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Skyrme interaction and spectra of light nuclei

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The original three-body term in the Skyrme interaction is replaced by a two-body explicit density dependent term to reproduce simultaneously the excited and ground states of nuclei. Care has been taken to remove the spin instability of the Hartree-Fock ground state in nuclear matter and also the antipairing nature of the interaction inherent in the original Skyrme interaction. The spin-isospin dependent parameter introduced in the density dependent term is determined from the average asymmetry ratio and asymmetry energy. The modified Skyrme force is used to calculate the low-lying states of ^{18}O, ^{18}F, ^{42}Ca, ^{42}Sc, and ^{16}O, ^{40}Ca. In the light of these calculations the relative importance of the different Skyrme variants is studied.

[NUCLEAR STRUCTURE Ground and excited state properties of nuclei with modified Skyrme interaction, spectra of ^{18}O, ^{18}F, ^{42}Ca, ^{42}Sc, ^{16}O, ^{40}Ca.]

I. INTRODUCTION

In recent years the Skyrme force has been extensively used for the study of nuclei. This interaction was first proposed by Skyrme[1] and later revived by Brink and Vautherin,[2] who used it in calculating ground state properties of doubly close nuclei in the framework of the Hartree-Fock (HF) model. Since then several[3,4] self-consistent HF calculations have been carried out to reproduce most of the ground state properties of both spherical and deformed nuclei. This interaction consists of a two-body momentum dependent zero-range part and a three-body zero-range part. The popularity of the interaction lies in its simplicity because it leads to a local HF energy density and hence the corresponding single-particle HF equation can be solved easily. Because of this simplicity, we[5,6] have been able to use this interaction for the study of high neutron-rich nuclei far from the valley of β stability and the study of polyneutron systems in HF model.

However, it has been observed[7,8] that the interaction is unable to reproduce the excited states of nuclei. Again,[8] the interaction has an antipairing property contrary to the usual pairing nature of the effective interaction. Furthermore, the calculation of random-phase approximation (RPA) states by Blaizot[7] reveals that the three-body force produces unstable spin-saturated ground states in nuclear matter and even-even nuclei. The same has also been pointed out by Chang[9] in his model study of spin-saturated ground states and by Backman *et al.*[10] in their calculation of Landau parameters for nuclear matter. The three-body term in the Skyrme interaction is found to be equivalent to a two-body density dependent term $(t_3/6)(1+P_\sigma)\times\rho[\frac{1}{2}(\vec{r}_1+\vec{r}_2)]\delta(\vec{r}_1-\vec{r}_2)$ in HF theory and it can easily be seen that this term vanishes in the case of like nucleons, i.e., proton-proton or neutron-neutron. However, the analysis of Kohler *et al.*[11] shows that the density dependent interaction for like nucleons may not be negligible.

In the present study we have attempted to remove the above discomfitures by modifying the effective interaction and to see how far we can explain simultaneously the properties of ground as well as excited states such as two-particle and particle-hole states. Krewald *et al.*[12] have modified the Skyrme interaction and have calculated the ground and particle-hole states in close-shell nuclei. They have not checked if two-particle spectra are reproduced. Sharp and Zamick have made an extensive study to see if the particle-hole and two-particle spectra could be simultaneously described by the Skyrme interaction and find that only particle-hole spectra could be reasonably well described. We have used the modified interaction for the calculation of low-lying states of ^{18}O,^{18}F, ^{42}Ca,^{42}Sc, and ^{16}O,^{40}Ca in a very simplified manner. In Sec. II we present the proposed modification along with the basis of redetermination of the parameters. Then the spin stability of the HF ground state of nuclear matter is studied. Section III is devoted to the study of the spectra of the above nuclei. In Sec. IV we calculate the parameters for the droplet model of nuclei and compare with those of Myers and Swiatecki.[13]

II. MODIFICATION OF THE SKYRME FORCE

It has been mentioned earlier that the three-body term of the Skyrme force gives rise to the spin instability and also mainly contributes to the antipairing nature of the force. Hence, as a first step we have chosen to replace the three-body term $t_3\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3)$ by a two-body density dependent term $t_3/6(1+x_3P_\sigma)\rho[\frac{1}{2}(\vec{r}_1+\vec{r}_2)]\delta(\vec{r}_1-\vec{r}_2)$. It may be recalled here that in HF theory the three-body term is equivalent to a two-body density dependent term $t_3/6(1+P_\sigma)\rho[\frac{1}{2}(\vec{r}_1+\vec{r}_2)]\times\delta(\vec{r}_1-\vec{r}_2)$. That is why we have chosen the above term so as not to disturb drastically the ground state properties of nuclei. The parameter x_3 is introduced in order to have density dependence among both like and unlike uncleons. The full interaction in a generalized form may be written as

$$V=t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2)+\frac{t_1}{2}[\vec{k}'^2\delta(\vec{r}_1-\vec{r}_2)+\delta(\vec{r}_1-\vec{r}_2)\vec{k}^2]$$
$$+t_2\vec{k}'\delta(\vec{r}_1-\vec{r}_2)\vec{k}+\frac{t_3}{6}(1+x_3P_\sigma)\rho^\alpha\left[\frac{\vec{r}_1+\vec{r}_2}{2}\right]\delta(\vec{r}_1-\vec{r}_2)+iW(\vec{\sigma}_1+\vec{\sigma}_2)\vec{k}'\delta(\vec{r}_1-\vec{r}_2)\vec{k}, \quad (1)$$

where $\vec{k}$ is the relative momentum operator $(\vec{\nabla}_1-\vec{\nabla}_2)/2i$ acting on the right and $\vec{k}'$ is the operator $-(\vec{\nabla}_1-\vec{\nabla}_2)/2i$ acting on the left. P_σ is the spin-exchange operator and σ's are the Pauli spin matrices. In order to keep our discussions and derivatons general, we have introduced the parameter α, which is the power of density in the density dependent term. Since the present parametrizations of the Skyrme force quite satisfactorily explain the ground state properties of nuclei, we have retained the values of the parameters t_0, t_1, t_2, t_3, and W. The remaining two parameters x_0 and x_3, which do not affect the ground state properties of $N=Z$ nuclei but affect the excited states, are determined from the following considerations.

