

Densities, Form Factors, Transitions and Multipole Moments in the s-d Shell, with the Skyrme Force*

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This paper reports the nuclear densities, radii, multipole moments, form-factors and transition probabilities obtained for the $A=4n$ type of nuclei in the s-d shell, using the Hartree-Fock wave functions calculated in Ref.(1) with the Skyrme force. Experimental data and theoretical values derived by others are shown for comparison.

Este trabalho apresenta as densidades, os raios, os momentos de multipolo, os fatores de forma e as probabilidades de transição nucleares obtidos para núcleos da camada s-d, do tipo $A = 4n$. usando as funções de onda de Hartree-Fock calculadas na ~ e.(1) com a força de Skyrme. Os resultados são comparados com medidas experimentais e com valores teóricos derivados por outros autores.

1. INTRODUCTION

In our previous ~ a ~ e we' applied the Hartree-Fock (HF) approximation with the Skyrme force to the $A=4n$ type of nuclei in the s-d shell. We used the Peierls and Yoccoz projection method to obtain wave functions of good angular momentum, energy levels and transition probabilities within the ground state band. The results were better than those obtained with more sophisticated two-body interactions. We had to assume the 0^{16} to be an inert core and the basis of independent particle wave

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functions was truncated to the s - d subspace. Time reversal and charge symmetry were also assumed.

The two-body part of the Skyrme² interaction is written in configuration space as

$$\begin{aligned}
 v_{12}(\vec{r}_1-\vec{r}_2) &= t_0(1+\chi_0 P^\sigma) \delta(\vec{r}_1-\vec{r}_2) + \frac{1}{2} t_1(1+\chi_1 P^\sigma) \cdot \\
 &\quad [\vec{k}^{\dagger 2} \delta(\vec{r}_1-\vec{r}_2) + \delta(\vec{r}_1-\vec{r}_2) \vec{k}^2] + \\
 &\quad + t_2 \vec{k}^\dagger \cdot \delta(\vec{r}_1-\vec{r}_2) \vec{k} + \\
 &\quad + i W_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \vec{k} \times \delta(\vec{r}_1-\vec{r}_2) \vec{k},
 \end{aligned} \tag{1}$$

where \vec{k}^\dagger and \vec{k} are relative momentum operators; P^σ is the spin-exchange operator, $\vec{\sigma}_1$ and $\vec{\sigma}_2$ are Pauli spin matrices. The three body term of the Skyrme force is also of zero-range

$$v_{123}(\vec{r}_1-\vec{r}_2, \vec{r}_2-\vec{r}_3) = t_3 \delta(\vec{r}_1-\vec{r}_2) \delta(\vec{r}_2-\vec{r}_3) \tag{2}$$

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

$$w_{12}(\vec{r}_1-\vec{r}_2) \rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) = \frac{1}{6} t_3 (1+P^\sigma) \delta(\vec{r}_1-\vec{r}_2) \rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) \tag{3}$$

In Ref.(1) we discuss how we performed the fitting to nuclear properties, that lead us to the following values for the parameters:

$$\begin{aligned}
 t_0 &= -1115.5 \text{ MeVfm}^3 & t_1 &= 314.6 \text{ MeVfm}^5 \\
 t_2 &= -106.7 \text{ MeVfm}^5 & t_3 &= 14992.8 \text{ MeVfm}^6 \\
 \chi_0 &= \chi_1 = 0.8 & W_0 &= 68.1 \text{ MeVfm}^5
 \end{aligned}$$

What we found was compared to the available experimental data and to some theoretical results derived by others.

D. Vautherin³ used two sets of parameters determined by Brink and himself (VB-I and VB-II) for the Skyrme force. A modified version of

Negele's effective interaction was used by Zofka and Ripka⁴ (ZR). Moszkowski⁵ also studied some s-d shell nuclei with his Modified Delta Interaction (MDI). We quote some of their results.

2. MULTIPOLE EXPANSION OF THE NUCLEAR DENSITY

The density of states distributions of a nucleus with A nucleons is given by

$$\rho(\vec{r}) = \sum_{i=1}^A |\phi_i(\vec{r})|^2, \quad (4)$$

the summation being over the occupied states described by the Hartree-Fock single particle wave functions $\phi_i(\vec{r})$. The above expression can be developed to the final form

$$\rho(\vec{r}) = \sum_L \rho_L(r) P_L(\cos \theta), \quad (5)$$

where the multipolar expansion coefficient is

$$\rho_L(r) = \rho_{016}(r) \delta_{L0} + \rho_L^{VN}(r) \quad (6)$$

The first contribution comes from the inert core and the second is from the valence nucleons, namely

$$\rho_{016}(r) = \frac{1}{\pi} \sum_{(n\ell)=(00)}^{(01)} (2\ell + 1) R_{n\ell}^2(r) \quad (7)$$

and

$$\rho_L^{VN}(r) = (1 + (-1)^L) \frac{2L+1}{2\pi} \sum_{\substack{n\ell jm \\ n' \ell' j'}} \rho_{\alpha' \alpha}^{HF} R_{n\ell}(r) R_{n' \ell'}(r) \\ [(2\ell+1)(2\ell'+1)]^{1/2} (L0\ell'0 | \ell 0) (L0j'm | jm) \\ W(L \ell' j \frac{1}{2}; \ell j') \quad (8)$$

Besides the Clebsch-Gordan and Racah coefficients, the $R_{nl}(r)$ are radial wave functions, $\rho_{\alpha\alpha}$ is the HF density of states; a stands for the set of harmonic oscillator quantum numbers n, R, j, m . In the $s-d$ shell, the contributing L values are $L = 0$ (monopole), $L = 2$ (quadrupole) and $L = 4$ (hexadecapole).

