PHYSICAL REVIEW C VOLUME 12, NUMBER 2 AUGUST 1975

Hartree-Fock-Bogoliubov calculations for odd-mass nuclei in the $0f$-$1p$ shell

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(Received 5 February 1975)

Employing the Hartree-Fock-Bogoliubov approximation and the Kuo-Brown interaction, results for odd-mass nuclei in the $0f$-$1p$ shell are reported. A ^{40}Ca core has been assumed. The blocking effect due to the presence of the odd nucleon has been taken into account. The ground-state energies, the intrinsic and ground-state quadrupole moments, reduced transition rates, and the pickup strengths are calculated and compared with the corresponding available experimental values.

[NUCLEAR STRUCTURE Odd isotopes of Ti, Cr, Fe, Ni, Zn, Ge, V, Mn, Co, Cu, Ga, As; calculated single-particle binding energies, ground-state energies, intrinsic and ground-state quadrupole moments, reduced transition rates, pick-up strengths. Hartree-Fock-Bogoliubov method. Kuo-Brown interaction.]

I. INTRODUCTION

In recent years considerable theoretical as well as experimental effort has been expended to understand the structure properties of the $0f$-$1p$ shell nuclei.[1] From the theoretical point of view the simplest way to study these nuclei is to assume a ^{40}Ca core while studying the lighter nuclei and a ^{56}Ni core for studying the heavier $0f$-$1p$ shell nuclei. However, recent observations and calculations[2-7] show that the assumption of ^{56}Ni as a closed core is not a good one and one must include $0f_{7/2}$ orbital in addition to the other p-f shell orbits in order to study nuclei heavier than ^{56}Ni. It is well known that the increase in the number of valence nucleons coupled with the consideration of all the $0f$-$1p$ single particle orbitals, makes a shell model study of these nuclei an unmanageable task. On the other hand, such calculations are quite tractable within the framework of Hartree-Fock (HF), Hartree-Fock-Bogoliubov (HFB), and Bardeen-Cooper-Schrieffer (BCS) approximations.

Recently, a study of the ground-state properties of the even-even $0f$-$1p$ shell nuclei using the above mentioned self-consistent approximations had been reported.[8] A ^{40}Ca core was assumed and the axial symmetric solutions were explored. Similar calculations for the $1s$-$0d$ shell even-even nuclei had been reported by Satpathy, Goss, and Banerjee.[9] Investigation of asymmetric shapes in the $1s$-$0d$ and $0f$-$1p$ shell nuclei had been carried out by Banerjee, Levinson, and Stephenson[10] and Chandra and Rustgi.[11] It was found by Chandra and Rustgi that the inclusion of $T=1$ pairing, yielded axially symmetric HFB solutions for $N=Z$ nuclei. A recent study by Sandhu, Rustgi, and Goodman[12] following the work of Goodman, Struble, Bar-Touv, and Goswami[13] shows that the $T=0$ pairing is not at all important for these nuclei. Further it may be mentioned that according to Geoke, Garcia, and Faessler[14] and Whitehead and Watt[15] there is little experimental evidence for $T=0$ pairing correlations in ^{24}Mg, ^{32}S, and ^{20}Ne nuclei in the $1s$-$0d$ shell. For $N\neq Z$ nuclei, it is known from the work of Wolter, Faessler, and Sauer[16] that it is a good assumption to consider only the proton-proton and neutron-neutron pairing.

In the present paper the work of Chandra and Rustgi is extended to odd-A nuclei. At present such a study for odd-A nuclei employing realistic interaction does not exist in the literature for $0f$-$1p$ shell. For even-even nuclei, the proton-neutron and time-reversal symmetries are known to produce fourfold degeneracy of the orbits. These symmetries, however, do not hold for odd-A nuclei. In the HFB approximation, the pairing interaction acts on a nucleon pair occupying the degenerate time-reversed orbits and makes it to jump to other orbits. But the presence of the odd nucleon in one of the orbits prevents the pair from jumping to that orbit, an effect referred to as the blocking effect.

In the following section, the HFB equations for odd nuclei are introduced. The numerical calculations are given in Sec. III. These calculations are carried out for Kuo-Brown[17] interaction. In Sec. IV a summary and conclusions of the study are given.

II. HFB EQUATIONS FOR ODD-A NUCLEI

The shell-model Hamiltonian of the system in the second quantized form is given by

$$H=\sum_{\alpha,\beta}\langle\alpha|\epsilon|\beta\rangle a_\alpha^\dagger a_\beta+\tfrac{1}{4}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\beta|V_A|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma\,, \tag{1}$$

where ϵ represents the single-particle energy and $\langle\alpha\beta|V_A|\gamma\delta\rangle$ represents the two-body matrix element between the antisymmetrized states. The creation and annihilation operators for a nucleon with quantum number $\alpha(nljm)$ are denoted by $a_\alpha^\dagger$ and a_α, respectively.

In the HFB approximation the pairing correlations are taken into account by introducing the generalized Bogoliubov quasiparticle transformation given explicitly in Ref. 8 [Eq. (9)]. Since this transformation does not conserve the particle number, the chemical potentials λ_n and λ_p are introduced as Lagrange multipliers to keep the expectation value of the nucleon numbers to the assigned value.

