Revista Brasileira de Ffsica, Vol. 7, Nº 3, 1977

Energy Levels and BE(2) Transition Rates in the Hartree-Fock Approximation with the Skyrme Force*

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Recebido em 16 de Julho de 1977

The Hartree-Fock approximation, with the Skyrme force, is applied to the $A=4n$ type of nuclei in the s-d shell. Energy levels and electric quadrupole transition probabilities within the ground state band are calculated from the projected states of good angular momentum. Strong approximations are made but the results concerning the spectra are better than those obtained with more sophisticated density independent two-body interactions. The transition rates are less sensitive to the interactions, as previously verified.

A aproximação de Hartree-Fock, com a força de Skyrme, é aplicada a núcleos da camada s-d, do tipo $A = 4n$. A partir dos estados projetados, com momento angular bem definido, calculam-se os níveis de energia e as probabilidades de transição de quadrupolo elétrico da banda fundamental. Apesar das aproximações feitas, os espectros de energia são melhores que os obtidos com interações mais sofisticadas, de dois corpos, independentes da densidade. As probabilidades de transição são menos sensíveis às interações, conforme já constatado.

† Work partially supported by FINEP (Brazil).
* With a fellowship from FAPESP (Brazil).
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1. INTRODUCTION

In the past few years, the density-dependent effective interactions have been used, in the Hartree Fock approximation, to explain many structure properties of the spherical and deformed nuclei[1-3]. In that line, the work of D. Vautherin and D.M. Brink (hereafter referred to as VB) used the Skyrme interaction to study spherical nuclei. Later on, D. Vautherin[4] used the same interaction to obtain some properties of axially symmetric nuclear systems. Zofka and Ripka[5] (ZR) studied the light deformed nuclei using a modified version of Negele's effective interaction. Among others, one should mention the Modified Delta Interaction (MDI) of Moszkowiski[6], who also studied *s-d* shell nuclei.

In this paper, we calculate several nuclear properties, using the HF approximation with the Skyrme force. Our results contribute with an extra information that the previous papers did not include; we performed the angular momentum projections of the HF wave functions in order to obtain the nuclear eriergy levels of the quasi-rotational spectra. This has been done many times in the past, by different authors[7,8], with density independent two-body interactions.

One could still use the same computational programs, but the storage of the interaction matrix elements would become impossible due to the new density dependence. As we had in mind to work with the light nuclei of the *s-d* shell, we assumed the O^{16} to behave as an inert core, and we had to truncate the expansion of independent particle wave functions to the small *s-d* subspace of shell model wave-functions. There were 24 single particle states available to our valence nucleons. Time reversal and charge symmetry allowed of a further reduction.

Our initial aim was to study all A = $4n$, *s-d* shell, nuclei. However, projection was used to obtain the energy levels of the fundamental band of Ne^{20}, Mg^{24} and Si^{28} only, because it would be highly expensive to repeat the calculation for S^{32} and Ar^{36}. The B(E2) transition rates, being essentially given by matrix elements of a one-body operator, allowed the calculation to go up to S^{32}; there are no available experimental data on B(E2) rates for Ar^{36}. We assumed these nuclei to be axially symmetric, although Mg^{24} and S^{32} could be considered as tri-axial.

As we truncate the space of single particle wave functions, keeping the O^{16} nucleus as a core, the expression for the HF ground state energy will contain a term belonging exclusively to the core, plus a term containing only valence nucleon states, and an extra term coupling the two systems, i.e., valence nucleons and core. This coupling term does not appear when one deals with density independent interactions. Now, its presence would make the hypothesis of an inert core inapplicable as one cannot separate the two distinct systems, namely, the inert coreand the valence nucleons. In order to perform the HF approximation followed by the projection, we assumed this term to be a constant with respect to the variational HF procedure. After determining the HF wave functions, the coupling term can be easily computed, and we assumed the corresponding energy equally distributed among all the nucleons; part of it, $16/A$ of its total value, will be incorporated to the core energy; the remaining $(A-16)/A$ fraction will be absorbed by the valence nucleons.

