Self-Consistent Calculations for Even Ti, Cr, and Fe Isotopes

Harish Chandra* and M. L. Rustgi
Nuclear Physics Laboratory, Department of Physics, State University of New York, Buffalo, New York 14214
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Results of self-consistent calculations with Hartree-Fock (HF), Hartree-Fock-Bogoliubov (HFB), and spherical BCS approximations obtained with the central Yukawa (CY) interaction and with renormalized Kuo and Brown matrix elements for the Hamada-Johnston (HJ) interaction are reported for even Ti, Cr, and Fe isotopes. The calculated ground-state energies, corrected for Coulomb interaction amongst the extracore protons, are compared with the experimental values, and a better agreement for the HJ interaction is obtained than for the CY although they do not differ much with respect to each other. It is found that in the HFB approximation, the HJ interaction favors prolate solutions over oblate or spherical ones. Unlike the CY, the HFB approximation for $Z<N=28$ nuclei with the HJ interaction does not converge to spherical minima with lowest energy. It is also seen that the pairing contribution to the spherical BCS energy minimum is considerably larger for the HJ interaction as compared to the CY. The desirability of spherical solutions for $Z<N=28$ nuclei for the HJ interaction is discussed, and it is argued that it cannot be obtained by including n-p pairing in the $T=1$ state. Modification of the Kuo and Brown renormalized matrix elements is suggested. Results for the oblate and prolate HFB solutions for Fe^{58} with HJ interaction are discussed, as these solutions have very close energy minima.

I. INTRODUCTION

One of the most engrossing problems in nuclear many-body theory is to formulate a program, both fundamental as well as practical, in which the properties of finite nuclei can be derived from the free nucleon-nucleon interaction. Since the publication of the pioneering work by Brueckner and collaborators in this field, a number of papers have appeared. The most straightforward way to carry out such a program is to use the Hartree-Fock theory, which may be regarded as a first approximation to the general scheme of Brueckner and which leads immediately to a shell-model description of nuclei. A recent improvement over the Hartree-Fock (HF) theory of nuclei has been given by Baranger,[1] who has incorporated into it the pairing aspect of the two-body interaction, employing the generalized Bogoliubov-Valatin transformation. This modified procedure, which goes by the name of Hartree-Fock-Bogoliubov (HFB) theory, has met with considerable success in the s-d shell for nuclei.

Results of a self-consistent calculation for the even Ti, Cr, and Fe isotopes for the HF, HFB, and spherical BCS approximations had been reported in a recent publication by one of the authors.[2] These calculations were carried out with a central potential having a Yukawa shape with its exchange mixture suitably adjusted to reproduce the energy levels of O^{18} and F^{18}. In that paper the main emphasis was put on the comparison of the prolate solutions obtained from HF and HFB approximations. The effect of pairing on such properties as the ground-state energies and intrinsic quadrupole moments was also studied. It was found that compared with HFB solutions, the spherical BCS solutions, in general, had higher ground-state energies and more pairing contributions to them; but for nuclei with $Z<N=28$, the BCS and HFB results were identical, both converging to spherical minima.

A serious drawback of this calculation was that the neutron and proton single-particle energies were taken to be the same; the effect of Coulomb repulsion amongst protons inside the Ca^{40} core as well as of the extracore protons was completely ignored. Consequently the ground-state energies obtained from the self-consistent calculations could not be compared with the experimental values.

In the present calculations, both the realistic Hamada-Johnson (HJ) and the same central Yukawa (CY) interactions are used and the effect of Coulomb interaction amongst the intracore protons is taken into account by taking different single-particle energies for protons and neutrons as obtained from the experimental data. For the extracore protons we make the Coulomb correction to the energy minima.

The choice for using the renormalized Kuo and Brown matrix elements[3] (KBRME) for the self-consistent calculations has been made primarily because they are the matrix elements of the realistic HJ interaction. Kuo and Brown have already demonstrated that the renormalized matrix elements give improved agreement, as compared with the bare ones, with the observed spectra and binding energy for the extracore nucleons of Ca^{42} and Sc^{42}. Their suitability in other nuclear-struc-

ture calculations has also been tested.[4] However, it may be mentioned here that both of these calculations include the $1g_{9/2}$ orbit, which is completely ignored in our self-consistent calculation. A calculation for the Sc^{42} spectrum, ignoring the $1g_{9/2}$ orbital, represents the trend of the spectrum as well as that obtained by Kuo and Brown; however, the binding energy of the extracore nucleons is decreased by about 0.5 MeV. The CY interaction also reproduces the Sc^{42} spectrum quite well. As the present work is limited to only the restricted-type of self-consistent calculations, bringing in $1g_{9/2}$ state along with the active p-f orbits will not cause any change in the properties associated with the intrinsic structure as it will enter as an unoccupied orbital in HF calculations. Since the $1g_{9/2}$ orbital has parity opposite to those of the p-f orbitals, it cannot mix with them because of parity conservation. It can affect the result only when other orbits of the same parity inside the core are also considered active in the calculation. Thus, even though inclusion of $1g_{9/2}$ improves the shell-model results, it cannot do so in the restricted type of self-consistent HF calculations. One might, in principle, expect an effect in a self-consistent HFB calculation because the $1g_{9/2}$ orbital might acquire an occupation probability greater than zero, which could renormalize the HF field in the HFB approximation. However, a little reflection shows that the renormalization of single-particle energies due to the addition of extracore nucleons lowers the single-particle energies of the p-f orbits but does not affect the $1g_{9/2}$ single-particle energy. Consequently its occupation probability will not be enough to affect the HFB results significantly.

The calculation with the HJ matrix elements will also enable us to make a direct comparison with the HF results obtained by Parikh and Svenne[5] for the p-f shell nuclei employing the matrix elements of Shakin, Waghmare, and Hull[6] for the Yale potential.[7]

As has been mentioned, the earlier[2] self-consistent HFB calculations were made only for the prolate shape, as their HF counterpart favored a prolate shape over oblate ones. But as the energy differences between prolate and oblate solutions were not very pronounced, one cannot be very sure that switching on the pairing force will not bring the oblate HFB solution down below the corresponding prolate HFB solution. Also, it is not very certain that all interactions favor a HF minimum of a specific shape. This has prompted us to report prolate as well as oblate solutions along with their characteristic properties derived from their intrinsic wave functions. Spherical BCS calculations for both the interactions (HJ and CY) are performed for the same reason.

The single-particle energies in MeV for neutrons are taken to be −8.35, −2.85, −6.28, and −4.22 and those for protons −1.07, 4.83, 0.72, and 2.43 corresponding to $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, and $2p_{1/2}$ states, respectively.

As in Ref. 2, the strengths corresponding to different two-nucleon states, of the CY interaction

$$V_{ST}(r) = V^0_{ST} e^{-r/\beta}/(r/\beta) \tag{1}$$

are given below:

$$V^0_{31} = -46.9 \text{ MeV}, \quad V^0_{13} = -34.4 \text{ MeV},$$

$$V^0_{33} = 19.4 \text{ MeV}, \quad V^0_{11} = 40.9 \text{ MeV}.$$

The range of the interaction is taken to be equal to the Compton wavelength of the pion.