According to Bloch and Messiah,[18] the generalized Bogoliubov transformation could be decomposed into three successive transformations. The first transformation transforms the particle operators $a_\alpha^\dagger$ from spherical basis into a set of particle operators $b_\beta^\dagger$ in the deformed basis,

$$b_\beta^\dagger=\sum_\alpha C_\alpha^\beta a_\alpha^\dagger\,. \tag{2}$$

The second transformation converts $b_\beta^\dagger$ into quasiparticle operators $A_\beta^\dagger$,

$$A_\beta^\dagger=U_\beta b_\beta^\dagger+V_\beta b_{\bar\beta}\,, \tag{3}$$

where a bar over the subscript indicates that the operator belongs to the time reversed states, i.e.,

$$b_{\bar\beta}^\dagger=\sum_\alpha(-)^{j_\alpha-m_\alpha}C_\alpha^\beta a_{j_\alpha,m_\alpha}^\dagger\,. \tag{4}$$

The third transformation mixes the quasiparticle operators among themselves. Since we are interested only in the ground-state properties, we can assume the last transformation to be unity.

The ground state of an even-even system in the HFB approximation may be written as

$$|\Phi_{\rm even}\rangle=\prod_i(U_i^p-V_i^p b_{ip}^\dagger b_{\bar ip}^\dagger)(U_i^n-V_i^n b_{in}^\dagger b_{\bar in}^\dagger)|0\rangle\,, \tag{5}$$

where $p(n)$ denotes proton (neutron) and the rest of the symbols have their usual meaning and are defined in Ref. 8.

For odd nuclei there is a nucleon which does not have any pairing correlations with the rest of the nucleons in the nucleus (we consider only n-n and p-p correlations), but interacts with the rest of the nucleons so as to contribute only to the HF field. Such an odd-A system can be described by the one quasiparticle state, i.e.,

$$|\Phi_{\rm odd}\rangle=A_n^\dagger|\Phi_{\rm even}\rangle\,, \tag{6}$$

where $n(\neq i)$ represents all the quantum numbers of the states occupied by the odd nucleon. In the following the quantum numbers of the odd nucleon are represented by n and those of the rest even number of nucleons by i. The symbols j, k, and l represent any general state.

From Eqs. (3) and (6) it is clear that a wave function possessing time reversal symmetry may be written as

$$|\Phi_{\rm odd}\rangle=\frac{b_n^\dagger+b_{\bar n}^\dagger}{\sqrt{2}}|\Phi_{\rm even}\rangle\,. \tag{7}$$

This wave function, however, lacks axial symmetry.

Following the same procedure as in the case of even-even system, we get the following expression for the energy of the ground state of the odd-A nucleus,

$$E_{\rm HFB}=\sum_{\tau_z}[{\rm Tr}^{\tau_z}(\epsilon\rho)_{\tau_z}+\tfrac{1}{2}{\rm Tr}^{\tau_z}(\Gamma\rho)+\tfrac{1}{2}{\rm Tr}^{\tau_z}(\Delta\chi)]\,, \tag{8}$$

where

$$\rho_{jj'}^m=\sum_{j_1}C_{jm}^{j_1m}C_{j'm}^{j_1m}V_{j_1m}{}^2\,, \tag{9}$$

$$\chi_{jj'}^m=-\sum C_{jm}^{j_1m}C_{j'm}^{j_1m}V_{j_1m}U_{j_1m}\,, \tag{10}$$

$$\Gamma_{jj'}^{\tau_z}=\sum_{\substack{j_1j_2\\ m_1\tau_z'}}\langle jm\tau_z,j_1m_1\tau_{z'}|V_A|j'm\tau_z,j_2m_1\tau_{z'}\rangle\rho_{j_1j_2}^{m_1\tau_z'}\,, \tag{11}$$

$$\Delta_{ii'}^{\tau_z}=\tfrac{1}{2}\sum_{i_1i_2m_1}\langle im\tau_z,i'\bar m\tau_z|V_A|i_1m_1\tau_z,i_2\bar m_1\tau_z\rangle\chi_{i_1i_2}^{m_1\tau_z} \tag{12}$$

with

$$V_n{}^2=U_n{}^2=\tfrac{1}{2} \tag{13}$$

and

$$\Delta_{n\bar n}=\Delta_{in}=0\,. \tag{14}$$

The expression (8) can be reduced to the following form

$$E_{\rm HFB}=\frac{1}{2}\sum_i(\epsilon_{ii}+\lambda-E_i)V_i{}^2+\frac{1}{2}\sum_{n,\bar n}(\epsilon_{nn}+e_n)V_n{}^2\,, \tag{15}$$

where

$$\epsilon_{ii} = \sum_{i'} \epsilon_i C_i^{i'} C_i^{i'} , \tag{16}$$

$$E_i^2 = \delta_i^2 + e_i^2 . \tag{17}$$

The quantities e_k and δ_i are obtained from

$$\sum_k \tilde{\Gamma}_{jk} C_k^l = e_l C_j^l , \tag{18}$$

and

$$\delta_i = \sum_{j,k} \Delta_{jk} C_j^i C_k^i , \tag{19}$$

where

$$\tilde{\Gamma}_{jk} = \Gamma_{jk} + \epsilon_j \delta_{jk} - \lambda \delta_{jk} . \tag{20}$$

The chemical potential λ is determined from

$$N = \frac{1}{2} \sum_i \left(1 - \frac{e_i - \lambda}{E_i} \right) + 1 . \tag{21}$$

