         | $\nu^4\pi^4 - \nu^{-2}\pi^{-2}$ | -364.45        | 60.40          | 6.46                        | -369.12         | 0.530     | 0.523     |
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Figure 1: The neutron single particle energy levels in $^{40}$Ca as a function of quadrupole deformation $\beta_C$. The levels are indicated by the spherical quantum numbers at zero deformation and the asymptotic quantum numbers at large deformation. Continuous (dashed) lines represent positive (negative) parity levels.