The harmonic-oscillator wave functions used to evaluate the matrix elements for the CY interaction correspond to the oscillator range parameter $b = 2.0 \times 10^{-13}$ cm, in agreement with the value used by Kuo and Brown. However, this value is slightly different from the one used earlier[2] ($b = 2.05 \times 10^{-13}$ cm).

In order to make the paper self-contained, we give a brief description of the self-consistent formalism in Sec. II. The results of the calculation are described in Sec. III. Section IV contains the summary and discussion.

II. SELF-CONSISTENT FORMALISM

The self-consistent equations for HF and HFB calculations are obtained by invoking certain assumptions about the nuclear shapes and symmetries. These assumptions have been given in Ref. 2. However, it has been pointed out in the paper of Banerjee, Levinson, and Stephenson, Jr.[8] that the existence of symmetries under time reversal, reflection in the x-z plane, and rotation through π about the x or z axis in the HF density matrix follows directly from the general exchange character and finite range of the effective shell-model interaction. As a consequence of this one would not expect parity maxing in the single-particle wave functions. In an earlier paper Bassichis, Kerman, and Svenne[9] have shown that parity mixing is energetically unfavorable unless the tensor force is increased to nearly twice the normal strength. Systematic alteration of the HF shapes of the s-d-shell $N = Z$ nuclei as obtained in the calculation of Bar-Touv and Kelson[10] follows from the above mentioned features of the interaction.

There seems to be at present no reason to think that these conclusions should be restricted only to the intrinsic structure of the s-d-shell nuclei. A natural extension of these results would be their application to the study of the p-f shell nuclei.

However, in the present calculation the shape of the nuclei is restricted to axially symmetric only, and thus the test for the possible alteration of the shape for $N=Z$, as well as other cases, is out of the question. This will, however, be considered in a future work.

We would also like to mention the fact that the natural symmetries of the density matrix properties of the nuclear interaction are tested by Banerjee, Levison, and Stephenson, Jr.[8] only for the HF case; however, the same could be extended for the HFB density matrix without any contradiction.

One of the main conclusions in Ref. 2 was that the HFB formalism, as developed in the most general way by Baranger, when applied to specific cases yielded results identical to the use of the HF, implying an absence of pairing. In some other cases it yielded solutions identical to spherical BCS results. As HF equations, worked out by many authors, are available in the literature, we do not find it essential to provide those derivations here. The same is true in some sense for BCS equations derived for potentials with finite range (i.e., different from schematic potentials such as $Q\cdot Q$ and the pairing force), and for rigorous details one is referred to another paper of Baranger.[11] Also, the explicit results for the BCS equations incorporating pairing between n-n and p-p pairs outside a doubly closed core can be found in the Appendix of Ref. 2. We shall avoid repeating these equations as well. In order to make the paper brief but self-contained, we shall simply outline those steps of the HFB procedure which are essential and relevant for this paper.

A. HFB Procedure

The starting point will be the many-body Hamiltonian written below in the second-quantized form as

$$H=\sum_{\alpha\beta}\langle\alpha|\epsilon|\beta\rangle a_\alpha^\dagger a_\beta+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V_A|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \tag{2}$$

where ϵ in the present calculation corresponds to the single-particle energies for the neutron and proton outside the Ca^{40} core. The two-particle matrix elements are evaluated, as usual, between the antisymmetric two-particle states.

As usual, the pairing correlation in the HFB wave function is introduced by introducing the Bogoliubov transformation as given in Eqs. (7) and (8) of Ref. 2. Since this transformation does not conserve the number of particles, one introduces the parameters λ_n and λ_p, referred to as chemical potentials, and the Hamiltonian takes the modified form

$$\mathcal{H}=H-\lambda_n n_n-\lambda_p n_p. \tag{3}$$

Here n_n and n_p are the neutron and proton number operators. The ground state of the system in the HFB approximation is defined by the vacuum for the quasiparticle operator. The HFB equations can then be derived following either of the procedures given in work of Chandra[2] and Satpathy, Goss, and Banerjee.[12]

The HFB matrix that one obtains has the form

$$W=\begin{pmatrix}\tilde{\Gamma} & \Delta\\ \Delta & -\tilde{\Gamma}\end{pmatrix}, \tag{4}$$

where $\tilde{\Gamma}$ and Δ are given by

$$\tilde{\Gamma}_{jj'}^{m\tau_z}=(\epsilon_j-\lambda_{\tau_z})\delta_{jj'}+\sum_{j_1j_2m_1\tau_z'}\langle jm\tau_z, j_1m_1\tau_z'|V_A|j'm\tau_z, j_2m_1\tau_z'\rangle\rho_{j_1j_2}^{m_1\tau_z'}, \tag{5}$$

$$\Delta_{jj'}^{m\tau_z}=\tfrac{1}{2}\sum_{j_1j_2m_1}\langle jm\tau_z, j'\bar{m}\tau_z|V_A|j_1m_1\tau_z, j_2\bar{m}_1\tau_z\rangle\chi_{j_1j_2}^{m_1\tau_z}, \tag{6}$$

and all the symbols are defined in Ref. 2. It is obvious that in the absence of pairing, the matrix χ, and consequently Δ, is identically zero. This will make the HFB density matrix identical to that of the HF approximation. The matrix W can be diagonalized by a real orthogonal matrix[2] given by $0=\left(\begin{smallmatrix}u & -v\\ v & u\end{smallmatrix}\right)$; ρ and χ in terms of the u and v matrices are given as

$$\rho=v\bar{v},\quad \chi=-v\bar{u}. \tag{7}$$

It is trivial to show that ρ and χ commute with each other. This implies that these matrices can be simultaneously diagonalized by a real orthogonal matrix R. As $Rv\bar{v}\tilde{R}$ and $Rv\bar{u}\tilde{R}$ are diagonal, one can choose another orthogonal matrix Q such that

$$Rv\tilde{Q}Q\bar{v}\tilde{R}=V\tilde{V}=VV \tag{8a}$$

and

$$Rv\tilde{Q}Q\bar{u}\tilde{R}=V\tilde{U}=VU \tag{8b}$$

or

$$V=Rv\tilde{Q};\quad U=Ru\tilde{Q}, \tag{8c}$$

where V and U are diagonal matrices. These results imply that the quasiparticle transformation is carried out in three successive operations as shown by the following matrix relation:

$$\begin{pmatrix}A^\dagger\\ \bar{A}\end{pmatrix}=\begin{pmatrix}\tilde{Q} & 0\\ 0 & \tilde{Q}\end{pmatrix}\begin{pmatrix}U & V\\ -V & U\end{pmatrix}\begin{pmatrix}R & 0\\ 0 & R\end{pmatrix}\begin{pmatrix}a^\dagger\\ \bar{a}\end{pmatrix}. \tag{9}$$

The series of transformations as shown in preceding equation were also obtained in a general form by Bloch and Messiah.[13] As a result of these

transformations the HFB wave function written in the following BCS form also satisfies Eq. (9) of Ref. 2.