In deriving Eq. (15) use has been made of the following relations

$$U_i V_i = \frac{\Delta_i}{2E_i} , \tag{22}$$

$$V_i^2 = \frac{1}{2} \left(1 - \frac{e_i - \lambda}{E_i} \right) \tag{23}$$

and

$$U_i^2 + V_i^2 = 1 . \tag{24}$$

III. NUMERICAL RESULTS

As mentioned earlier, the Kuo-Brown matrix elements for the Hamada-Johnson interaction are used for numerical computations. The single-particle energies (in MeV) are −8.35, −2.85, 6.28, and 4.22 for neutrons and −1.07, 4.83, 0.72, and 0.43 for protons corresponding to $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ orbitals, respectively. The results of the self-consistent HFB calculations for the odd-neutron even proton and odd-proton even-neutron nuclei are given in Tables I–V. Wherever possible the calculated values are compared with the experimental results. Since the particle number projection has been found[14] to have negligible effect on the intrinsic wave function, its effects are not studied.

A. Binding energies and separation energies

The results for the binding energies given with respect to the ^{40}Ca core and separation energies are listed in Tables I and II. Since we have not performed projection calculations, for reasons given above the separation energies are calculated as the difference between the self-consistent energy minima of the neighboring nuclei.

The binding energies agree fairly well with the experimental values[19] though as one goes very far from the core (Zn, Ge isotopes) the calculated values are found to be slightly higher. This could be due to the fact that we use the same oscillator parameter for the entire f-p shell which is not a very good assumption. One needs larger values of the oscillator parameter for the heavier nuclei. However, for realistic interactions the renormalized matrix elements are not available for different values of the oscillator parameter and calculating them is a very time consuming job.

From Table I it is clear that as one adds neutrons, both the neutron separation energies and neutron pair separation energies ($E_{\text{even(odd)}} - E_{\text{even-2(odd-2)}}$) decrease. Agreement with the experimental values is good for the lighter isotopes. As the neutron excess increases, the decrease in the theoretical separation energies is slower than what is observed. This feature is more pronounced for the heavier nuclei (Ni, Zn, and Ge). The fluctuations in the separation energies are fairly well reproduced. It is also noted that for a particular set of isotopes the calculated binding energy comes closer to the observed values as one adds more neutrons.

To study the effects of the addition of protons, results for the different sets of isotones are given in Table II. For neutron numbers 24, 26, 28, and 30 the theoretical binding energy is consistently smaller than the observed value. Unlike in the case of isotopes where the difference between observed and calculated values became less with the addition of neutrons, here in case of these isotones the difference does not decrease. Inclusion of n-p pairing might improve the situation. For neutron numbers 32, 34, 36, and 38 the calculated binding energy is generally greater than the observed value and may be understood in terms of the employment of a smaller oscillator parameter than what is needed. The saturation of the calculated binding energy for a fixed number of neutrons is more rapid than what is observed, as can be seen from the proton separation energies. Only for the neutron number 38 is the decrease in calculated proton separation energy slower than the experimental value. For neutron number 24, 26, and 28 the calculated proton pair sepatation energies are reasonably close to the experimental values, and the rate of decrease in it as one adds more protons is also in good agreement with experiments. For the neutron numbers 36 and 38 the calculated proton pair separation energy ΔE_{pp} is generally greater than experiment, but the rate

TABLE I. Comparison of the calculated binding energies (B. E.) of odd-neutron nuclei with respect to ^{40}Ca core, neutron separation energies (ΔE_N), and neutron pair separation energies (ΔE_{NP}) with the corresponding experimental values. All energies are given in MeV. The value of intrinsic quadrupole moment using effective charge $e = 0.8$ are given in the last column.