(i) In our[5,14] study of exotic nuclear systems we observe that maximum asymmetry depends strongly upon the spin-isospin force parameters x_0 and x_3. Under the extreme condition of particle stability, the asymmetry ratio would be decided from the equation $e_q^f=0$, where e_q^f is the Fermi energy of either the proton or the neutron. Using nuclear matter approximations, the corresponding expression for neutron stability with interaction (1) can be written as[14]

$$e_n^f\equiv\frac{\hbar^2k_f{}^2}{2m}(1+\beta)^{2/3}+t_0\rho\left[\left[1+\frac{x_0}{2}\right]-(x_0+\tfrac{1}{2})\frac{(1+\beta)}{2}\right]$$
$$+\frac{t_1}{16}\rho k_f{}^2\{(3-\beta)(1+\beta)^{2/3}+\tfrac{3}{5}[(1+\beta)^{5/3}+2(1-\beta)^{5/3}]\}$$
$$+\frac{t_2}{16}\rho k_f{}^2\{(5+\beta)(1+\beta)^{2/3}+\tfrac{3}{5}[3(1+\beta)^{5/3}+2(1-\beta)^{5/3}]\}$$
$$+\frac{t_3}{12}\rho^{\alpha+1}\left\{(\alpha+2)(1+x_3/2)-(x_3+\tfrac{1}{2})\left[\frac{\alpha}{2}(1+\beta^2)+1+\beta\right]\right\}=0\ , \quad (2)$$

where k_f is the Fermi momentum and β is the asymmetry ratio, i.e., $\beta=(N-Z)/(N+Z)$. The value of this quantity both from theoretical calculations[5] and experimental derivations (Garvey-Kelson[15]) is found to be 0.3 on the average.

(ii) Secondly, it has been observed that these two parameters x_0 and x_3 do not affect the binding energy of $N=Z$ nuclei but affect $N\neq Z$ nuclei. The quantity which controls this aspect is given by asymmetry energy:

$$a_\tau=\frac{\hbar^2 k_f{}^2}{6m}-\frac{t_0\rho_0}{4}(\tfrac{1}{2}+x_0)-\frac{t_3}{24}(\tfrac{1}{2}+x_3)\rho_0^{\alpha+1}+\frac{t_2}{6}\rho k_f{}^2, \tag{3}$$

which has been used in determining the parameters.

(iii) Finally, the equation of state of pure neutron matter has been taken into account because of its connection with the study of high dense matter. In this regard we have taken that of Siemans and Pandharipande[16] as the guiding equation of state in order to find the two parameters as proposed by Lattimer and Ravenhall.[17] The quantity which controls the equation of state of pure neutron matter is the binding energy of pure neutron matter, for which the expression with Skyrme force can be written as

$$\frac{E}{N}=\frac{3\hbar^2}{10m}k_n^f+\frac{t_0}{4}(1-x_0)\rho_n+\tfrac{3}{40}(t_1+3t_2)\rho_n k_n^{f^2}+\frac{t_3}{24}\rho_n^{\alpha+1}(1-x_3). \tag{4}$$

Thus, the above three aspects have been taken into account so as to get the best fit for the two parameters x_0 and x_3. The values of these two parameters, along with the other parameters for different Skyrme forces, are given in Table I. Since S_{II} and S_{III} give comparatively better results for ground state properties of nuclei, we have chosen them only for reparametrizations. It has also been generally believed that fractional power of density such as $\rho^{1/3}$ is more appropriate. So we have chosen Kohler's parametrization in our study. Ground state properties that have been calculated with this interaction are found to be in good agreement with experiment. We would like to see how far the spectra of light nuclei could be described with this interaction. The parameters determined by Kohler[11] are also presented in Table I.

We would like to check whether these interactions have the requisite property to produce spin stability in the HF ground state of nuclear matter. Here we have taken two different approaches for studying this. In the final approach,[9] it is assumed that in the ground state, single particle levels (plane waves) with $|\vec{k}|\le k_L$ are occupied by both spin-up and spin-down pairs of nucleons, while levels with $k_L\le|\vec{k}|\le k_f$ are occupied by one proton and one neutron with spin-up (say). Then the degree of unsaturation would be given by $D=k_L/k_f$ and the ground state energy of unsaturated nuclear matter can be obtained using the Skyrme interaction (1) in the HF model as

$$\begin{aligned}E/A(D,k_f)={}&\frac{3\hbar^2 k_f{}^2}{10m}\frac{(1+D^5)}{(1+D^3)}+\frac{t_0 k_f{}^3}{8\pi 2}\left[(1+D^3)+\frac{2x_0-1}{3}\frac{(1-D^3)}{(1+D^3)}\right]\\&+\frac{k_f{}^5}{80\pi^2}\left[(3t_1+5t_2)(1+D^5)+(t_2-t_1)\frac{(1-D^3)}{(1+D^3)}(1-D^5)\right]\\&+\frac{t_3}{24}\left[\frac{k_f{}^3}{3\pi^2}\right]^{\alpha+1}[\tfrac{3}{2}(1+D^3)^2+(x_3-\tfrac{1}{2})(1-D^3)^2](1+D^3)^{\alpha-1},\end{aligned} \tag{5}$$

TABLE I. The values of parameters t_0 (MeV fm^3), t_1 (MeV fm^5), t_2 (MeV fm^5), t_3 (MeV fm^6), W (MeV fm^5), x_0, x_3, and α for different Skyrme variants. The units of the parameter t_3 for S_{ka} are in MeV fm^4.

Model	t_0	t_1	t_2	t_3	W	x_0	x_3	α
S_{II}	−1169.9	585.6	−27.1	9331.1	105.0	0.34		
S_{III}	−1128.75	395.0	−95.0	14 000.0	120.0	0.45		
S_{II}^M	−1169.9	585.6	−27.1	9331.1	105.0	0.229	1.2693	1.0
S_{III}^M	−1128.75	395.0	−95.0	14 000.0	120.0	0.4025	0.7744	1.0
S_{ka}	−1602.88	570.88	−67.7	8000.0	125.0	−0.02	−0.286	1.33

where the density is given by

$$\rho=\frac{1+D^3}{3\pi^2}k_f{}^3 .$$

But with the three-body term in the Skyrme force, the last term in expression (5) would be simply $t_3k_f{}^6D^3/36\pi^4$. Now, the condition that the spin-saturated system $D=1$ would be stable follows to be

$$\left\{\left[\frac{\partial^2(E/A)}{\partial k_f\partial D}\right]^2-\frac{\partial^2(E/A)}{\partial k_f{}^2}\frac{\partial^2(E/A)}{\partial D^2}\right\}_{D=1}\le 0. \quad (6)$$

For the two-body Skyrme force, in general, the above inequality simplifies to the condition

$$a_\tau \ge \gamma, \quad (7)$$

where a_τ is given by Eq. (3) and γ is given by

$$\gamma=-\frac{t_0x_0\rho_0}{2}-\frac{t_3x_3}{12}\rho_0^{\alpha+1}. \quad (8)$$

It is important to specify here that the second term in γ arises purely because of two-body density dependence of the effective interaction and hence that term is absent in the case of three-body contact interaction. Furthermore, this particular term effectively reduces the quantity γ and hence helps in getting the spin stability condition (7) satisfied. In actual calculation this has been clearly borne out (see Table II).