$$|\Phi_{\mathrm{HFB}}\rangle = \prod_i (U_i^p - V_i^p\, b_{i\nu}{}^{\dagger} b_{i\bar{\nu}}{}^{\dagger})(U_i^n - V_i^n\, b_{i\pi}{}^{\dagger} b_{i\bar{\pi}}{}^{\dagger})|0\rangle\,, \tag{10}$$

where the generalized particle operator $b^{\dagger}$ is related to particle operator $a^{\dagger}$ through the matrix R in the following way:

$$b_{i\tau_z}{}^{\dagger} = \sum_g R_{ig}^{\tau_z} a_{g\tau_z}{}^{\dagger}. \tag{11}$$

Fluctuation in the number of pairs of neutrons and protons results from the fact that $|\Phi_{\mathrm{HFB}}\rangle$ does not conserve the number of particles and can be easily evaluated in terms of U and V by using Eq. (10) in the following equation:

$$\sigma_{\tau_z}{}^2 = \langle\Phi_{\mathrm{HFB}}|n_{\tau_z}{}^2|\Phi_{\mathrm{HFB}}\rangle - \langle\Phi_{\mathrm{HFB}}|n_{\tau_z}|\Phi_{\mathrm{HFB}}\rangle^2. \tag{12}$$

This gives

$$\sigma_{\tau_z}{}^2 = \sum_i (U_i^{\tau_z} V_i^{\tau_z})^2. \tag{13}$$

$\sigma_{\tau_z}{}^2$ is the dispersion in the probability distribution of number of pairs around its mean value.

In order to start the HFB calculation an initial choice of the matrices u and v is essential. The appropriate choice of these matrices is not trivial. We first diagonalize the single-particle Hamiltonian H'

$$\langle m|H'|j'm\rangle = \epsilon_j \delta_{jj'} + \eta\langle jm|Q_0{}^2|j'm\rangle \tag{14}$$

for a suitable deformation parameter η with a negative or positive value for it according to whether an oblate- or prolate-shape calculation is needed. We then multiply each element of the first $N_{\tau_z}^0$ eigenvectors of the orthogonal matrix by a factor a, and the remaining eigenvectors by a factor a'. This will yield the starting matrix v. Similarly, a multiplication of the first $N_{\tau_z}^0$ eigenvectors by b and the remaining ones by b' will give us the matrix u. The multiplicative factors satisfy the following conditions:

$$a^2 + b^2 = 1; \quad b^2 \ll a^2 < 1; \tag{15a}$$

$$a'^2 + b'^2 = 1; \quad a'^2 = (1 - a^2)N_{\tau_z}^0/(N - N_{\tau_z}^0). \tag{15b}$$

In the above, a, b, a', and b' are taken to be positive; $N_{\tau_z}^0$ is the number of nuclear pairs of isotopic spin τ_z. N is the order of the orthogonal matrix.

From this set of u and v, initial ρ and χ matrices are set up and then iteration is continued until the self-consistent solution with desired accuracy is achieved.

The HFB matrix can also yield results identical to spherical BCS provided the initial values of u and v are chosen with the orthogonal matrix obtained for $\eta = 0$, and equal occupation probability is assigned to the states which have the same j value but differ in the projection quantum number.

III. DISCUSSION OF SELF-CONSISTENT RESULTS

A. Energy Minima for Self-Consistent Shapes

The computational results of the self-consistent calculations with the CY interaction and with the KBRME for the $2p$-$1f$ shell are given in Tables I and II, respectively. In calculating these we have used Eqs. (27)–(29) of Ref. 2.

As has been mentioned earlier, we have used different single-particle energies for the neutrons and protons and a different oscillator range parameter, so the numbers in Table I are bound to be different from those that appeared in Ref. 2. It is

TABLE I. Comparison of energy minima for Ti, Cr, and Fe isotopes obtained from the HF, HFB, and BCS solutions for the central Yukawa interaction. Pairing contributions to the solutions are compared. The energies are given in MeV.

	E_{HF}		E_{HFB}			Pairing energy for HFB		Pairing energy for
Isotope	Prolate	Oblate	Prolate	Oblate	E_{BCS}	Prolate	Oblate	BCS
Ti^{44}	−28.14	−25.74	−28.14	−25.92	−25.90	−0.00	−2.65	−4.29
Ti^{46}	−48.55	−46.52	−48.75	−47.24	−47.14	−1.42	−3.58	−5.21
Ti^{48}	−67.94	−66.60	−68.42	−67.74	−67.74	−2.19	−4.27	−4.81
Ti^{50}	−87.11	−86.78	−87.48	−87.48	−87.48	−2.05	−2.05	−2.04
Cr^{48}	−59.58	−56.77	−59.58	−57.26	−57.02	−0.02	−3.90	−6.03
Cr^{50}	−81.80	−79.96	−82.17	−80.93	−80.86	−1.70	−4.51	−5.51
Cr^{52}	−102.98	−102.73	−103.88	−103.88	−103.88	−2.84	−2.84	−2.85
Cr^{54}	−124.13	−120.86	−124.12	−122.52	−122.52	−0.11	−5.41	−5.82
Fe^{52}	−94.62	−92.40	−94.62	−93.37	−93.38	−0.02	−4.54	−4.95
Fe^{54}	−118.83	−118.54	−119.66	−119.66	−119.66	−2.36	−2.36	−2.36
Fe^{56}	−141.28	−138.75	−141.55	−140.53	−140.52	−1.82	−5.30	−5.54
Fe^{58}	−161.47	−161.19	−162.29	−161.62	−160.55	−3.28	−3.76	−6.90

clear from Table I that the HFB energy minima for the CY potential favor prolate shapes for the nuclei under consideration. The HFB solutions for $N=Z$ nuclei converge to the HF solutions for prolate shapes; but the oblate solutions for these cases converge to lower energy minima as compared to their corresponding HF minima. They have a considerable pairing effect, as is evident from the pairing energy for oblate shapes. For $Z<N=28$ nuclei, the oblate as well as the prolate HFB solutions converge to the energy minima for a spherical shape. In fact, the pairing energies for these nuclei are identical for both the prolate and oblate cases.

The results appearing in Table II for the KBRME have gross features which are quite similar to those of Table I. With the exception of Fe^{58}, for which the prolate and oblate HFB solutions are quite close to each other, the HFB solutions corresponding to prolate shapes have lower energy minima. For Fe^{58}, the oblate solution is only 0.01 MeV above the prolate solution. The HFB solutions for $N=Z$ nuclei are also similar to those of the CY interaction. There is some pairing for Cr^{48}, and the HFB solution is lower than the HF solution by 0.02 MeV. Unlike those for the CY, the HFB results for $Z<N=28$ nuclei with the HJ potential do not converge to spherical solutions. The spherical BCS minima lie considerably above the corresponding HFB minima. More specifically, $E_{\mathrm{HFB}}-E_{\mathrm{BCS}}$ for Ti^{50}, Cr^{52}, and Fe^{54} is -2.26, -6.92, and -9.15 MeV, respectively. In fact, the HFB solutions for these nuclei, with the exception of Ti^{50}, are similar to their corresponding HF solutions because in these cases the pairing is not very large. For Ti^{50}, the pairing energy is not very large. For Ti^{50}, the pairing energy is $\frac{1}{2}$ the amount of pairing energy corresponding to the BCS solution, whereas for Cr^{52} and Fe^{54} it is less than $\frac{1}{10}$ of its value for the BCS solution.