Nucleus	B.E. Calc.	B.E. Expt.	ΔE_N Calc.	ΔE_N Expt.	ΔE_{NP} Calc.	ΔE_{NP} Expt.	Q_0 ($e\times10^{-24}$ cm^2)
^{44}Ti	27.94	33.43	...	...	...	...	1.06
^{45}Ti	39.21	42.95	11.27	9.52	...	...	1.12
^{46}Ti	50.11	56.15	10.91	13.20	22.17	22.72	1.23
^{47}Ti	59.81	65.02	9.70	8.87	20.60	22.07	1.20
^{48}Ti	69.98	76.65	10.17	11.63	19.87	20.50	1.26
^{49}Ti	79.23	84.80	9.25	8.15	19.42	19.78	1.24
^{50}Ti	88.82	95.74	9.59	10.94	18.84	19.09	1.27
^{51}Ti	97.24	102.12	8.42	6.38	18.01	17.32	1.16
^{48}Cr	60.61	69.42	...	...	...	...	1.64
^{49}Cr	73.06	80.06	12.45	10.64	...	...	1.74
^{50}Cr	84.37	93.00	11.31	12.94	23.76	23.58	1.82
^{51}Cr	96.97	102.26	12.60	9.26	23.91	22.20	1.84
^{52}Cr	106.53	114.30	9.56	12.04	22.16	21.30	1.85
^{53}Cr	117.26	122.24	10.73	7.94	20.29	19.98	1.84
^{54}Cr	126.24	131.96	10.98	9.72	19.71	17.66	1.79
^{55}Cr	135.39	138.22	9.15	6.26	18.13	15.98	1.68
^{52}Fe	94.44	105.66	...	...	...	...	2.31
^{53}Fe	108.05	116.34	13.61	10.68	...	...	2.28
^{54}Fe	119.73	129.72	11.68	13.38	25.29	24.06	2.24
^{55}Fe	131.91	139.02	12.18	9.30	23.86	22.68	2.26
^{56}Fe	142.39	150.22	10.48	11.20	22.66	20.50	2.15
^{57}Fe	153.20	157.22	10.81	7.00	21.29	18.20	2.00
^{58}Fe	163.07	167.91	9.87	10.69	20.68	17.69	1.90
^{59}Fe	173.32	174.00	10.25	6.09	20.12	16.78	−1.64
^{56}Ni	133.06	141.95	...	...	...	...	−2.33
^{57}Ni	146.01	157.87	12.95	15.92	...	...	−2.32
^{58}Ni	157.35	164.42	11.34	6.55	24.29	22.47	−2.27
^{59}Ni	170.21	173.42	12.86	9.00	24.20	15.55	−2.24
^{60}Ni	181.28	184.81	11.07	11.39	23.93	20.39	−2.19
^{61}Ni	193.78	192.63	12.50	7.82	23.57	19.21	−2.16
^{62}Ni	204.74	203.23	10.96	10.60	23.46	18.42	−2.12
^{63}Ni	215.50	210.07	10.76	6.84	21.72	17.44	−1.96
^{64}Ni	224.34	219.73	8.84	9.66	19.60	16.50	−1.77
^{65}Ni	234.60	225.82	10.26	6.09	19.10	15.75	−1.02
^{61}Zn	180.06	183.42	...	...	...	...	2.40
^{62}Zn	192.34	196.03	12.28	12.61	...	...	−2.09
^{63}Zn	206.92	205.20	14.58	9.17	26.86	21.78	−1.96
^{64}Zn	219.57	217.06	12.65	11.86	27.23	21.03	−2.02
^{65}Zn	232.19	225.04	12.62	7.98	25.27	19.84	−1.80
^{66}Zn	242.49	236.09	10.30	11.05	22.92	19.03	−1.57
^{67}Zn	254.89	243.15	12.40	7.06	22.70	18.11	−1.36
^{65}Ge	218.87	213.92	...	...	...	...	−1.84
^{66}Ge	232.19	227.81	13.82	13.95	...	...	−1.85
^{67}Ge	247.00	236.15	14.81	8.28	28.13	22.23	−1.68
^{68}Ge	258.37	248.47	11.37	12.32	26.18	20.60	−1.44
^{69}Ge	272.98	256.94	14.61	8.47	25.98	20.79	−1.20

of decrease as the proton number increases agrees well with the experiment.

B. Intrinsic quadrupole moments and transition probabilities

In Tables I and II, the values of the intrinsic quadrupole moment (Q_0) are given in the last column and are evaluated by using the expression

$$Q_0 = \left(\frac{16\pi}{5}\right)^{1/2} \sum_{k,\alpha,\beta} \langle \alpha | e_k r_k^2 Y_{20} | \beta \rangle C_\alpha^k C_\beta^k V_k^2 ,$$

where e_k is the effective charge, i.e., $e_{\text{proton}} = 1 + e$ and $e_{\text{neutron}} = e$. The values of Q_0 is positive for the

TABLE II. Comparison of the calculated binding energies (B. E.) of odd-proton nuclei with respect to ^{40}Ca core, proton separation energies (ΔE_p), and proton pair separation energies (ΔE_{pp}) with the corresponding experimental values. All energies are given in MeV. The values of intrinsic quadrupole moment using effective charge $e = 0.8$ are given in the last column.