The second approach[10] for the study of spin stability of nuclear matter involves the calculation of Landau[18] Fermi-liquid parameters as has been done by Backman *et al.*[10] In this approach the bulk properties of nuclear matter are written in terms of the two-body interaction on the Fermi surface, and this may be expressed as the second derivative of the total energy of nuclear matter with respect to the occupation number at the Fermi surface. Conventionally, one can write this as

$$\langle \vec{k}_1,\vec{k}_2 \mid V \mid \vec{k}_1,\vec{k}_2\rangle = N_0{}^{-1}[F(\theta)+F'(\theta)\vec{\tau}_1\cdot\vec{\tau}_2 + G(\theta)\vec{\sigma}_1\cdot\vec{\sigma}_2 + G'(\theta)(\vec{\sigma}_1\cdot\vec{\sigma}_2)(\vec{\tau}_1\cdot\vec{\tau}_2)], \quad (9)$$

where $N_0{}^{-1}=\hbar^2\pi^2/(2k_fm^*)$ and m^* is the effective mass. As both the particles are on the Fermi surface, all the parameters F, F', G, and G' are functions of the angle θ between the wave vectors $\vec{k}_1$ and $\vec{k}_2$, and hence these parameters can be identified as the coefficients in the Legendre expansion. Then it follows that for spin stability, all the coefficients F_L, F_L', G_L', and G_L should be greater than $-(2L+1)$. Retaining the terms up to $L=1$ (higher order coefficients are, in fact, small), we have for the two-body density dependent interaction, in general,

$$F_0=\frac{N_0}{8}\left\{6t_0+(3t_1+5t_2)k_f{}^2 + t_3\rho_0^\alpha\left[\frac{\alpha(\alpha+3)}{2}+1\right]\right\},$$

$$F_1=-\frac{N_0}{8}(3t_1+5t_2)k_f{}^2,$$

$$F_0'=-\frac{N_0}{8}\left[2t_0(2x_0+1)+\frac{t_3}{3}\rho_0^\alpha(2x_3+1) + k_f{}^2(t_1-t_2)\right],$$

$$F_1'=G_1=G_1'=\frac{N_0}{8}(t_1-t_2)k_f{}^2, \quad (10)$$

$$G_0=\frac{N_0}{8}\left[2t_0(2x_0-1)+(2x_3-1)\frac{t_3\rho_0^\alpha}{3} - (t_1-t_2)k_f{}^2\right],$$

$$G_0'=-\frac{N_0}{8}\left[2t_0+\frac{t_3\rho_0^\alpha}{3}+(t_1-t_2)k_f{}^2\right],$$

$$N_0=\frac{k_f}{\pi^2}\left[\frac{\hbar^2}{2m}+\frac{\rho}{16}(3t_1+5t_2)\right]^{-1}.$$

However, with the three-body interaction, the corresponding expression for all the quantities except F_0', G_0, and G_0' remain invariant. These expressions may be listed here for the sake of comparison:

$$F_0'=-\frac{N_0}{8}\left[2t_0(2x_0+1)+t_3\rho+(t_1-t_2)k_f{}^2\right],$$

$$G_0=\frac{N_0}{8}\left[2t_0(2x_0-1)-t_3\rho-(t_1-t_2)k_f{}^2\right], \quad (11)$$

$$G_0'=-\frac{N_0}{8}\left[2t_0+t_3\rho+(t_1-t_2)k_f{}^2\right].$$

TABLE II. The values of the calculated Landau-Migdal parameters and spin-stability condition parameters a_τ (MeV) and γ (MeV) for different Skyrme variants.

Force	a_1	γ	F_0	F_1	F_0'	$F_1=G_1=G_1'$	G_0	G_0'	N_0^{-1}
$S_{\rm II}$	34.16	29.51	−0.06	−1.26	0.69	0.48	−0.77	−0.04	271.57
$S_{\rm III}$	28.15	36.83	0.30	−0.71	0.87	0.49	−1.57	−0.35	207.87
$S_{\rm II}^M$	27.04	−1.86	−0.06	−1.26	0.34	0.48	0.43	0.39	271.57
$S_{\rm III}^M$	29.35	13.94	0.30	−0.71	0.92	0.49	−0.002	0.46	207.87
S_{ka}	32.91	13.43	−0.26	−1.17	0.66	0.55	−0.02	0.32	252.22

In Table II we have presented all these quantities for the old, modified, and Kohler's version of the Skyrme force. It can easily be seen both for the modified and Kohler's version that the spin stability condition is satisfied.

The other important property of an interaction is the pairing nature. To check this we have calculated the matrix elements of the type $\langle j^2J=0, T=1 \mid V_{sk} \mid j^2J=0, T=1\rangle$. In our calculation of all the matrix elements, the density ρ has been assumed to be due to the core only. Thus, for ^{18}F and ^{18}O we take the density ρ due to ^{16}O in the matrix element calculation. Similarly, the density of ^{40}Ca has been used for the calculation of matrix elements in the corresponding region. In Table III we have presented some pairing matrix elements of the above type with the Skyrme forces $S_{\rm II}$ and $S_{\rm III}$, modified Skyrme forces $S_{\rm II}^M$ and $S_{\rm III}^M$, and Kohler's version S_{ka}. It is clearly evident that the antipairing effect which was present in $S_{\rm II}$ and $S_{\rm III}$ has disappeared in $S_{\rm II}^M$ and $S_{\rm III}^M$. In the Kohler interaction antipairing is also absent.

III. SPECTRA OF LIGHT NUCLEI

In order to test the suitability of the Skyrme force to describe the excited states, we have calculated the low-lying states of some of the light nuclei. The calculations have been carried out in the shell-model approach. The spectra for different nuclei are obtained in the configuration mixing calculations using the harmonic oscillator basis states. The single particle energy eigenvalues are taken from experiment. The oscillator length parameter "b" is obtained from comparison of the corresponding rms radii.