As for the CY, an over-all gain in binding energy due to pairing is not large for prolate shapes and the HJ potential. This conclusion is also true for the oblate HF and HFB solutions.

An oblate HF solution for Fe^{56} corresponding to the HJ potential is not obtained. However, if convergence is attempted, the solution should have an energy minimum higher that the corresponding oblate HFB solution, which, as one can see from Table II, is higher that the prolate HF and HFB solutions.

It would be interesting to compare the ground-state energies for the KBRME with the HF results of Parikh and Svenne[5] for the Yale potential. A comparison of these numbers shows that the HF ground-state energies for the HJ interaction are consistently lower than their corresponding values for the Yale potential. It is also seen that whereas for the HJ potential the HFB oblate solution for Fe^{56} lies above the prolate solution, the HF solution for an oblate shape favors a lower minimum for the Yale interaction. For Fe^{58}, convergence for the prolate HF solution for the Yale potential was not achieved,[5] but as mentioned earlier, for the HJ potential the oblate and prolate HFB solutions are quite close to each other.

In Table III we compare the calculated ground-state energies corresponding to solutions favoring minimum energies with the experimental values obtained with respect to the Ca^{40} core. The theoretical energies are corrected for Coulomb interaction amongst the extracore protons by using the work of Seeger.[14]

It is found that the theoretical binding energies

TABLE II. Comparison of energy minima for Ti, Cr, and Fe isotopes obtained from the HF, HFB, and BCS solutions for the Kuo and Brown renormalized matrix elements. Pairing contributions to the solutions are also compared. The energies are given in MeV.

	E_{HF}		E_{HFB}			Pairing energy for HFB		Pairing energy for
Isotope	Prolate	Oblate	Prolate	Oblate	E_{BCS}	Prolate	Oblate	BCS
Ti^{44}	-28.59	-26.41	-28.60	-26.71	-26.39	-0.00	-2.97	-5.81
Ti^{46}	-50.75	-47.72	-50.77	-48.37	-47.56	-0.58	-3.58	-7.55
Ti^{48}	-69.54	-67.86	-70.63	-68.91	-67.90	-2.85	-4.29	-8.16
Ti^{50}	-89.02	-87.92	-89.46	-88.33	-87.20	-3.64	-4.36	-8.33
Cr^{48}	-63.23	-57.97	-63.25	-58.80	-57.00	-0.17	-4.86	-9.31
Cr^{50}	-86.87	-81.23	-86.97	-82.95	-80.19	-1.12	-5.04	-9.83
Cr^{52}	-109.06	-105.86	-109.10	-106.73	-102.18	-0.88	-2.22	-9.85
Cr^{54}	-128.39	-124.70	-128.78	-126.79	-123.07	-2.67	-5.24	-10.86
Fe^{52}	-100.32	-95.25	-100.31	-96.97	-91.65	-0.04	-4.48	-10.38
Fe^{54}	-125.50	-124.67	-125.53	-125.26	-116.38	-0.97	-1.88	-10.18
Fe^{56}	-148.06		-148.25	-147.25	-139.88	-1.48	-4.49	-12.14
Fe^{58}	-167.68	-167.11	-168.74	-168.73	-162.98	-4.41	-4.90	-11.88

TABLE III. Comparison of ground-state energy minima (corrected for Coulomb energy) with the experimental binding energies for Ti, Cr, and Fe isotopes. The symbols P, O, and Sp in the parentheses stand for prolate, oblate, and spherical shapes, respectively. The energies are given in MeV.

	Central Yukawa		Kuo and Brown renormalized matrix elements		Experimental binding energy with respect to Ca^{40} core
Isotope	Nature of the solution	Energy minimum with Coulomb correction	Nature of the solution	Energy minimum with Coulomb correction	
Ti^{44}	HF(P)	−27.48	HF(P)	−27.94	−33.53
Ti^{46}	HFB(P)	−48.09	HFB(P)	−50.11	−56.13
Ti^{48}	HFB(P)	−67.77	HFB(P)	−69.98	−76.64
Ti^{50}	BCS(Sp)	−86.80	HFB(P)	−88.82	−95.73
Cr^{48}	HF(P)	−56.94	HFB(P)	−60.61	−69.66
Cr^{50}	HFB(P)	−79.57	HFB(P)	−84.37	−92.99
Cr^{52}	BCS(Sp)	−101.31	HFB(P)	−106.53	−114.29
Cr^{54}	HF(P)	−121.59	HFB(P)	−126.24	−131.95
Fe^{52}	HF(P)	−88.74	HF(P)	−94.44	−105.63
Fe^{54}	BCS(Sp)	−113.86	HFB(P)	−119.73	−129.69
Fe^{56}	HFB(P)	−135.82	HFB(P)	−142.39	−150.20
Fe^{58}	HFB(P)	−156.62	HFB(P≅O)	−163.07	−167.89

are quite close to the experimental numbers. It is also seen that the numbers for the HJ interaction show better agreement. This is not surprising, since the $T=1$ force in the CY is somewhat weaker than in the HJ interaction. It is also interesting to note that the theoretical binding energy per nucleon improves and comes closer to the experimental value with the increase in neutron number.

B. Fluctuation in the Number of Pairs

Fluctuation in the number of pairs as calculated by using Eq. (13) is presented in Table IV along with the chemical potentials. The pairing energy shown in Tables I and II shows the over-all effect of pairing on the binding energy, but it does not tell us anything about its origin. A calculation on fluctuation is able to provide us with this information.

From Table IV it is clear that there is no pairing in Ti^{44} and Fe^{52} for either of the two interactions. This conclusion is arrived at by examining the pairing energy for the prolate HFB solution. For the CY potential, pairing between neutron pairs is effective only for Ti^{46}, Ti^{48}, Cr^{50}, and Fe^{58} and between protons for all nuclei with $Z<N=28$ and Fe^{56}. In the solitary case of Fe^{58}, pairing between neutron as well as proton pairs is found to be effective. This is due to the fact that the HF gap for protons (G_p) and neutrons (G_n) is quite small (less than 1.0 MeV). In fact, for neutrons it is only 0.48 MeV. The HF gap is defined as the energy difference between the last occupied and first unoccupied state.

TABLE IV. Comparison of neutron and proton chemical potentials (in MeV), fluctuation in the number of neutron and proton pairs corresponding to prolate HFB solutions with Yukawa potential (CY) and KBRME. The values are also given for the oblate HFB solution with the HJ interaction for Fe^{58}.