Nucleus	B.E. Calc.	B.E. Expt.	ΔE_p Calc.	ΔE_p Expt.	ΔE_{pp} Calc.	ΔE_{pp} Expt.	Q_0 ($e \times 10^{-24}$ cm^2)
^{46}Ti	50.11	56.15	•••	•••	•••	•••	1.23
^{47}V	55.87	61.28	5.76	5.13	•••	•••	1.44
^{48}Cr	60.61	69.42	4.74	8.14	10.50	13.27	1.64
^{48}Ti	69.98	76.65	•••	•••	•••	•••	1.26
^{49}V	77.44	83.37	7.46	6.72	•••	•••	1.52
^{50}Cr	84.37	93.00	6.93	9.63	14.39	17.35	1.82
^{51}Mn	90.33	98.23	5.96	5.23	12.89	14.86	2.04
^{52}Fe	94.44	105.66	4.11	7.43	10.07	12.66	2.31
^{50}Ti	88.82	95.74	•••	•••	•••	•••	1.27
^{51}V	97.89	103.76	9.07	8.02	•••	•••	1.56
^{52}Cr	106.53	114.30	8.64	10.54	17.71	18.56	1.85
^{53}Mn	114.02	120.82	7.49	6.52	16.13	17.06	2.08
^{54}Fe	119.73	129.72	5.71	8.90	13.20	15.42	2.24
^{55}Co	127.29	134.73	7.56	5.01	13.27	13.91	−2.12
^{53}V	116.50	119.56	•••	•••	•••	•••	1.48
^{54}Cr	126.24	131.96	9.74	12.40	•••	•••	1.79
^{55}Mn	135.03	139.99	8.79	8.03	18.53	20.43	2.00
^{56}Fe	142.39	150.22	7.36	10.23	16.15	18.26	2.15
^{57}Co	150.46	156.20	8.07	5.98	15.43	16.21	2.20
^{58}Ni	157.35	164.42	6.89	8.22	14.96	14.20	−2.27
^{57}Mn	154.52	156.05	•••	•••	•••	•••	1.80
^{58}Fe	163.07	167.91	8.55	11.86	•••	•••	1.90
^{59}Co	172.81	175.24	9.74	7.33	18.29	19.19	−1.96
^{60}Ni	181.28	184.81	8.47	9.57	18.21	16.90	−2.19
^{61}Cu	188.02	189.56	6.74	4.75	17.21	14.32	−2.08
^{62}Zn	192.34	196.03	4.32	6.47	11.06	11.22	−2.09
^{61}Co	195.00	192.07	•••	•••	•••	•••	−1.88
^{62}Ni	204.74	203.23	9.74	11.16	•••	•••	−2.12
^{63}Cu	213.23	209.31	8.49	6.08	18.23	17.24	−2.08
^{64}Zn	219.57	217.06	6.34	7.75	14.83	13.83	−2.02
^{65}Ga	218.87	213.92	−0.70	−3.14	5.64	4.61	−2.00
^{66}Ge	232.19	227.87	13.32	13.95	12.62	10.81	−1.85
^{64}Ni	224.34	219.73	•••	•••	•••	•••	−1.77
^{65}Cu	234.49	227.13	10.15	7.40	•••	•••	−1.60
^{66}Zn	242.49	236.09	8.00	8.96	18.15	16.36	−1.57
^{64}Ga	251.71	241.36	9.22	5.27	17.22	14.23	−1.18
^{68}Ga	258.37	248.47	6.66	7.11	15.88	12.38	−1.44
^{67}Cu	255.06	243.31	•••	•••	•••	•••	−1.24
^{68}Zn	264.86	253.34	9.80	10.03	•••	•••	−1.19
^{69}Ga	275.94	259.95	11.08	6.61	20.88	16.64	
^{70}Ge	284.07	268.48	8.13	8.53	19.21	15.14	−1.06
^{71}As	294.82	273.10	10.75	4.62	18.88	13.15	−0.04

prolate shape and negative for the oblate shape of the nucleus. From Table I it is noted that the Ti, Cr, and Fe isotopes (except ^{59}Fe) are prolate in shape. For Ti isotopes the deformation first increases and then it is constant for ^{48,49,50}Ti isotopes. For the Cr isotopes it increases gradually and then drops for ^{54,55}Cr. For Fe isotopes the deformation decreases consistently. This is in contradiction to what was found with Rosenfeld-Yukawa interaction.[20] All the Ni, Zn (except ^{61}Zn), and Ge isotopes are oblated in shape.

For the nuclei with neutron numbers $N = 24$, 26, 28, and 30 the nuclei are prolate and the deformation increases with the addition of protons. For $N = 32$, 34, 36, and 38 except for ^{57}Mn and ^{58}Fe all the nuclei are oblate and the deformation increases with the addition of protons.

In this paper because the projection of good angular momentum states has not been attempted, the quadrupole moment of the ground states (Q_I) and

TABLE III. The projection quantum number K of the state occupied by the odd nucleon as calculated by the HFB approximation is compared with the experimental ground-state spin I. Calculated ground state quadrupole moment Q_I and $B(E2)$ values are compared with the experimental values whenever possible. The Q_I values are also compared with those calculated by Scholtz and Malik (SM).

			Q_I ($e\times10^{-24}$ cm^2)			$B(E2)$ ($e^2\times10^{-50}$ cm^4)		
Nucleus	K	I	Calc.	Expt.	SM	Transition	Calc.	Expt.
^{45}Ti	$\frac{3}{2}$	$\frac{7}{2}$	−0.20	...	−0.587	$\frac{5}{2}\rightarrow\frac{7}{2}$	0.46	...
^{47}Ti	$\frac{5}{2}$	$\frac{5}{2}$	0.44	0.29	+0.880	$\frac{7}{2}\rightarrow\frac{5}{2}$	0.85	2.8
^{49}Cr	$\frac{1}{2}$	$\frac{5}{2}$	0	...	+0.873	...	...	...
^{51}Cr	$\frac{5}{2}$	$\frac{7}{2}$	0.12	...	−0.423	$\frac{5}{2}\rightarrow\frac{7}{2}$	2.00	...
^{53}Fe	$\frac{5}{2}$	$\frac{7}{2}$	−0.16	...	...	$\frac{5}{2}\rightarrow\frac{7}{2}$	3.08	...
^{59}Ni	$\frac{3}{2}$	$\frac{3}{2}$	−0.44	...	...	$\frac{5}{2}\rightarrow\frac{3}{2}$	4.28	...
^{61}Zn	$\frac{3}{2}$	$\frac{3}{2}$	0.48	...	...	$\frac{5}{2}\rightarrow\frac{3}{2}$	4.92	...
^{63}Zn	$\frac{5}{2}$	$(\frac{3}{2},\frac{5}{2})$	−0.68	...	...	$\frac{7}{2}\rightarrow\frac{5}{2}$	2.26	...
^{67}Zn	$\frac{3}{2}$	$\frac{5}{2}$	0.08	...	...	$\frac{3}{2}\rightarrow\frac{5}{2}$	1.57	1.8
^{47}V	$\frac{3}{2}$	$\frac{7}{2}$	−0.29	...	−1.194	$\frac{5}{2}\rightarrow\frac{7}{2}$	0.62	...
^{49}V	$\frac{3}{2}$	$\frac{7}{2}$	−0.32	...	−1.194	$\frac{5}{2}\rightarrow\frac{7}{2}$	0.82	...
^{51}V	$\frac{3}{2}$	$\frac{7}{2}$	−0.32	−0.05	−0.985	$\frac{5}{2}\rightarrow\frac{7}{2}$	0.86	1.7
^{53}V	$\frac{3}{2}$	$\frac{5}{2}$	−0.12	...	...	$\frac{3}{2}\rightarrow\frac{5}{2}$	1.86	...
^{55}Co	$\frac{5}{2}$	$\frac{7}{2}$	−0.12	...	...	$\frac{5}{2}\rightarrow\frac{7}{2}$	2.66	...
^{57}Co	$\frac{5}{2}$	$\frac{7}{2}$	0.16	...	...	$\frac{5}{2}\rightarrow\frac{7}{2}$	2.86	...
^{61}Cu	$\frac{3}{2}$	$\frac{3}{2}$	−0.12	...	...	$\frac{5}{2}\rightarrow\frac{3}{2}$	1.68	...
^{65}Cu	$\frac{3}{2}$	$\frac{3}{2}$	−0.32	...	...	$\frac{5}{2}\rightarrow\frac{3}{2}$	2.20	...
^{67}Cu	$\frac{3}{2}$	$\frac{3}{2}$	−0.24	...	...	$\frac{5}{2}\rightarrow\frac{3}{2}$	1.32	...