In Section 2, we describe how the Skyrme force parameters were fitted. The HF equations with the density dependent interaction are discussed in Section 3. Energy levels and B(E2) transition probabilities, obtained with good J projected wave functions, are presented in Section 4 and they are followed by a short conclusion.

2. THE PARAMETERS FOR THE SKYRME FORCE

The two-body part of the Skyrme interaction we have used is written in configuration space as

$$
\begin{aligned}
v_{12}(\underset{\sim}{r}_1 - \underset{\sim}{r}_2) = {} & t_0(1 + \chi_0 P^\sigma)\delta(\underset{\sim}{r}_1 - \underset{\sim}{r}_2) + \tfrac{1}{2} t_1(1 + \chi_1 P^\sigma) \times \\
& \times \left[\underset{\sim}{k}^{\dagger 2}\delta(\underset{\sim}{r}_1 - \underset{\sim}{r}_2) + \delta(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)\underset{\sim}{k}^2\right] + \\
& + t_2\, \underset{\sim}{k}^{\dagger} \cdot \delta(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)\, \underset{\sim}{k} + \\
& + i W_0 (\underset{\sim}{\sigma}_1 + \underset{\sim}{\sigma}_2)\underset{\sim}{k}^{\dagger} \times \delta(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)\underset{\sim}{k} \quad , \qquad (2.1)
\end{aligned}
$$

where $\underset{\sim}{k}^{\dagger}$ and $\underset{\sim}{k}$ are relative momentum operaiors acting on the bra and *ket* respectivel ly; P^{σ} is the spin-exchange operator, and $\underset{\sim}{\sigma}_1$ and $\underset{\sim}{\sigma}_2$ are Pauli spin-matrices. The three-body term of the Skyrme force is also of zero-range

$$v_{123}(\underset{\sim}{r}_1-\underset{\sim}{r}_2,\underset{\sim}{r}_2-\underset{\sim}{r}_3) = t_3\ \delta(\underset{\sim}{r}_1-\underset{\sim}{r}_2)\delta(\underset{\sim}{r}_2-\underset{\sim}{r}_3)\ , \tag{2.2}$$

and, for HF calculations of even-even nuclei, this force is equivalent to a two-body density dependent interaction

$$w_{12}(\underset{\sim}{r}_1-\underset{\sim}{r}_2)\rho\left(\frac{\underset{\sim}{r}_1+\underset{\sim}{r}_2}{2}\right) = \frac{1}{6}\,t_3(1+P^{\sigma})\delta(\underset{\sim}{r}_1-\underset{\sim}{r}_2)\rho\left(\frac{\underset{\sim}{r}_1\ \underset{\sim}{r}_2}{2}\right). \tag{2.3}$$

Instead of using the parameters obtained by Vautherin and Brink, we performed our own fitting, with harmonic oscillator wave functions, such that t_0, t_1, t, and t_3 should reproduce

a) the experimental binding energy of O^{16};

b) the experimental value of the weighted sumof the valence neutron separation energies in O^{17} ,

$$\sum_{nlj\ \in\ 1s0s} (2j+1)\left[E_{nlj}(O^{17}) - E(O^{16})\right]\ ; \tag{2.4}$$

c) the empirical value of the nuclear matter energy per particle, $(E/A)_{NM}$;

d) also, that the O^{16} binding energy should be a minimum with respect to the harmonic oscillator parameter $b_{O^{16}}$.

The set of four equations obtained from the conditions above were solved severa1 times, assuming different values of $b_{O^{16}}$, k_F and $(E/A)_{NM}$, each one spanning a range of acceptabie values. Moreover, we used the parameters t_0, t_1, t, and t_3 to calculate the O^{16} and Ca^{40} s-d shell single-particle energies.

	t_0	t_1	t_2	t_3	χ_0	W_0
VB - I	-1057.3	235.9	-100.0	14463.5	0.56	120.0
VB - II	-1169.9	585.6	- 27.1	9331.1	0.34	105.0
This Work	-1115.5	314.6	-106.7	14992.8	0.8	68.1

Table 1. Skyrme's force parameters determined by Vautherin and Brink, VB-I and VB-II, and those obtained in this work, The dimensions are: t_0 (in MeV fm^3), t_1 (in MeV fm^5), t_2 (in MeV fm^5), t_3 (MeV fm^6), W_0 (MeV fm^5) and χ_0 is dimensionless.