	No. of neutron pairs	No. of proton pairs	Fluctuation in number of pairs				Chemical potential			
			CY		KBRME		CY		KBRME	
Isotope			σ_n^2	σ_p^2	σ_n^2	σ_p^2	λ_n	λ_p	λ_n	λ_p
Ti^{44}	1	1	0.00	0.00	0.00	0.00	−11.759	−4.498	−12.213	−4.951
Ti^{46}	2		0.52	0.00	0.16	0.00	−10.077	−6.093	−10.465	−7.096
Ti^{48}	3		0.72	0.00	0.81	0.00	−9.614	−7.344	−9.661	−8.450
Ti^{50}	4		0.00	0.77	0.80	0.09	−9.018	−8.336	−9.112	−9.760
Cr^{48}	2	2	0.00	0.00	0.04	0.04	−12.130	−4.888	−12.692	−5.426
Cr^{50}	3		0.63	0.00	0.36	0.00	−11.060	−6.499	−11.498	−7.530
Cr^{52}	4		0.00	1.04	0.32	0.00	−10.365	−8.051	−10.423	−9.138
Cr^{54}	5		0.00	0.00	0.75	0.00	−9.480	−9.469	−9.493	−10.357
Fe^{52}	3	3	0.00	0.00	0.00	0.00	−12.868	−5.595	−13.317	−6.062
Fe^{54}	4		0.00	0.81	0.16	0.27	−11.789	−7.722	−11.934	−7.874
Fe^{56}	5		0.00	0.63	0.25	0.36	−10.944	−8.474	−10.759	−9.456
Fe^{58}	6		0.72	0.54	0.72	0.54	−10.183	−10.101	−10.128	−10.571
Fe^{58} (0)	6				0.72	0.72			−10.617	−11.381

With the HJ potential, pairing is found to be effective only in neutron pairs in Ti^{46}, Ti^{48}, Cr^{50}, Cr^{52}, and Cr^{54}. There are no cases where pairing correlation between proton pairs exists. In almost all other cases pairing is effective between both types of pairs. For Cr^{48} there is practically no pairing correlation for either of the two interactions, and examination of the Hf gap shows that G_n and G_p are quite large (~2.5 MeV) for both cases.

It is quite interesting to note that for $Z < N = 28$ nuclei, pairing exists between proton pairs for the CY and is very strong between neutron pairs and weak between proton pairs for the HJ interaction. We offer the following explanation for understanding this.

With the CY potential, the occupied single-particle neutron states have wave functions with maximum components corresponding to $j = \frac{7}{2}$. When pairing is switched on, it tries to increase the occupation probability in the neutron $j = \frac{7}{2}$ state. This is possible only when the HF field for neutrons is modified, which has the effect of modifying the proton density matrix. This induces occupation probabilities in proton states which were unoccupied in the HF approximation. When the HFB minimum is approached for these cases, the $j = \frac{7}{2}$ state is completely occupied with neutrons, thus giving no pairing contribution. On the other hand, the protons in such a situation only partially occupy the $j = \frac{7}{2}$ state and extend a little over other single-particle states, giving rise to pairing, which is shown by the fluctuation in the number of proton pairs.

The HJ interaction is quite different from the simple CY in structure and has quite different HF spectra for these nuclei. The wave functions for the four occupied neutron states in this case do not have the largest component corresponding to $j = \frac{7}{2}$. This makes one of the HF states having a $j = \frac{7}{2}$ component unity in the family of unoccupied HF states. When pairing is introduced, it tries to occupy this state as well, and since other states exist between $m = \frac{7}{2}$ and the upper-most occupied state, they also become partially populated. As a consequence the $j = \frac{7}{2}$ spherical state does not become fully occupied by eight neutrons but instead shares the neutrons with other single-particle states because of the partial occupation probability of the deformed HF states.

C. Chemical Potential

When the pairing force is identically zero, the chemical potential denotes the Fermi energy level. In HFB calculations it indicates the approximate position of the Fermi level. As a result of this, one could study the changes in the approximate position of the Fermi levels for neutrons and protons as a pair of neutrons or protons is added to the system in the presence of pairing. In Table IV we list the chemical potential for protons and neutrons for both interactions corresponding to HFB shapes with minimum energies.

A comparison of neutron and proton chemical potentials (λ_n and λ_p) shows that except for Fe^{56} and Fe^{58} these quantities are usually higher (less negative) for the CY interaction. It is also noted that, for both interactions, the addition of neutron pairs for a fixed number of protons increases the neutron chemical potential λ_n somewhat linearly, but the value of λ_p decreases much faster than the increase in λ_n. Such a trend in the shift of chemical potential is not surprising and can be easily understood by closely examining the behavior of

TABLE V. Comparison of quadrupole moment (in units of $b^2 = 4.0 \times 10^{-26}$ cm^2) and hexadecapole moments (in units of b^4) for Ti, Cr, and Fe isotopes for shapes corresponding to minimum energies and obtained from the central Yukawa potential (CY) and KBRME. The values for Fe^{58} for the oblate shape with the HJ interaction are also given. P, O, and Sp stand for prolate, oblate, and spherical shapes.

	CY					KBRME			
Isotope	Solution	Q_n^2	Q_p^2	Q_n^4	Q_p^4	Solution	Q_n^2	Q_p^2	Q_n^4	Q_p^4
Ti^{44}	HF(P)	10.20	10.33	33.39	33.50	HF(P)	10.15	10.29	32.78	32.90
Ti^{46}	HFB(P)	12.07	10.12	25.70	32.22	HFB(P)	14.81	10.48	25.97	32.17
Ti^{48}	HFB(P)	10.04	9.36	18.35	30.24	HFB(P)	15.68	10.59	13.64	31.50
Ti^{50}	BCS(Sp)	0.00	0.00	0.00	0.00	HFB(P)	16.10	10.47	3.59	28.85
Cr^{48}	HF(P)	14.52	14.67	22.78	22.64	HFB(P)	15.70	15.82	24.61	24.23
Cr^{50}	HFB(P)	16.64	14.95	13.53	21.22	HFB(P)	20.59	16.16	16.47	22.12
Cr^{52}	BCS(Sp)	0.00	0.00	0.00	0.00	HFB(P)	21.61	16.11	−0.87	20.35
Cr^{54}	HF(P)	13.79	14.06	15.94	20.80	HFB(P)	19.95	15.98	−9.23	19.23
Fe^{52}	HF(P)	10.66	10.76	−12.27	−12.30	HF(P)	22.33	22.16	14.91	12.72
Fe^{54}	BCS(Sp)	0.00	0.00	0.00	0.00	HFB(P)	22.12	21.29	−6.26	9.09
Fe^{56}	HFB(P)	13.93	14.24	12.09	9.37	HFB(P)	22.61	19.83	−19.62	4.59
Fe^{58}	HFB(P)	14.78	14.88	−8.85	−1.61	HFB(P)	17.78	18.48	−17.64	0.93
Fe^{58}						HFB(O)	−19.49	−15.85	4.63	22.72

the HF field. The HF field depends on the $T=1$ and $T=0$ force, as well as on the density matrix for protons and neutrons. This matrix changes as the number of protons or neutrons changes. An increase in the number of neutrons changes the density matrix, which directly affects the HF field for protons. For a fixed number of protons, even if we assume that the proton density matrix remains unchanged in the $|jm\rangle$ representation, as the number of neutrons increase, the HF field for the protons in the upper-most occupied orbit is modified by $T=1$ and $T=0$ neutron-proton forces. Since the $T=1$ and $T=0$ force has an over-all interaction, the upper-most occupied orbit is lowered with an increase in neutron number. Hence the value of the chemical potential for protons is lowered. The neutron chemical potential, on the other hand, is mostly affected by the added neutrons and very little by protons. Therefore, only the $T=1$ force modifies the HF field for neutrons. This lowers to some extent the state which is now occupied by the added neutrons but was previously unoccupied. A similar argument will hold for the behavior of λ_p as the proton number is changed.