the reduced transition rates $[B(E2)]$ for the lowest transitions cannot be calculated exactly. However, one can follow the suggestion due to Villars[21] that the rotational model approximation is reasonably good for the lower levels. Thus we use the relations

$$Q_I=\frac{3k^2-I(I+1)}{(2I+3)(I+1)}Q_0\,,$$

$$B(E2)=\frac{5}{16\pi}\begin{bmatrix} I & 2 & I' \\ k & 0 & k \end{bmatrix}^2 Q_0{}^2\,,$$

where [ ] denotes the Clebsch-Gordan coefficient in the convention of Rose.[22] The theoretical values of Q_I and $B(E2)$ shown in Table III have been calculated for $e=0.8$. Our values of Q_I correctly predict the sign and are slightly in better agreement than the calculations of Scholtz and Malik[23] based on the Coriolis-coupling model. For the odd-neutron and odd proton nuclei, the $B(E2)$ values obtained are very similar to the one obtained with the Rosenfeld-Yukawa interaction[20] except for a few nuclei. It is hoped that in the future more data will become available to test the results.

C. Pickup strengths

The pickup strengths obtained from the equation

$$S_j^{\tau_z}=\sum_{\alpha m} V_{\alpha m}{}^2(C_{jm}{}^{\alpha\tau_z})^2$$

are given in Tables IV and V for odd-neutron and odd-proton nuclei, respectively. Experimentally these can be found from one-nucleon transfer reactions. For even isotopes agreement for the pickup strengths was found[8] to be quite satisfactory. For odd isotopes not much experimental data are available except for ^{47}Ti and ^{49}Ti and in both these cases the data seem not to satisfy the sum rule $\Sigma S_j=N$, where N is the number of neutrons or protons outside the ^{40}Ca core. For the Ti isotopes it is the $f_{7/2}$ shell which gets most of the contribution as we add more neutrons and the proton pickup strengths remain almost constant. A similar observation is also made for the other isotopes.

In V isotopes (Table V) as we go from lighter to heavier isotopes, one notices that the proton pickup strength for the $f_{7/2}$ shell decreases and there is a corresponding increase in the values corre-

TABLE IV. Neutron and proton pickup strengths are given for odd-neutron nuclei. The available experimental values are given in parentheses.

Nucleus	Neutron pickup strengths				Proton pickup strengths			
	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$f_{7/2}$	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$f_{7/2}$
^{45}Ti	0.11	0.47	0.19	2.23	0.12	0.46	0.12	1.30
^{47}Ti	0.14	0.64	0.30	3.92	0.10	0.48 (0.18)	0.11	1.30 (2.35)
^{49}Ti	0.34	1.18	0.53	4.95	0.11	0.55	0.08	1.26
^{51}Ti	0.49	1.71	0.65	6.15	0.11	0.55	0.07	1.27
^{49}Cr	0.33	0.85	0.62	3.20	0.13	0.78	0.22	2.87
^{51}Cr	0.56	1.07	0.99	4.38	0.12	0.86	0.20	2.82
^{53}Cr	0.63	1.58	1.41	5.38	0.10	0.88	0.17	2.85
^{55}Cr	0.71	2.16	1.66	6.47	0.09	0.85	0.15	2.91
^{53}Fe	0.65	1.21	0.93	4.21	0.73	1.22	0.74	3.31
^{55}Fe	0.71	1.63	1.35	5.31	0.68	1.29	0.50	3.53
^{57}Fe	0.80	2.56	1.86	5.78	0.63	1.40	0.31	3.66
^{59}Fe	1.40	2.93	1.71	6.96	0.38	1.83	0.29	3.50
^{57}Ni	0.73	2.32	1.56	4.39	0.77	2.33	0.91	3.99
^{59}Ni	1.00	2.56	1.86	5.58	0.73	2.41	0.73	4.13
^{61}Ni	1.11	2.77	2.51	6.61	0.69	2.46	0.52	4.33
^{63}Ni	1.60	3.32	2.67	7.41	0.54	2.58	0.37	4.51
^{65}Ni	1.72	3.86	3.54	7.88	0.37	2.41	0.22	4.99
^{61}Zn	0.82	2.13	2.49	5.56	0.90	1.94	1.75	5.41
^{63}Zn	1.56	3.00	1.78	6.66	1.11	2.82	0.76	5.31
^{65}Zn	1.64	3.39	2.68	7.29	0.99	2.85	0.58	5.59
^{67}Zn	1.76	3.85	3.54	7.85	0.99	2.85	0.58	5.59
^{65}Ge	1.60	3.79	0.85	6.76	1.54	3.09	1.09	6.30
^{67}Ge	1.66	3.46	2.70	7.18	1.56	3.13	0.75	6.56
^{69}Ge	1.80	3.84	3.53	7.82	1.48	3.27	0.23	7.02