In Table 1, we show the set of parameters we have obtained, andthetwo sets determined by Vautherin and Brink. As the first and second terms of expression (2.1) correspond to S-wave interactions, we assumed $\chi_0 = \chi_1$. This parameter, which determines symmetry effects, was adjusted to give a value of the order of 30 MeV for the symmetry-energy coefficient in nuclear matter. The parameter W_0 was adjusted to reproduce the splitting of the Od levels in O^{17}. As the b value we found for O^{16} was very close to the one we would obtain with the formula proposed by Blomqvist and Molinari[9],

$$b = \left[\frac{\hbar^2/m}{45\, A^{-1/3} - 25\, A^{-2/3}} \right]^{1/2}, \qquad (2.5)$$

we chose to use this last formula for the various nuclei studied here. In Table 2, the experimental or empirical values of the nuclear properties are compared with the ones reproduced with our set of parameters, with the two sets of Vautherin and Brink VB-I and VB-II, and with those of Zofka and Ripka.

	VB-I	VB-II	ZR	This Work	Exp. or Emp.
$\varepsilon_{1s_{1/2}}(O^{16})$	- 3.27	- 2.14		- 1.42	- 3.27
$\varepsilon_{0d_{3/2}}(O^{16})$				0.57	0.94
$\varepsilon_{0d_{5/2}}(O^{16})$	- 8.16	- 5.31		- 4.51	- 4.14
$\varepsilon_{1s_{1/2}}(Ca^{40})$	-15.7	-17.1		-13.5	-18.1
$\varepsilon_{0d_{3/2}}(Ca^{40})$	-15.0	-17.5		-15.2	-15.6
$\varepsilon_{0d_{5/2}}(Ca^{40})$	-22.2	-23.3		-20.9	-21.7
$BE/A(O^{16})$	9.17	8.84	8.33	8.93	8.93
$BE/A(Ca^{40})$	10.51	10.28	9.97	10.41	10.42
$r_c(O^{16})$	2.68	2.75	2.72	2.68	2.73
$r_c(Ca^{40})$	3.41	3.49	3.50	3.43	3.49
$b\ (O^{16})$	1.71	1.76	1.67	1.74	
$b\ (Ca^{40})$			1.71	1.94	
$(BE/A)_{MNS}$	16.	16.	16.5	16.5	16.
k_F	1.32	1.30	1.30	1.30	1.36
C_{av}	29.3	34.1		32.0	31.5
K	370.	342.	313.	366.	

Table 2. Properties of the O^{16} and Ca^{40} spherical nuclei and of the symmetric nuclear matter. Values obtained by Vautherin and Brink, VB-I and VB-II, Zofka and Ripka, ZR, and in this work. The last column contains the corresponding experimental or empirical values. In the first six rows, we have the s-d shell single particle energies (in MeV); BE/A is the binding energy per nucleon (in MeV); r_c is the nuclear charge radius, and b the harmnic oscillator constant (both in fm). The last four rows contain the nuclear matter binding energy per particle (in MeV), the Fermi mmentum (fm^{-1}), the symmetry-energy coefficient (in MeV), and the incompressibility coefficient (in MeV).

3. THE HARTREE-FOCK APPROXIMATION

Consider an even-even nucleus with A nucleons, whose ground state is a Slater determinant $|\Psi_0>$, of its single particle occupied states $|i>$. The Hamiltonian containing the Skyrme density-dependent interaction will have an expectation value in the state $|\Psi_0>$ given by

$$E_0(A) = \sum_{i=1}^{A} <i|\hat{t}|i> + \frac{1}{2} \sum_{i,j=1}^{A} <ij|v_{12}+w_{12}\rho_A|ij> , \qquad (3.1)$$

where $\hat{t}$ is the kinetic energy operator, ρ_A is the density of the system considered, and the two-body matrix elements are anti-symmetrized. In the HF approximation the states $|i>$, or the corresponding wave functions ϕ_i, are chosen to give the lowest possible value of $E_0(A)$.