A. Two-particle spectra

For calculating low-lying states, the nuclei ^{18}O, ^{18}F, ^{42}Ca, and ^{42}Sc may be considered as consisting of an inert core of ^{16}O or ^{40}Ca (as the case may be) plus two valence nucleons confined to the *sd* or *pf* shell. Then, to a first approximation the spectra may be obtained by diagonalizing the two nucleon secular matrix in the model space of the *sd* or *pf* shell corresponding to the nuclei ^{18}O,^{18}F and ^{42}Ca,^{42}Sc, respectively. However, it has been observed that the Skyrme interaction bears a strong resemblance with a realistic interaction and, in fact, it has been shown by Negele[19] that the Skyrme interaction is nothing but an effective G matrix. Hence, it will be too simplistic to expect to get satisfactory results by mere diagonalization of the G matrix. To have an adequate representa-

TABLE III. Some model pairing matrix elements of the form $\langle j_a{}^2J=0,T=1 \mid V_{sk} \mid j_a{}^2J=0,T=1\rangle_{AS}$ for different Skyrme variants.

	$S_{\rm II}$	$S_{\rm III}$	$S_{\rm II}^M$	$S_{\rm III}^M$	Ska
$j_a=0d_{5/2}$	2.13	2.76	−2.14	−1.75	−2.83
$j_a=0s_{1/2}$	4.50	6.20	−1.40	−0.63	−0.14
$j_a=0d_{3/2}$	1.36	1.63	−1.49	−1.38	−2.04
$j_a=0f_{7/2}$	1.99	2.49	−1.42	−0.61	−1.68
$j_a=0f_{5/2}$	1.46	2.12	−1.10	−0.26	−1.35
$j_a=1p_{1/2}$	1.69	2.06	−0.28	0.18	−0.05

tion, one should take into account the core-polarization[20] correction due to 3p1h, as has been done by Kuo and Brown.[21] Finally, one should diagonalize the total G matrix, i.e., $G + G_{3\text{p1h}}$ known as the model interaction to get the spectra. The method of the 3p1h core-polarization calculation has been given in detail by Kuo and Brown[21] and hence we are just listing here the final formulas for ready reference:

$$\langle (ab)JT \mid G_{3\text{p1h}} \mid (cd)JT \rangle_{AS} = \frac{(-1)^{j_a+j_b+j_c+J+T}}{[(1+\delta_{ab})(1+\delta_{cd})]^{1/2}} \times \sum_{\text{ph}J''T''} (-1)^{J''+T''} U(\tfrac{1}{2}TT''\tfrac{1}{2};\tfrac{1}{2}\tfrac{1}{2})$$
$$\times [\, U(j_aJJ''d_c;d_bj_d)L(j_c,j_b)L(j_a,j_d) + U(j_aJJ''j_d;j_bj_c)L(j_d,j_b)L(j_a,j_c)(-1)^{J+T+1}$$
$$+ U(j_bJJ''j_c;j_aj_d)L(j_c,j_a)L(j_b,j_d)(-1)^{J+T+1}U(j_bJJ''j_d;j_aj_c)L(j_d,j_a)L(j_b,j_c)] ,$$

$$L(j_a,j_b) \equiv L(\text{ph}J''T''j_a;j_b) = (-1)^{j_\text{p}+j_\text{h}+J''+T''+1} \sum_{J'''T'''} \left[\frac{2J''+1}{2j_b+1} \; \frac{2T'''+1}{2} \right]^{1/2} U(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2};T'''T'')$$
$$\times U(j_aj_\text{p}j_bj_\text{n};J'''J'')\langle (b\text{h})J'''T''' \mid G \mid (\text{p}a)J'''T''' \rangle_{AS},$$

where a, b, c, d, and p are particle states and h denotes hole states. For parity conservation, we may have either the hole in the $0p$ shell and the particle in the $1p$-$0f$ shell or the hole in the $0s$ shell and the particle in the $1s$-$0d$ shell in the case of ^{18}O and ^{18}F nuclei. Similarly, in the case of ^{42}Ca and ^{42}Sc, the hole is kept confined to the $0p$ or $1s$-$0d$ shell and the particle p to the $0f$-$1p$ or $0g$-$1d$-$2s$ shell, respectively. For the value of $\hbar\omega$, we have taken an average value of 14 MeV for sd shell nuclei and 10 MeV for pf shell nuclei.

The spectra for ^{18}O and ^{18}F, obtained by diagonalizing the model interaction in the sd shell two-nucleon subspace, are shown in Figs. 1 and 2 along with the experimental values. The experimental spectra for ^{18}O and ^{18}F are taken from standard tables. Then the absolute ground state energies shown in the figures are determined as follows. Using the binding energy (E_B) data, the ground state energies of valence nucleons are taken to be

$$-E_B(^{18}\text{O})-E_B(^{16}\text{O})+2E_B(^{17}\text{O}) = -3.90 \text{ MeV (for } ^{18}\text{O})$$

and

$$-E_B(^{18}\text{F})-E_B(^{16}\text{O})+E_B(^{17}\text{O})+E_B(^{17}\text{F}) = -5.00 \text{ MeV (for } ^{18}\text{F}).$$

The diagonalization has been carried out for different Skyrme variants (S_{II}, S_{II}^M, S_{III}^M, and S_{ka}). The original S_{III} force almost gives similar characteristic results compared to the other Skyrme variants, hence, we have shown the results only for S_{II}. It can clearly be seen from the spectrum of ^{18}O that for the S_{II} force the levels do not match at all both qualitatively (ordering of the levels) and quantitatively (in magnitude) with those of experiment. Rather, the ground state energy level comes above the excited states. This is, however, expected from the observed antipairing nature of the effective interaction. On the contrary, the modified version gives much better results compared to the original three-body Skyrme force. This is again the result of the pairing property of the effective interaction. Comparing the results of S_{II}^M and S_{III}^M, one can see that the former compares better with the experiment than the latter. The two low-lying states