TABLE V. Neutron and proton pickup strengths for odd-proton nuclei.

Nucleus	Neutron pickup strengths				Proton pickup strengths			
	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$f_{7/2}$	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$f_{7/2}$
^{47}V	0.11	0.61	0.24	3.04	0.12	0.59	0.17	2.12
^{49}V	0.37	1.01	0.58	4.04	0.13	0.68	0.14	2.04
^{51}V	0.56	1.30	0.83	5.30	0.13	0.75	0.12	2.00
^{53}V	0.67	2.00	1.19	6.13	0.12	0.74	0.11	2.04
^{51}Mn	0.58	1.09	0.89	3.43	0.42	1.03	0.51	3.04
^{53}Mn	0.64	1.18	1.00	5.18	0.43	1.06	0.47	3.04
^{55}Mn	0.72	1.95	1.71	5.62	0.44	1.15	0.29	3.11
^{57}Mn	0.85	2.77	1.88	6.51	0.43	1.21	0.22	3.14
^{55}Co	0.75	2.35	0.94	3.93	0.80	2.33	0.53	3.34
^{57}Co	0.76	1.89	1.88	5.47	0.76	1.44	0.45	4.34
^{59}Co	1.04	2.64	2.09	6.22	0.35	1.94	0.59	4.12
^{61}Co	1.50	2.80	2.55	7.15	0.31	1.99	0.42	2.27
^{59}Cu	0.78	1.89	1.89	5.44	0.83	1.70	1.13	5.35
^{61}Cu	1.08	2.70	2.12	6.10	0.72	2.61	0.72	4.95
^{63}Cu	1.57	2.92	2.60	6.91	1.05	2.63	0.48	4.84
^{65}Cu	1.70	3.69	2.93	7.69	0.54	2.75	0.35	5.36
^{67}Cu	1.74	3.90	4.41	7.95	0.38	2.48	0.21	5.93
^{65}Ga	1.57	2.97	2.63	6.83	1.05	2.89	1.16	5.89
^{67}Ga	1.71	3.68	2.99	7.61	0.99	3.09	0.55	6.37
^{71}As	1.98	3.97	4.15	7.89	1.00	3.95	0.11	7.94

sponding to $p_{3/2}$ shell. This is so because as the number of neutrons increases, the structure of the HF field in the HFB approximation for different states becomes more dissimilar and this shows up in the calculation of pickup strengths through the wave function.

D. Single-particle levels

The single-particle levels for neutrons and protons are displayed in Fig. 1 for the Ti isotopes. The number to the right of each level is twice the projection quantum number of the level. The level occupied by the odd nucleon is represented with a solid circle on it. The dashed lines show the Fermi levels.

For Ti isotopes we see that the first occupied $m = \frac{1}{2}$ level is far removed from the rest of the levels. Except for ^{49}Ti, the Fermi level is always below the level occupied by the odd nucleon. As we go from lighter to heavier isotopes, the order of the levels does not change though the separation between them does. For the Cr and Fe isotopes (not displayed here), the Fermi level is always below the level occupied by the last nucleon, though ^{59}Fe has a different order of the single-particle levels than the rest of the isotopes and has its Fermi level above the level occupied by the last neutron. Similar features are also seem in other nuclei. In all the nuclei studied, it is found that, in general, the effect of the addition of a neutron (proton) is that the neutron (proton) single-particle spectrum becomes more compressed accompanied by a lowering of all the proton (neutron) single-particle levels and thus increasing binding energy of the nucleus. This last feature could be attributed to an increased neutron-proton interaction through the Hartree-Fock field. This feature is most prominent in Ni, Zn, and Ge isotopes.