We assume the nucleus of O^{16} to be a core and the states available to the extra-core particles in Ne^{20}, Mg^{24}, Si^{28}, S^{32}, Ar^{36} are confined to the *s-d* shell only. Assuming time reversal and charge symmetry, the (A-16) valence nucleons will have six possible states to occupy, with a fourfold degeneracy. The expression for the nuclear energy (3.1) will now contain terms involving separately, the core, the valence nucleons, plus an extra term, $E_{C\text{-}VN}$, mixing core and valence nucleon states, so that the required condition for the inert core approach is not reproduced:

$$E_0(A) = E_0(O^{16}) + \sum_{i=17}^{A} <i|\hat{s}|i> + E_R + E_{C\text{-}VN}$$

$$+ \frac{1}{2} \sum_{i,j=17}^{A} <ij|v_{12}+ w_{12}\ \rho_{O^{16}}|ij> , \qquad (3.2)$$

where

$$<i|\hat{s}|i> = <i|\hat{t}|i> + \sum_{j=1}^{16} <ij|v_{12}+w_{12}\ \rho_{O^{16}}|ij> +$$

$$+\frac{1}{2}\sum_{k,j=1}^{16}\langle kj|w_{12}\ \delta\rho_i\ |ij\rangle\ , \tag{3.3}$$

$$E_R=\frac{1}{2}\sum_{i,j,k=17}^{A}\langle ij|w_{12}\ \delta\rho_k|ij\rangle\ , \tag{3.4}$$

$$E_{C\text{-}VN}=\sum_{i=1}^{17}\sum_{j,k=17}^{A}\langle ij|w_{12}\delta\rho_k\,|\,ij\rangle\ , \tag{3.5}$$

$$\delta\rho_i=|\,\phi_i\,(\frac{\underset{\sim}{r}_1+\underset{\sim}{r}_2}{2})\,|^2\ . \tag{3.6}$$

Density independent two-body interactions do not give rise to such terms as E_R, the rearrangement energy, or, when an inert core is introduced, to the mixing term, $E_{C\text{-}VN}$. The latter shows that the inert core approximation should be inadequate with density dependent two-body forces. Our procedure was as follows: the variational calculation was performed assuming $E_{C\text{-}VN}$ to be a constant with respect to it. We also assumed that $E_{C\text{-}VN}$ should be equally distributed over the A nucleons, and therefore the O^{16} ground state energy was taken as

$$E_0'(O^{16})=E_0(O^{16})+(16/A)\,E_{C\text{-}VN}=\text{Exp.value}\,. \tag{3.7}$$

The single particle energies $\langle i|\hat{\varepsilon}|i\rangle$ were taken as the experimental energy levels of O^{17}; $E_{0d_{5/2}}=-4.14$ MeV, $E_{1S_{1/2}}=-3.27$ MeV, $\varepsilon_{0d_{3/2}}=0.94$ MeV.

The HF approximation was carried out for Ne^{20}, Mg^{24}, Si^{28}, S^{32} and Ar^{36}, assuming that they are axially symmetric. A prolate and an oblate solution were tried for each nucleus, keeping the one with the lowest energy. A HF single-particle state $|pm\rangle$ is expressed in terms of the s-d shell orbitals as

$$|pm\rangle=\sum_{nlj\ 6\ \text{Odls}}^{P}C_{nlj}\,|\,nljm\,\rangle\ . \tag{3.8}$$