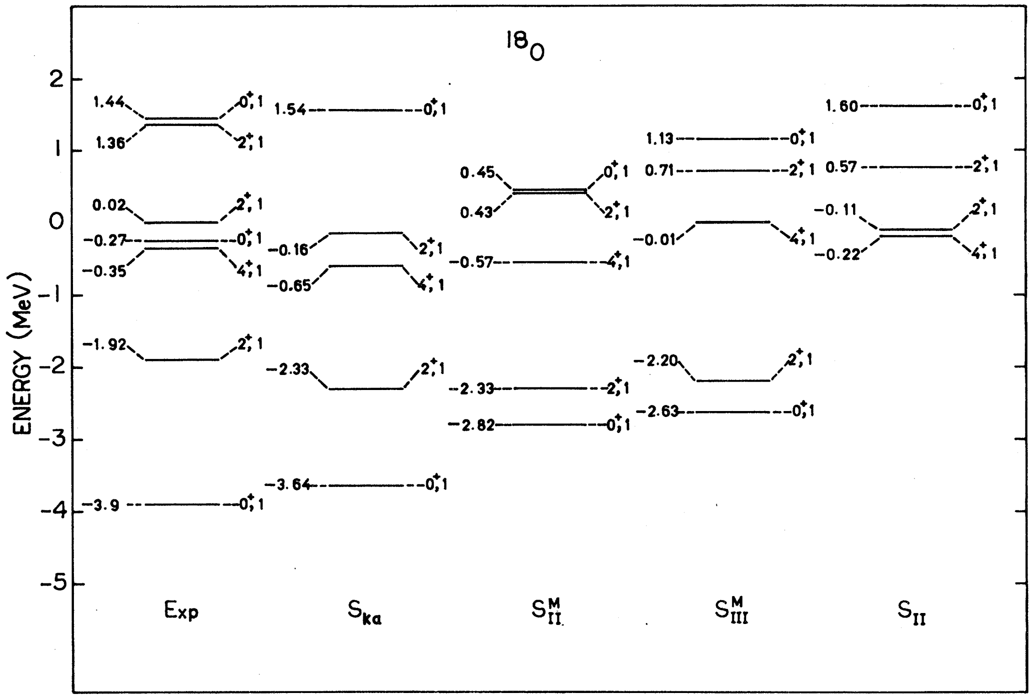

FIG. 1. Low lying states of ^{18}O calculated with the original and modified Skyrme interaction, are compared with the experimental results.

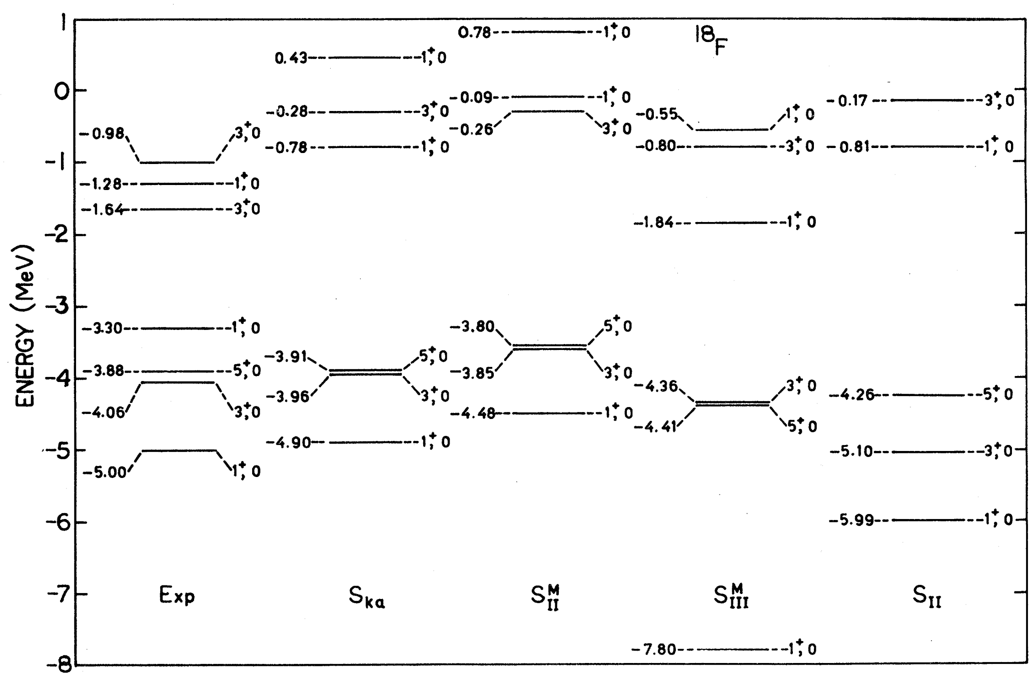

FIG. 2. Low lying states of ^{18}F calculated with the original and modified Skyrme interaction, are compared with the experimental results.

$(2^+,1)$ and $(4^+,1)$ are almost reproduced in the calculation. However, the ground state energy level $(0^+,1)$ comes a little bit above (by about 1 MeV) the corresponding experimental level. We have expected that the core-polarization contribution would lower the above level to the requisite extent. But in actual calculation, we find that this correction is not spectacular and it affects only marginally but nonetheless it cannot be neglected. To substantiate our argument we have presented a few of the matrix elements in Table III and this clearly bears out the above fact. However, our results with S_{ka} are in much better agreement with experiment. It must be noted that the basic difference between $S_{\rm II}^M$ and S_{ka} lies only in density dependence of the interaction. In our modification scheme we have retained the simplicity of linear density dependence $(\alpha=1)$ so as to have close resemblance with the original three-body force. On the other hand, Kohler has introduced fractional density dependence $(\alpha=\frac{1}{3})$ and this lowers the compressibility of nuclear matter in better agreement with experiment. This Skyrme variant will be referred to in the text as S_{ka}. With S_{ka}, however, we find that the $(0^+,1)$ level in the ^{18}O spectrum compares quite well with the experiment level (see Fig. 1).

As regards the ^{18}F spectrum, we see from Fig. 2 that the low-lying states 1^+, 3^+, 5^+, and $T=0$ with S_{ka}, $S_{\rm II}^M$ compare very well with those of the experiment, whereas with the original $S_{\rm II}$ and $S_{\rm III}$, the corresponding levels come much deeper (by about 1 MeV). However, the calculated higher excited states compare poorly with those of the experiment. This is, of course, expected as these high lying states are likely to be affected more, due to higher oscillator states in addition to the *sd* shell for proper description. This is also applicable to the higher excited states of ^{18}O. Similar results are also obtained by Kuo and Brown[21] in their calculations.