IV. SUMMARY AND CONCLUSIONS

A study of all the odd-A nuclei in the $0f$-$1p$ shell is carried out. By comparing the present results

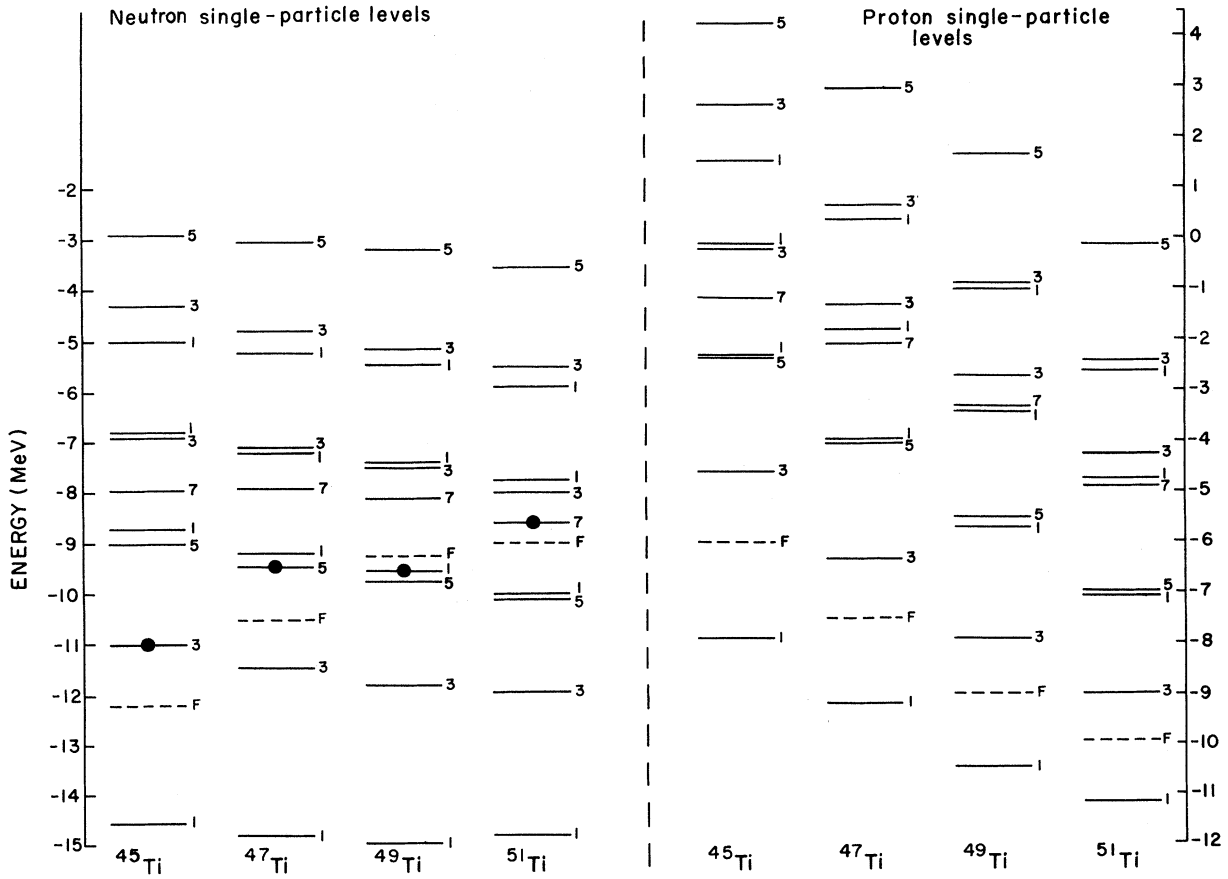

FIG. 1. Positions of the self-consistent neutron and proton single-particle energy levels for Ti isotopes for the Kuo-Brown interaction. The dashed lines show the Fermi levels. The level occupied by the odd neutron is represented by a solid circle.

with the ones for even nuclei, an attempt to study the effects of the addition of a neutron or a proton has been made.

The binding energies, the saturation of separation energies, and the fluctuation of separation energies are fairly satisfactorily reproduced. The addition of a neutron or a proton does not, in general, change the shape of the nuclei and the sequence of single-particle levels as classified by their m value. The separation between the levels does change and there is a crossing over of the levels in case they are very close to each other.

As one adds more neutrons (protons), the neutron (proton) single-particle spectrum is more and more compressed and the proton (neutron) levels go down and gain more binding energy. This last feature could be attributed to increased neutron-proton interaction through the Hartree-Fock field. This effect is most prominent in Ni, Zn, and Ge isotopes.

The quadrupole moments and $B(E2)$ values as calculated employing the rotational model approximation compare favorably with a few pieces of data that are available and give better agreement than obtained by Scholtz and Malik[23] on the Coriolis coupling model. Unfortunately not enough experimental data are available to make the comparison of neutron and proton pickup strengths meaningful. In the only case where the data are available, it is found that the observed pickup strengths do not satisfy the sum rule $\Sigma S_j = N$.

It might be remarked that in our calculations we have not considered the n-p pairing in $T=1$ states. However, it has been concluded in the work of Chen and Goswami[24] that the contribution from this pairing decreases as the difference in the number of neutron and proton increases and should be therefore unimportant for most of the nuclei considered here. Similar conclusions have also been reached at by Wolter *et al.*[16] The $T=0$ pairing has been shown to be unimportant by Sandhu *et al.*[12] Also we have not attempted particle number projection since the nuclei studied here do not exhibit a rotational spectrum and it has been found[14] that particle number projection has negligible effect on the intrinsic wave function. Further the interaction considered here does not have any density dependence.[25,26]

ACKNOWLEDGMENTS

It is a great pleasure for one of the authors (M.L.R.) to express his deep appreciation to Professor G. E. Brown for providing the facilities and stimulation to carry out this work during his stay at the State University at Stony Brook. Many discussions with Dr. D. Vautherin about density-dependent interactions are also gratefully acknowledged. The authors would also like to take this opportunity to thank Professor G. Breit for several conversations.

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