	$\|pm\rangle$	$1s_{1/2}$	$0d_{3/2}$	$0d_{5/2}$	ε_p
Ne^{20}	1/2	-0.4538	-0.3273	0.8288	-14.20
	-3/2	0.	0.2044	0.9789	-10.30
Prolate	1/2'	**0.7005**	0.4438	0.5589	- 7.57
	5/2	0.	**0.**	1.	- 7.27
	1/2''	-0.5507	0.8342	0.0279	**- 5.40**
	-3/2'	**0.**	**0.9789**	-0.2044	- 2.22
Mg^{24}	1/2	-0.4430	-0.2241	0.8680	-19.14
	-3/2	0.	0.2690	0.9631	-16.52
	1/2'	0.4592	**0.7749**	0.4344	-13.57
Prolate	5/2	0.	**0.**	1.	-11.93
	1/2''	0.7700	**-0.5911**	0.2404	-10.03
	-3/2'	0.	0.9631	-0.2690	- 7.05
Si^{28}	5/2	0.	0.	**1.**	-22.80
	-3/2	0.	**-0.5751**	0.8180	**-20.11**
	1/2	0.7002	-0,1708	0.6933	-19.53
Oblate	3/2'	0.	**0.8181**	0.5751	-14.86
	1/2'	**0.5377**	-0.5128	-0.6693	-14.65
	1/2''	0.4698	0.8414	-0.2672	-10.24
S^{32}	1/2	-0.3098	-0.0591	0.9490	-25.11
	-3/2	0.	0.1694	**0.9855**	-24.17
	5/2	0.	0.	1.	-21.75
Prolate	1/2'	**0.**6049	0. 7578	0. 2446	-20.33
	1/2''	0.7335	-0.6498	0.1990	-17.92
	3/2'	0.	**0.9855**	-0.1694	-16.96
Ar^{36}	5/2	0.	0.	1.	-27.96
	-3/2	0.	**-0.1756**	**0.9844**	-26.54
	1/2	0.3569	**0.0808**	0.9306	-25.73
Oblate	1/2'	**0.7920**	**-0.5544**	-0.2556	**-21.83**
	3/2'	0.	**0.9845**	**0.1756**	-21.67
	1/2''	**0.4953**	0.8283	-0.2618	-18.66

Table 3. The **expansion** coefficients C^{p}_{nljm} **and** the HF **single**-particle energies **(in MeV).** The dashed lines **separate** the occupied from the non-occupied orbits.

The expansion coefficients and the HF single particle energies are shown in Table 3. The dotted lines separate the occupied from the non-occupied states. In Table 4, we show the ground state E_0, the rearrangement E_R and the mixing term E_{C-VN} energies per particle. In the last two columns, we have the energy gap and the oscillator constant bcalculated from formula (2.5). As Zofka and Ripka, we also found that the density dependence reduces the energy gap by a factor of two, as compared with the ones obtained with density independent two-body interactions.

	$\frac{E(A) - E_0(O^{16})}{A - 16}$		$\frac{E_R}{A-16}$	$\frac{E_{C-NV}}{A}$	Δ	b
	Exp.	Th.				
Ne^{20}	- 9.77	- 8.78	0.50	0.54	3.90	1.77
Mg^{24}	-10.73	-10.34	0.53	0.98	2.95	1.82
Si^{28}	-11.20	-11.28	0.81	1.64	4.68	1.85
S^{32}	-11.27	- 11.97	0.92	2.02	2.41	1.88
Ar^{36}	-11.33	-12.34	1.22	2.55	3.01	1.91

Table 4. All energies in MeV. The experimental and calculated ground state energies, the rearrangement and mixing term energies, per nucleon; the energy gap. The harmonic oscillator constant (in fm) obtained from the Blomqvist and Molinari formula.

4. ENERGY LEVELS AND B(E2) TRANSITIONS

Most of the formalism on the HF approximation and the projection of states of good angular momentum J can be found in Ref.7. An irreducible tensor operator will have the following matrix elements between the projected states $|\Phi^J_{MK}\rangle$:

$$\langle \Phi^{J_1}_{M_1K_1} | T^{(k)}_q | \Phi^{J_2}_{M_2K_2} \rangle = \frac{2J_2+1}{2\, C^*_{J_1K_1} C_{J_2K_2}} (J_2M_2kq|J_1M_1) \quad \times$$