The spectra for the nuclei ^{42}Ca and ^{42}Sc have similarly been obtained by diagonalizing the model interaction in the two-nucleon subspace of the *pf* shell with ^{40}Ca as the core. The results along with experimental values are displayed in Figs. 3 and 4, respectively. Again the experimental ground state energies shown in the figures are determined using binding energy (E_B) data. The ground state energies of the valence nucleons are taken to be

$$-E_B(^{42}\text{Ca})-E_B(^{40}\text{Ca})+2E_B(^{41}\text{Ca})$$
$$=-3.11\text{ MeV (for }^{42}\text{Ca)}$$

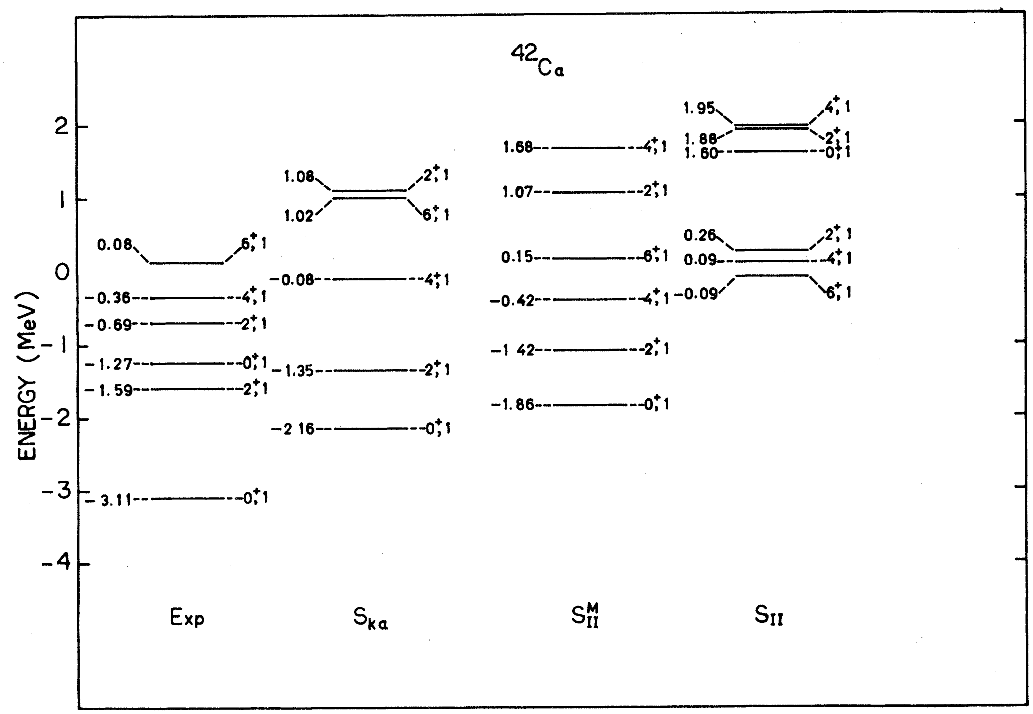

FIG. 3. Low lying states of ^{42}Ca calculated with the original and modified Skyrme interaction, are compared with the experimental results.

and

$$-E_B(^{42}\mathrm{Sc})-E_B(^{40}\mathrm{Ca})+E_B(^{41}\mathrm{Ca})+E_B(^{41}\mathrm{Sc})$$
$$=-2.59\ \mathrm{MeV}\ (\text{for } ^{42}\mathrm{Sc})$$

Exactly like ^{18}O and ^{18}F, we observe similar features in the spectra of the nuclei ^{42}Ca and ^{42}Sc. In the case of ^{42}Ca, calculated low-lying states 2^+, 4^+, and 6^+ are almost in agreement with experiment for the Skyrme variants S_{II}^{M} and S_{ka}. But the ground state 0^+ level calculated with modified Skyrme force does not agree to a satisfactory extent with the experimental value. However, there is slight improvement in agreement for S_{ka}. In the overall picture we are of the view that lack of adequate pairing strength in the Skyrme force is responsible for such a poor agreement. Though we are able to avoid the antipairing property in the modified Skyrme interaction, the pairing strength perhaps is not sufficient to lower the 0^+ level to come on par with experiment. Hence we would like to point out that one has to introduce an additional pairing term into the interaction particularly for such a kind of spectroscopic calculation. Waroquier *et al.*[23] used an extended form of the Skyrme interaction to calculate the spectrum in the case of ^{42}Ca only.

Regarding ^{42}Sc, we see that all the low-lying energy levels are reproduced with S_{ka}, S_{II}^{M}, and S_{II}. This is because pairing is not important for $T=0$ levels. However, with S_{III}^{M} all the low-lying states except $(1^+,0)$ is well reproduced. Similar features have also been oberved for the nucleus ^{18}F with S_{III}^{M}. Thus, comparing the results of S_{II}^{M} and S_{III}^{M}, we see that the former gives better results than the latter.

B. Particle-hole states

We have calculated the odd-parity states of close-shell nuclei such as ^{16}O and ^{40}Ca in the usual shell model approach. We consider particle-hole excitations only over $1\hbar\omega$ states, i.e., exciting particles to the next higher shell from the last occupied shell. In the case of ^{16}O we excite one particle from the occupied $0p$ shell to the sd shell while for ^{40}Ca the same has been done to the pf shell from the occupied sd shell. The results are presented in Figs. 5 and 6. We clearly see that the whole spectrum for ^{16}O with the Skyrme variants S_{ka}, S_{II}^{M},