D. Intrinsic Multipole Moments

The values of neutron and proton intrinsic quadrupole and hexadecapole moments are displayed in Table V. These quantities are evaluated by using the following expressions:

$$Q_{\tau_z}{}^2 = \left(\frac{16\pi}{5}\right)^{1/2} \sum_{ij} \langle i|r^2 Y_2^0(\theta,\phi)|j\rangle \rho_{ij}^{\tau_z}, \tag{16}$$

$$Q_{\tau_z}{}^4 = \left(\frac{16\pi}{9}\right)^{1/2} \sum_{ij} \langle i|r^4 Y_4^0(\theta,\phi)|j\rangle \rho_{ij}^{\tau_z}, \tag{17}$$

where $|i\rangle$ stands for $|jm\rangle$. Since these quantities involve density matrices for neutrons and protons separately, a study of these numbers gives an insight into the structure of the single-particle wave functions.

An inspection of the above-mentioned table shows that the respective values of multipole moments

TABLE VI. Comparison of neutron and proton pickup strengths calculated from the intrinsic wave functions corresponding to solutions with minimum energies and obtained for the central Yukawa potential (CY) and KBRME. P, O, and Sp stand for prolate, oblate, and spherical shapes.

Isotope	Interaction	Solution	Neutron pickup strength				Proton pickup strength			
			$j=\frac{1}{2}$	$j=\frac{3}{2}$	$j=\frac{5}{2}$	$j=\frac{7}{2}$	$j=\frac{1}{2}$	$j=\frac{3}{2}$	$j=\frac{5}{2}$	$j=\frac{7}{2}$
Ti^{44}	CY	HF(P)	0.1089	0.3987	0.1837	1.3087	0.1227	0.4216	0.1694	1.2862
	KBRME	HF(P)	0.1030	0.4040	0.1581	1.3349	0.1167	0.4286	0.1452	1.3096
Ti^{46}	CY	HFB(P)	0.1164	0.4584	0.2244	3.1984	0.1062	0.4096	0.1278	1.3560
	KBRME	HFB(P)	0.1256	0.5640	0.2598	3.0496	0.1188	0.4964	0.1098	1.2744
Ti^{48}	CY	HFB(P)	0.1080	0.4592	0.2622	5.1696	0.0722	0.3048	0.1086	1.5136
	KBRME	HFB(P)	0.2930	0.9900	0.4482	4.2656	0.1206	0.5488	0.0882	1.2392
Ti^{50}	CY	BCS(Sp)	0.0009	0.0068	0.0033	7.9888	0.0049	0.0146	0.0518	1.9287
	KBRME	HFB(P)	0.4656	1.4940	0.6012	5.4392	0.1222	0.5948	0.0720	1.2112
Cr^{48}	CY	HF(P)	0.0763	0.5216	0.1290	3.2731	0.0868	0.5533	0.1187	3.2412
	KBRME	HFB(P)	0.1134	0.6644	0.2580	2.9640	0.1264	0.6996	0.2346	2.9384
Cr^{50}	CY	HFB(P)	0.2792	0.7792	0.5298	4.4136	0.0900	0.6364	0.1038	3.1696
	KBRME	HFB(P)	0.4932	0.9824	0.8820	3.6408	0.1290	0.8328	0.2130	2.8256
Cr^{52}	CY	BCS(Sp)	0.0002	0.0016	0.0014	7.9967	0.0076	0.0234	0.0866	3.8825
	KBRME	HFB(P)	0.5924	1.1312	1.0926	5.1808	0.1130	0.8780	0.1806	2.8288
Cr^{54}	CY	HF(P)	0.4365	0.9719	0.9128	7.6789	0.0773	0.5130	0.0781	3.3316
	KBRME	HFB(P)	0.6808	1.9044	1.6134	5.8016	0.0974	0.8780	0.1608	2.8640
Fe^{52}	CY	HF(P)	0.0003	0.2074	0.0477	5.7445	0.0004	0.2241	0.0431	5.7324
	KBRME	HF(P)	0.6554	1.1686	0.9111	3.2649	0.7244	1.1991	0.7874	3.2891
Fe^{54}	CY	BCS(Sp)	0.0001	0.0006	0.0009	7.9984	0.0071	0.0227	0.0885	5.8818
	KBRME	HFB(P)	0.6686	1.2296	0.9828	5.1168	0.6764	1.2088	0.6894	3.4256
Fe^{56}	CY	HFB(P)	0.4838	1.0592	0.7998	7.6552	0.2080	0.7100	0.2712	4.8080
	KBRME	HFB(P)	0.7432	1.9168	1.8384	5.5016	0.6778	1.3488	0.3816	3.5928
Fe^{58}	CY	HFB(P)	0.6700	2.0240	1.7100	7.5968	0.2094	0.8316	0.1632	4.7944
	KBRME	HFB(P)	0.8592	2.7276	2.0490	6.3640	0.5650	1.3572	0.2994	3.7792
Fe^{58}	KBRME	HFB(O)	1.0844	2.6912	1.9326	6.2912	0.3940	1.7000	0.4200	3.4864

for Ti^{44} for both types of interactions are quite close to each other, which signifies that for Ti^{44} the occupied single-particle HF wave functions are not very different when their components are compared. This argument is true to some extent for the structure of the occupied states corresponding to Cr^{48}, since the quadrupole moment and hexadecapole moment for both types of interactions do not differ much. However, in the case of Fe^{52}, another $N=Z$ nucleus, the structure is expected to be quite different. This is because a comparison of the wave functions obtained from diagonalizing the Γ_{final} matrix of the HFB approximation for both cases shows that the equivalent occupied states for the CY interaction are $m=\frac{1}{2}$, $m=\frac{3}{2}$, and $m=\frac{5}{2}$ in increasing order of energy eigenvalue, whereas for the HJ interaction the upper-most occupied state is not $m=\frac{5}{2}$ but $m=\frac{1}{2}$, with the maximum component corresponding to the $j=\frac{5}{2}$ state. This change in the last occupied state causes a change in sign for the value of hexadecapole moment.

For nuclei with $Z<N=28$ the values for the multipole moments for the CY interaction are identically zero, but it is not so for the HJ potential. In fact their values for the HJ interaction are quite large. This is because for a given j value, the contribution to multipole moments with positive sign comes from the lower projection quantum numbers. Thus, when other states with lower projection quantum numbers come down and become occupied and the states with higher projection quantum numbers are pushed up, the contribution to the multipole moment becomes additive and thus more pronounced.