$$\times \sum_{\mu\nu} (J_2 K_2 k\nu | J_1 K_1) \int_0^{\pi} d\beta \ \text{sen}\,\beta \, d^{J_1}_{K\mu}(\beta) < \Psi_{K_1} | e^{-i\beta J_y} T^{(k)}_{\nu} | \Psi_{K_2} > , \quad (4.1)$$

where

$$|C_{JK}|^2 = \frac{2J+1}{2} \int_0^{\pi} d\beta \ \text{sen}\,\beta \ d^{J}_{KK}(\beta) < \Psi_K | e^{-i\beta J_y} | \Psi_K > , \quad (4.2)$$

$$d^{J}_{KM}(\beta) = < JK | e^{-i\beta J_y} | JM > ; \quad (4.3)$$

M and K are the projections of the total angular momentum on the z-axis of the laboratory system and body system, respectively. In our case, the ground state bands have $K = 0$. $T^{(k)}_q$ is replaced by the nuclear Hamiltonian for the energy levels calculation or by $(r^2 Y_{2q})$ for the B(E2) transition rates.

In Figs.1, 2a and 2b, we show the energy levels in MeV of Ne^{20}, Mg^{24} and Si^{28} fundamental bands. The calculations were made in a Burroughs 1400 computer. We could not repeat them for S^{32} and Ar^{36}, in spite of the minor changes required by the programs.

Hartree-Fock calculations with two-body density independent interactions were initially performed using simple two-body forces with an exchange mixture [7,8]. The projected energy spectrum looked reasonably good for Ne^{20} and too compressed for Si^{28}. This was usually considered to be a deficiency of the HF approximation. As soon as more sophisticated two-body forces were employed[10,11], namely, the renormalized matrix elements of an interaction proposed by Kahana, Lee and Scott[12], $(KLS)_R$, the quality of the Si^{28} spectrum improved. This has been the subject of a paper by Soyeur and Zucker[13]. In Figures 1 and 2b, we reproduce the spectra obtained in Ref.11 using the same matrix elements $(KLS)_R$. In the case of Ne^{20}, we have also calculated the energy levels, in our present scheme, using the two sets of parameters derived by Vautherin and Brink. VB-I and VB-II.