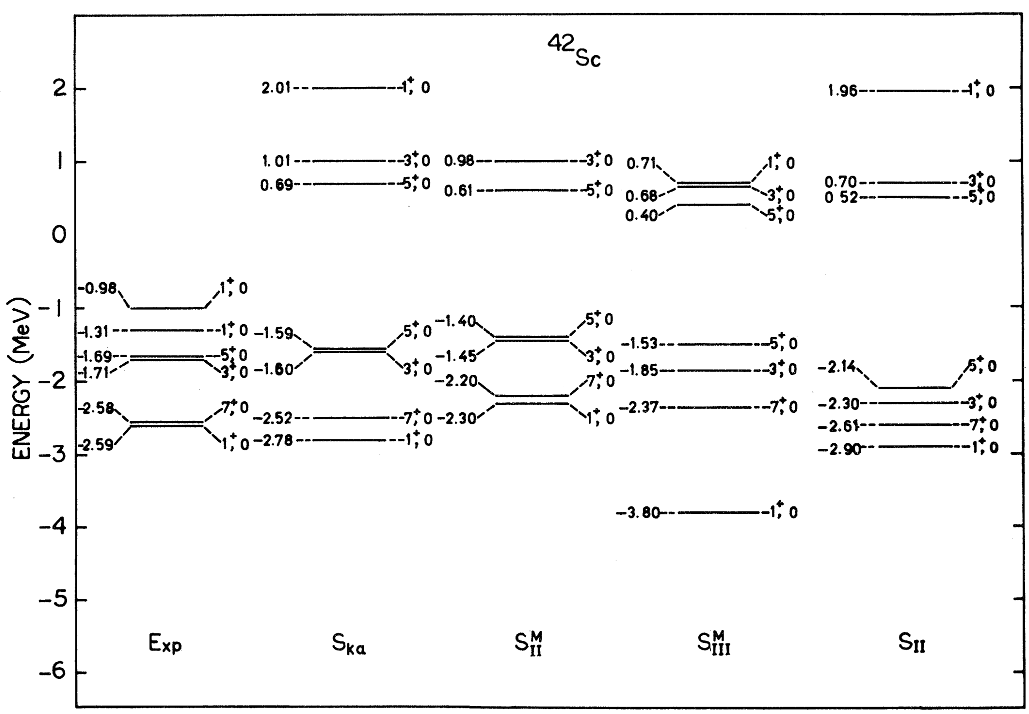

FIG. 4. Low Lying states of ^{42}Sc calculated with the original and modified Skyrme interaction, are compared with the experimental results.

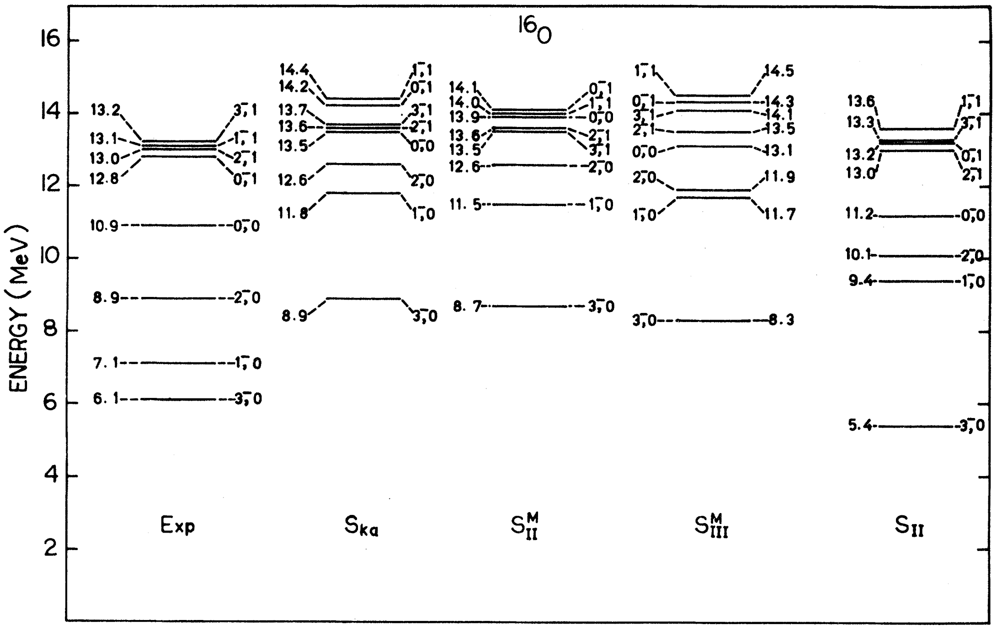

FIG. 5. Spectrum of ^{16}O calculated with the original and modified Skyrme interaction, are compared with the experimental results.

and S_{III}^{M} are raised by a fixed amount compared to the experimental spectrum. However, the ordering of the levels with total angular momentum J and isospin T (3,0), (1.0), (2.0), and (0,0) is maintained with experiment. But higher excited states corresponding to $T=1$ are not in order. In reality these levels are very close to each other and in actual calculation this is found to be so. These high lying states would need a larger basis for proper description. Similar features are also observed in the

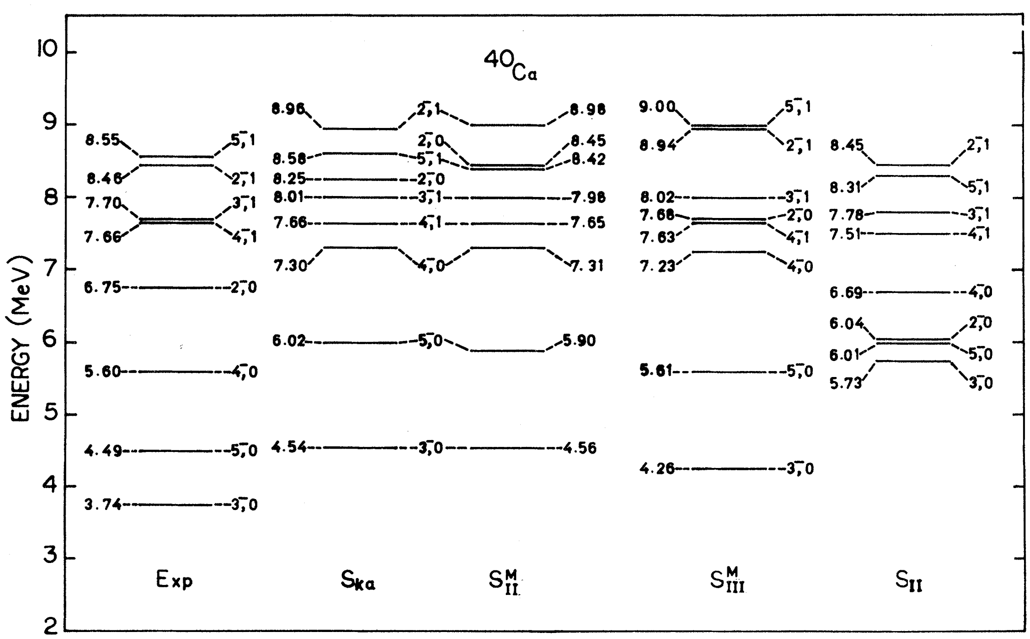

FIG. 6. Spectrum of ^{40}Ca calculated with the original and modified Skyrme interaction, are compared with the expeirmental results.

spectrum of ^{40}Ca. Thus the overall description of the spectra is qualitatively good.

IV. MASS FORMULA COEFFICIENTS

It is desirable to calculate the mass formula coefficients and compare them with those of Myers and Swiatecki.[13] This would guarantee a good fit to the actual nuclei without studying them in detail.