E. Spectroscopic Factor

We present here the pickup strengths for neutrons and protons separately in Table VI. The following expressions have been used to evaluate these strengths:

$$S_j^{\tau_z} = (2j+1)v_{j\tau_z}{}^2 \quad \text{(for BCS)}$$
$$= \sum_m^{\text{occ}} (C_{jm}^{\alpha\tau_z})^2 \quad \text{(for HF)} \tag{18a}$$
$$= \sum V_{\alpha m}{}^2 (C_{jm}^{\alpha\tau_z})^2 \quad \text{(for HFB)}, \tag{18b}$$

where $V_{\alpha m}$ is given by Eq. (8) and the $C_{jm}^{\alpha\tau_z}$'s are the components of the orthogonal matrix (R) which diagonalizes the HFB density matrix. It is to be noted that in the absence of pairing Eq. (18b) reduces to the HF value, and for no deformation it reduces to the BCS result.

The values of the pickup strengths for neutrons and protons corresponding to Ti^{44} calculated for both the interaction are almost equal. This follows from the fact that the overlaps of occupied states corresponding to both interactions are nearly 100%. The pickup strengths for Ti^{46} are also not very different for these interactions. The neutron pickup strength for Ti^{48} corresponding to the CY is somewhat different from its counterpart for the HJ interaction but the values for the proton pickup strength are not much different. For Ti^{50} the CY interaction gives a spherical HFB solution with a neutron pickup strength slightly smaller than 8 for this $j=\frac{7}{2}$ state. This is the value for complete occupation. Similarly, the proton pickup strength for the $j=\frac{7}{2}$ state is slightly smaller than the number of protons (i.e., two). For the HJ interaction the pickup strength for neutrons is distributed over all the single-particle states with $j=\frac{7}{2}$ and has the value 5.44. A similar thing happens for the proton case. The Cr isotopes also follow a somewhat identical trend. For Fe isotopes the differences in the individual values for the pickup strengths corresponding to these interactions are quite pronounced. This is so because as the number of neutrons and protons increases, the structure of the HF field in the HFB approximation for different states for these interactions becomes more dissimilar and this shows up in the calculation of pickup strengths through their wave functions.

F. Results for Fe^{58}

It has been pointed out that prolate and oblate HFB solutions for the HJ interaction for this isotope have energy minima which are very close to each other. In fact the prolate solution is lower than the oblate only by 0.01 MeV. This is somewhat interesting because of the fact that the corresponding solutions for the CY interaction are not so close to each other. However, even for the CY potential the prolate-oblate differences for this isotope are comparably much smaller than the differences in the prolate and oblate HFB minima for other nuclei under consideration, with the exception of $Z<N=28$ nuclei. For $Z<N=28$ nuclei the HFB solutions are spherical. We give here in Table VII results of the diagonalization of the Γ^{HFB} self-consistent matrices for prolate as well as oblate shapes for the HJ interaction. From Table IV it is seen that for this nucleus, fluctuation in the number of neutron and proton pairs for an oblate shape is equal to 0.72. The chemical potentials for this solution corresponding to neutrons and protons lie lower than their respective values in the prolate HFB solution. Obviously, intrinsic neutron and proton quadrupole moments will have negative values, which is seen from the Table V. The neutron pickup strengths for oblate solutions

do not differ much from the prolate values. However, they are somewhat different for protons.

IV. SUMMARY AND DISCUSSION

The main motivation of this work has been to make a comparative study of the properties of even Ti, Cr, and Fe isotopes with the CY potential and with the KBRME for the HJ potential. It is found that for the CY interaction, HFB calculations for prolate shapes have lower minima than their respective oblate solutions. The only exceptions to these are nuclei with $Z < N = 28$, for which the oblate and prolate HFB solutions converge to spherical ones with the same minima. For CY interactions, the oblate HFB solutions corresponding to $N = Z$ nuclei have considerable pairing correlation, a feature completely absent in the prolate solutions for these nuclei.

The HFB calculations with the HJ interaction also usually favor prolate minima over the oblate ones; the only exception being Fe^{58} for which both the prolate and oblate shapes have very close energy minima. However, in detail, the results for the HJ differ much from the results for the CY interaction. The prolate solutions for $N = Z$ nuclei with the HJ interaction do not favor pairing correlations except for Cr^{48}, where there is some correlation. All other nuclei, including $Z < N = 28$ have pairing correlations for prolate HFB shapes. With the HJ interaction, the spherical BCS solutions for all the nuclei under consideration have energy minima higher than their prolate and oblate counterparts. The BCS solutions with this interaction usually have pairing energies much larger than the BCS solutions for the CY. In some cases they are even slightly more than four times the value for the CY (see example Fe^{54} in Tables I and II).

TABLE VII. Single-particle energy eigenvalues and eigenfunctions for neutrons and protons for Fe^{58}. The eigenfunctions are obtained by diagonalizing the self-consistent prolate and oblate HF terms of the HFB matrices for the HJ interaction. In columns labeled $p_{1/2,k}$, $p_{3/2,k}$, ..., etc., the components corresponding to the projection quantum number are given.

Neutron wave functions						Proton wave functions					
ϵ_k	k	$p_{1/2,k}$	$p_{3/2,k}$	$p_{5/2,k}$	$f_{7/2,k}$	ϵ_k	k	$p_{1/2,k}$	$p_{3/2,k}$	$f_{5/2,k}$	$f_{7/2,k}$
					Fe^{58} (prolate)						
−4.9540	$\frac{5}{2}$			0.9803	0.1977	−0.6618	$\frac{5}{2}$			0.9770	0.2134
−7.8605	$\frac{1}{2}$	0.7814	0.3738	0.4778	0.1460	−4.2000	$\frac{1}{2}$	0.7339	0.3853	0.5330	0.1698
−8.7346	$\frac{3}{2}$		−0.4676	0.8834	0.0310	−4.8356	$\frac{3}{2}$		−0.4735	0.8808	0.0073
−9.7660	$\frac{7}{2}$				1.0000	−5.9160	$\frac{7}{2}$				1.0000
−10.1913	$\frac{3}{2}$		0.8073	0.4125	0.4220	−6.3933	$\frac{3}{2}$		0.7942	0.4233	0.4359
−11.8404	$\frac{1}{2}$	−0.1759	−0.5265	0.7842	−0.2772	−8.0335	$\frac{1}{2}$	−0.2734	−0.4899	0.7993	−0.2153
−13.6384	$\frac{5}{2}$			−0.1977	0.9803	−10.1748	$\frac{5}{2}$			−0.2134	0.9770
−14.6511	$\frac{1}{2}$	−0.5582	0.4500	0.3828	0.5825	−10.9298	$\frac{1}{2}$	−0.5870	0.4998	0.2620	0.5805
−17.0845	$\frac{3}{2}$		−0.3600	−0.2224	0.9061	−13.2862	$\frac{3}{2}$		−0.3808	−0.2122	0.9000
−19.1985	$\frac{1}{2}$	0.2164	−0.6169	−0.1005	0.7500	−14.9887	$\frac{1}{2}$	0.2051	−0.6014	−0.0919	0.7667
					Fe^{58} (oblate)						
−5.0725	$\frac{1}{2}$	−0.4093	0.2072	0.8837	−0.0928	−0.6625	$\frac{1}{2}$	−0.3872	0.2533	0.8777	−0.1244
−6.8782	$\frac{3}{2}$		0.2358	0.9310	−0.2787	−2.8668	$\frac{3}{2}$		0.2239	0.9236	−0.3111
−8.1631	$\frac{1}{2}$	0.3474	−0.7219	0.3789	0.4633	−4.0282	$\frac{1}{2}$	−0.2944	0.6974	−0.4039	−0.5136
−10.7398	$\frac{1}{2}$	−0.6428	0.0382	−0.2301	0.7297	−6.9549	$\frac{5}{2}$			0.8684	−0.4959
−10.9643	$\frac{5}{2}$			0.8486	−0.5291	−7.2658	$\frac{1}{2}$	−0.6585	0.1152	−0.2232	0.7094
−11.2890	$\frac{3}{2}$		−0.4359	0.3577	0.8259	−7.5310	$\frac{3}{2}$		−0.4217	0.3796	0.8235
−15.1066	$\frac{1}{2}$	0.5464	0.6591	0.1505	0.4943	−11.5074	$\frac{1}{2}$	−0.5743	0.6604	0.1289	0.4663
−15.2564	$\frac{5}{2}$			0.5291	0.8486	−11.7140	$\frac{5}{2}$			0.4959	0.8684
−16.0887	$\frac{3}{2}$		0.8686	−0.0732	0.4901	−12.3364	$\frac{3}{2}$		0.8787	−0.0532	0.4745
−18.3067	$\frac{7}{2}$				1.0000	−14.5216	$\frac{7}{2}$				1.0000