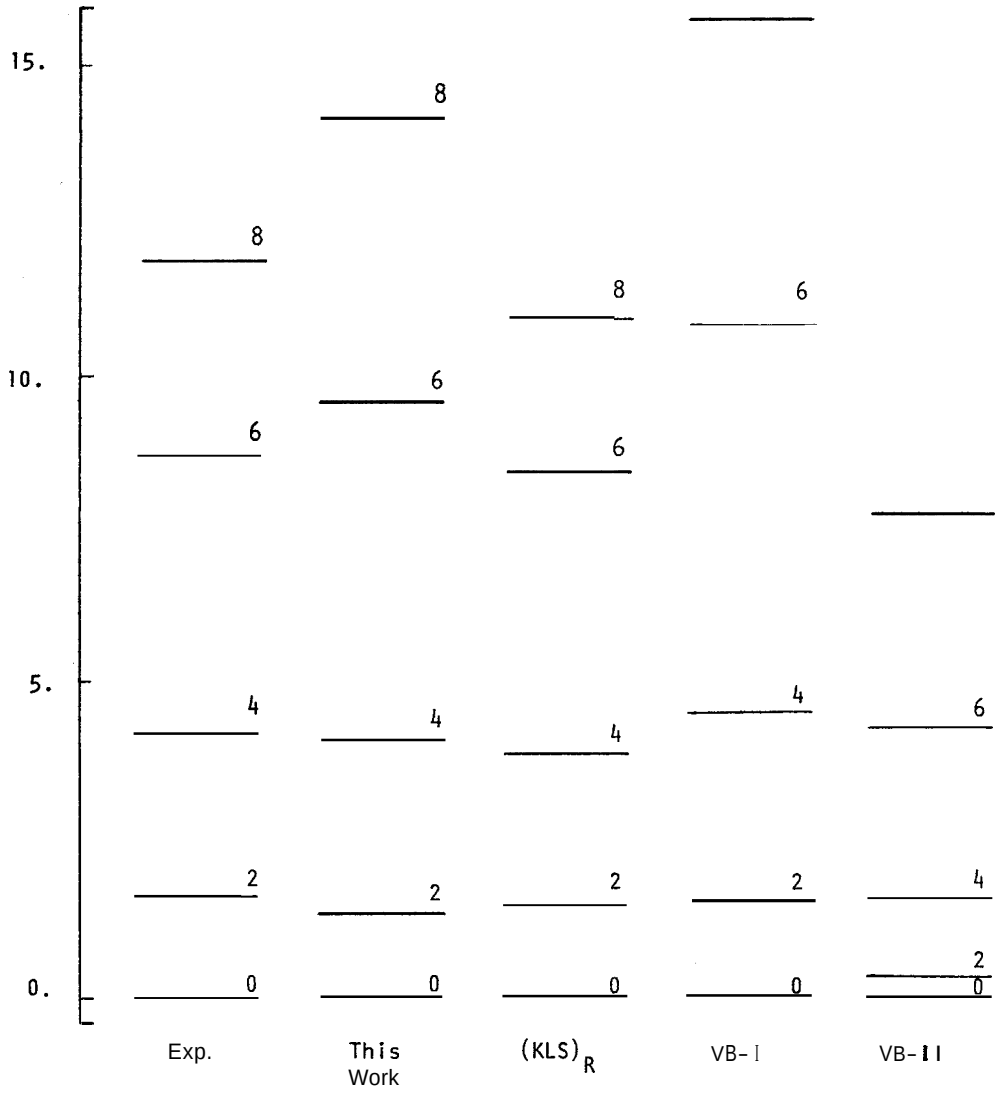

FIG.1 - Projected HF spectra of Ne^{20} using different interactions. The spin value is on the right of each level. The energies are in MeV.