In order to calculate these coefficients we took the usual procedure of expressing the energy of a nucleus (only volume term) as

$$E/A=-a_1+a_\tau\delta^2+\tfrac{1}{2}k\epsilon^2-L\epsilon\delta^2+\tfrac{1}{2}M\delta^4, \tag{12}$$

where

$$\delta=\frac{\rho_n-\rho_z}{\rho_n+\rho_z}$$

and

$$\epsilon=-\frac{1}{3}\frac{\rho-\rho_0}{\rho_0}.$$

The coefficient a_1 is the binding energy per particle of nuclear matter and a_τ is the asymmetry energy. The quantity K is the nuclear compressibility. The term in L gives the density dependence of the symmetry energy and M is the coefficient which specifies the deviation of the symmetry energy from a quadratic dependence on δ. Then the HF energy density obtained by using the Skyrme generalized interaction (1) can be expressed in the above form for nuclear matter. Then identifying the different terms, the corresponding coefficients are found to be

$$\begin{aligned}
L&=\frac{2\hbar^2k_f^{\,2}}{6m}-\frac{3t_0}{4}(\tfrac{1}{2}+x_0)\rho_0\\
&\quad-\frac{\alpha+1}{8}t_3(\tfrac{1}{2}+x_3)\rho_0^{\alpha+1}+\tfrac{5}{6}t_2\rho_0k_f^{\,2},\\
K&=\frac{6\hbar^2k_f^{\,2}}{10m}+\tfrac{9}{4}t_0\rho_0+\tfrac{3}{16}(2+3\alpha)t_3\rho_0^{\alpha+1}\\
&\quad+\tfrac{3}{4}(3t_1+5t_2)\rho_0k_f^{\,2},\\
M&=2\left[\frac{\hbar^2k_f^{\,2}}{162m}+\frac{(3t_1+t_2)}{648}\rho_0k_f^{\,2}\right].
\end{aligned} \tag{13}$$

Here we have listed only the relevant quantities. The expression for asymmetry energy has already appeared earlier [see Eq. (3)]. The values of these quantities along with the maximum asymmetry ratio are presented in Table IV. In general, we find that all the quantities except compressibility compare quite well with those of Myers and Swiatecki[13] (see Table V). However, the value of compressibility with S_{ka} force agrees well with those of the above. This is due to the fractional density dependence of the interaction.

TABLE IV. Some of the $T=1$ matrix elements both bare (G) and core-polarization $G_{3\text{p1h}}$ for S_{ka} and S_{II}^M Skyrme variants.

$j_aj_bj_cj_dj$	J	Ska G	Ska $G_{3\text{p1h}}$	S_{II}^M G	S_{II}^M $G_{3\text{p1h}}$
$0d_{5/2}0d_{5/2}0d_{5/2}0d_{5/2}$	0	−2.834	−0.200	−2.144	−0.250
	2	−1.073	0.108	−0.821	0.073
	4	−0.712	0.822	−0.605	0.728
$1s_{1/2}1s_{1/2}1s_{1/2}1s_{1/2}$	0	−0.140	0.003	−1.396	0.017
$0d_{5/2}0d_{5/2}0d_{3/2}0d_{3/2}$	0	−1.950	−0.206	−1.605	−0.264
	2	−0.567	−0.183	−0.526	−0.206
$0f_{7/2}0f_{7/2}0f_{7/2}0f_{7/2}$	0	−1.679	−0.280	−1.418	−0.268
	2	−0.567	−0.183	−0.526	−0.206
	4	−0.424	0.795	−0.370	0.246
	6	−0.315	1.718	−0.287	0.627
$1p_{1/2}1p_{1/2}1p_{1/2}1p_{1/2}$	0	−0.050	0.441	−0.280	0.198
$0f_{7/2}0f_{7/2}1p_{3/2}1p_{3/2}$	0	−0.544	−0.111	−0.287	−0.164
	2	−0.191	−0.093	−0.122	−0.095

TABLE V. Calculated values of mass formula coefficients in MeV units along with asymmetry ratio.

Quantity	Myers and Swiatecki	S_{II}	S_{III}	S_{II}^M	S_{III}^M	S_{ka}
Vol. energy	−15.98	−16.00	−15.87	−16.00	−15.87	−16.00
Symmetry energy	36.50	34.20	28.16	27.04	29.35	32.90
Compressibility K	240.00	342.00	356.00	342.00	356.00	237.17
Density dependence asymmetry L	100.00	50.01	10.13	21.72	20.90	72.02
Asymmetry M	0.00	1.10	0.83	1.10	0.83	1.05
Maximum asymmetry ratio $=\frac{N-Z}{N+Z}$		0.30	0.33	0.36	0.32	0.30

V. CONCLUSION

The main aim behind the present work has been to describe the ground state as well as the excited states of nuclei with the Skyrme force. This has been a problem because of the inherent nature of the antipairing property of the interaction. This has been accomplished to some extent in the present work by replacing the three-body term by a two-body density dependent term in the Skyrme force. In this density dependent term a spin-isospin dependent parameter x_3 is introduced in order to have density dependence between both like and unlike nucleons. In our modification scheme the newly introduced parameter x_3 along with x_0 is determined by fitting maximum asymmetry ratio, asymmetry energy, and energy per particle of pure neutron matter. Since most of the ground state properties are well reproduced by the original force, we have retained the values of the parameters t_0, t_1, t_2, t_3, and W. It is found in our calculation that spin-instability and antipairing property inherent in S_{II} and S_{III} force have vanished with the modification. Further from our calculation of low-lying states of ^{18}O, ^{18}F, ^{42}Ca, and ^{42}Sc we found that our modified version gives much better results compared to the original three-body Skyrme force. However, quantitatively speaking, the level $(0^+,1)$ is not well reproduced. In the overall picture, S_{II}^M gives a better result compared to S_{III}^M.

We have also investigated the suitability of the Skyrme force which has a density dependence with fractional power such as $\rho^{1/3}$. For this purpose, we have chosen Kohler interaction.[11] Our calculation of the spectra of nuclei with this interaction gives comparatively better agreement than the modified S_{II} and S_{III} force. Thus $\rho^{1/3}$ dependence is a better representation of the density dependence than the linear density dependence. With both Kohler interaction as well as with modified S_{II} and S_{III} interactions, the $(0^+,1)$ level in both ^{18}O and ^{42}Ca are in poor agreement with experiment. This is due to the lack of strong pairing strength which is reflected in weak $(0^+,1)$ matrix element and affects crucially this level.

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