It is interesting to see that the ground-state energies, corresponding to the solutions with minimum energies and corrected for Coulomb interaction due to extracore protons, are quite close to the experimental values for both the interactions. The agreement is somewhat better with the HJ than with the CY interaction.

With the addition of neutrons and protons to the Ca^{40} core, the self-consistent calculations for these isotopes show differences in the intrinsic structure obtained for these interactions. As a result, the multipole moments and pickup strengths for these isotopes evaluated from the self-consistent wave functions differ considerably, in general, as the atomic mass numbers of the isotopes change.

From the results with the CY interaction and the calculations of Rustgi *et al.*[15] for V^{51} and Cr^{52} and of Lips and McEllistrem[16] for p-f shell nuclei, it is desirable to obtain self-consistent spherical minima for $Z < N = 28$ nuclei, which the Kuo and Brown matrix elements used in this work fail to generate. This might suggest some modifications of the matrix elements which generate the desired HFB spherical solutions for these cases but preserve the ground-state energies around the experimental values. Of course, one might also consider the approximations used in our work. The most prominent looking might be n-p pairing in $T = 1$ states. However, it has been concluded in the work of Chen and Goswami[17] that the contribution from this pairing decreases rapidly as the difference in the number of neutrons and protons increases. According to this, the n-p pairing in $T = 1$ state should not be important for Ti^{50} where, if only extracore particles are compared, the number of neutrons is considerably larger than protons. Thus the absence of a spherical solution with the HJ interaction for Fe^{54}, and to a lesser extent for Cr^{52}, could be attributed to the absence of n-p pairing if this interaction had yielded a spherical HFB minimum with just the pairing between identical particles for Ti^{50}. One might advance one other concrete reason for considering n-p pairing. This could be that the matrix elements for n-p correlation exist just as do the matrix elements giving rise to n-n and p-p pairing. But the self-consistent minima are not determined just by the existence of these terms. As an example, for $N = Z$ nuclei the effect of pairing matrix elements corresponding to n-n and p-p, which are always there, is completely absent for the prolate solutions in the CY case and partially absent in HJ case. The effect, however, exists in spherical solutions, but they are not the solutions with minimum energies and there is no guarantee that using n-p pairing will bring them down below the axially symmetric solutions. In fact, it may happen that the inclusion of n-p pairing term might not at all affect the spherical solution and may be identical to the one obtained by just including n-n and p-p pairing. This is somewhat similar to HFB yielding HF solutions. Also, for writing HFB equations, one does not have to explicitly make such assumptions as

$$\langle \alpha\beta | V_A | \gamma\beta \rangle = 0 \quad \text{unless } \alpha \equiv \gamma,$$

$$\langle \alpha\beta | V_A | \gamma\bar{\gamma} \rangle = 0 \quad \text{unless } \bar{\alpha} = \beta,$$

which are essential for the derivation of the BCS equations for finite-range interactions. However, these matrix elements are ineffective in HFB solutions for $Z < N = 28$ nuclei with the CY interaction, where the solutions converge to BCS results.

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Energy per Particle of Neutron Matter near Nuclear Density*

Sara L. Schlenker† and E. L. Lomon
Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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The energy per particle of neutron matter in the density range 10^{13} to 10^{15} g/cm^3 was calculated self-consistently using recent nuclear potentials: the Bressel-Kerman-Rouben potential and the boundary-condition model of Feshbach and Lomon. At low densities the results are in good agreement with other calculations of the energy density of neutron matter. At higher densities, the predicted energy density depends more strongly on the specific potential used. More recent potentials yield somewhat lower pressures for neutron matter (hence a smaller mass range for neutron stars) than those predicted with the Levinger-Simmons potential which has been used as the basis for calculations of neutron-star structure.

I. INTRODUCTION

The matter of which real neutron stars are composed is a complicated substance. Near nuclear densities it will contain mostly a Fermi sea of neutrons, but at lower densities the neutrons will cluster with the remaining protons into nuclei, and at higher densities mesons and baryon isobars will be formed in such great numbers that the neutrons will no longer dominate. Even near nuclear density the effects of protons, electrons, and muons will be nonnegligible, and idealized neutron matter will only approximate the real situation. However, a good knowledge of the properties of idealized neutron matter is basic to understanding the behavior of neutron stars, since it does provide a starting point for perturbation calculations and extrapolations which take into consideration the more complex effects. A study of neutron matter can also serve to point out just what degree of uncertainty arises in the energy per particle due to the lack of knowledge of the nuclear potential.

This paper presents calculations of the energy per particle in neutron matter for two recent nuclear potentials with the matrix-inversion method of solving the Bethe-Goldstone equation[1,2] in Brueckner[3] theory. The potentials used are the Bressel-Kerman-Rouben potential[4] and the boundary-condition model of Feshbach and Lomon.[5] The calculations were made using existing nuclear-matter programs developed by Wang and Spencer,[6] with modifications introduced to make them applicable to neutron matter. These modifications consist of dropping $T=0$ nucleon pair contributions and replacing statistical factors of $\frac{1}{2}(2T+1)=\frac{3}{2}$ by unity, recognizing that neutron pairs are in $T=1$, $T_z=1$ states only. In addition, one need only note that the density of nuclear matter is twice that of neutron matter for a given Fermi momentum.

II. CALCULATIONS

The energy per particle in neutron matter is found using the Brueckner reaction matrix G which acts on free two-particle states and is defined by the Bethe-Goldstone equation:

$$G = v + v\frac{Q}{e}G, \tag{1}$$

where v is the internucleon potential, Q is an exclusion operator which limits the intermediate states to those above the Fermi sea, and e is an energy denominator involving the single-particle potentials. This formalism includes all the effects of two-body clusters of particles interacting via two-body forces, and has been described extensively elsewhere in the literature.[2]

In order to introduce a partial-wave separation of the Bethe-Goldstone equation, it is necessary to remove the angular dependence of the operators Q and e. For this work, Q was replaced by its an-