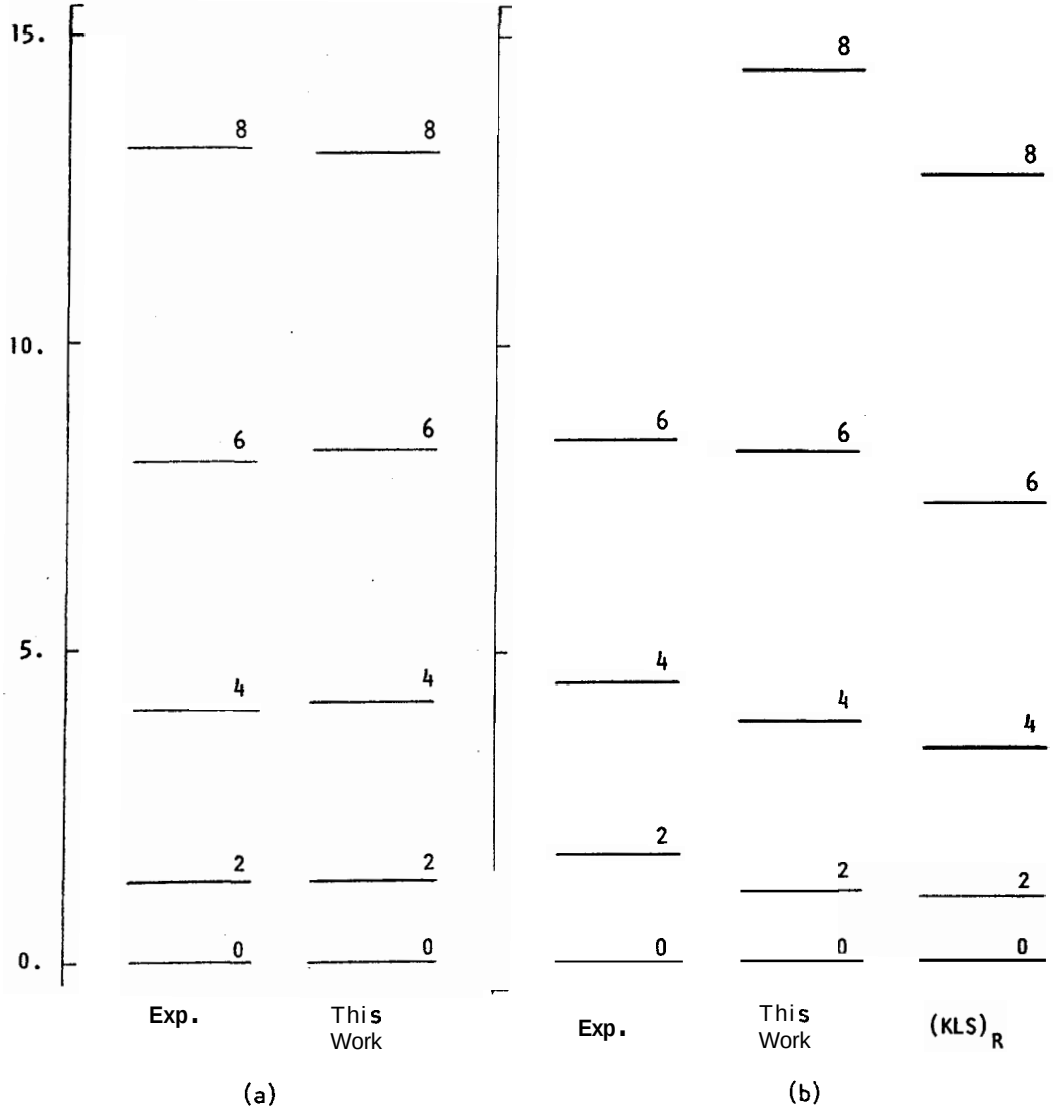

FIG.2 - Projected HF spectra (a) of Mg^{24} and (b) of Si^{28}. The spin value is on the right of each level. The energies are in MeV.

$J_i \to J_f$		Ne^{20}		Mg^{24}		Si^{28}		S^{32}	
		TH	EXP.(a)	TH.	EXP.(b)	TH.	EXP.(c)	TH	EXP.(d)
2	0	18.1	17.8 ± 2.5	21.5	20.5 ± 0.6	22.4	14. ± 4.	10.3	9.2 ± 2.8
4	2	23.2	21.9 ± 2.1	28.7	23. ± 4.	30.6	21. ± 5.	13.3	18.4 ± 4.5
6	4	19.8	20.4 ± 2.4	27.2	$34.^{+36}_{-10}$	30.7		12.2	
8	6	12.0		22.0	$16.^{+25}_{-6}$	26.9		8.8	
10	8			12.1		18.9		4.1	

Table 5. The electric quadrupole transition probabilities, in Weisskopf units. The calculated values are compared with (a) Ref. 14, (b) Ref.15, (c) Ref.16, (d) Ref.17.

One sees that the Skyrme force will give rise to an enlarged spectrum. The tendency towards Si^{28} to obtain a more compressed spectrum is maintained; however, the quality has been improved. The lower t_3 value in the set of parameters VB-II, diminishing the contribution of the density dependent term, may be the reason why its Ne^{20} spectrum came out too compressed.

In Table 5, we show the quadrupole reduced transition probabilities for Ne^{20}, Mg^{24}, Si^{28} and S^{32}, in Weisskopf units. In a previous paper[11], it was found that the B(E2) values were very much insensitive to the type of interaction being employed. The situation did not change now. The values obtained with the Skyrme force are very close to those calculated with density independent two-body forces. We use effective charges $e_p = 1.5e$ and $e_n = 0.5e$.

5. CONCLUSIONS

The simple Skyrme interaction has been successfully used by various authors to describe severa1 nuclear properties. In this paper, we present the K = 0 fundamental band of energies obtained from the HF ground state with the Peierls and Yoccoz projection method. In spite of some strong restrictions we had to make in order to perform the HF approximation, we found that the Skyrme force reproduces satisfactorily well the energy levels.

The density dependence is implicitly contained in the wave functions that were used to calculate the energy levels and the B(E2) transition rates matrix elements. The Hami1tonian operator further increases this dependence on the density when one calculates the energies. This is probably why the transition probabilities are not sensitive to the type of interaction being employed, as the operator involved does not contain the interaction.

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