As we neglect the Coulomb interaction and $N=Z$, the density of protons will be $\rho^p(\vec{r}) = \frac{1}{2} \rho(\vec{r})$, where the total density $\rho(\vec{r})$ is given by (5). Corrections due to the center of mass motion and to the finite size of proton⁶ were taken into account, such that one obtains the nuclear charge density distribution $\rho^c(\vec{r})$, which can be also written as a multipole expansion. The new coefficient $\rho_L^c(r)$ is a function of the old one given by expressions (6), (7) and (8).

With harmonic oscillator wave functions, the nuclear state can be written as a product of the center of mass w.f. times an intrinsic wave functions. The spurious states are eliminated by keeping the center of mass wave function in its ground state. The final expression of $\rho^c(\vec{r})$, containing both corrections, is the same as given by Negele⁶

$$\rho^c(\vec{r}) = \frac{1}{2[\alpha_p^2 - B^2]^{3/2}} \int d^3r' \exp\left[-\frac{(\vec{r}-\vec{r}')^2}{(\alpha_p^2 - B^2)}\right] \rho(\vec{r}') \quad (8')$$

where

$$B^2 = b^2/A$$

$$\alpha_p = \sqrt{2/3} r_p = \sqrt{2/3} \cdot 0,8 \text{ fm}$$

$$b = \text{h.o. constant}$$

The charge density distribution coefficients for $L = 0, 2, 4$ are shown in Figs. 1a, 1b for Ne^{20} , Mg^{24} , Si^{28} and S^{32} . Comparison with the experimental data will be made through the electron scattering form factors as the experimental densities are derived from them.

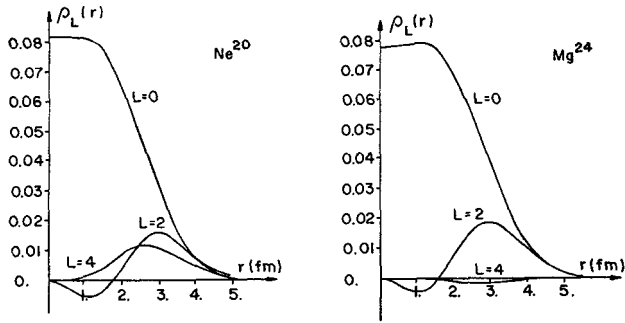


Fig.1a - Expansion coefficients for the Ne^{20} and Mg^{24} nuclear charge density distributions.

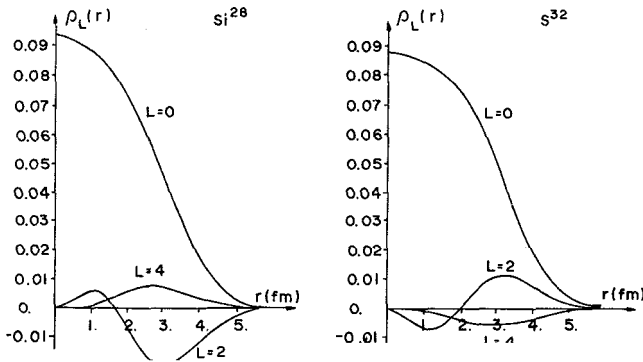


Fig.1b - Expansion coefficients for the Si^{28} and S^{32} nuclear charge density distributions.

3. RADII

The nuclear mass and charge distributions expressions are

$$\langle r_M^2 \rangle = \frac{4\pi}{A} \int_0^\infty \rho_0(x) r^4 dx \quad (9)$$

and

$$\langle r_c^2 \rangle = \frac{4\pi}{Z} \int_0^\infty \rho_0^c(x) r^4 dx, \quad (10)$$

respectively. $\rho_0(x)$ is given by (6) for $L = 0$, and $\rho_0^c(x)$ is the $L = 0$ expression for the charge distribution, taking into account the correc-

tions due to the center of mass motion and to the finite size of proton.

In Table 1 we compare the experimental values of the nuclear charge r.m.s. radius for Ne^{20} , Mg^{24} , Si^{28} , S^{32} and Ar^{36} with the ones obtained by various authors.

The mass radius, not including the corrections, is also shown; one sees that the net effect of the finite size of proton and the center of mass motion corrections increase the radius value.

The expression depend on the harmonic oscillator constant b . We used the Blomqvist-Molinari⁷ formula to calculate the value of b for each nucleus. What we found is in very good agreement with the data, indicating that their formula works quite well for light nuclei.

Table 1 - Nuclear charge radii (in fm) determined by various authors. In the last column we have the mass radius, without the corrections due to the center of mass motion and to the finite size of proton.

r_c	Exp.	VB-I	VB-II	MDI-I	ZR	This Work r_c	This Work r_M
Ne^{20}	$2.91 \pm 0.05^{(a)}$	2.88	3.02	2.96	3.05	2.87	2.80
Mg^{24}	$2.99 \pm 0.03^{(b)}$	3.01	3.15	3.12	3.24	3.04	2.97
Si^{28}	$3.11 \pm 0.03^{(b)}$	3.05	3.26		3.35	3.16	3.09
S^{32}	$3.24 \pm 0.03^{(b)}$	3.17	3.32	3.26	3.42	3.26	3.19
Ar^{36}		3.30	3.42	3.40	3.46	3.35	3.28

(a) Ref .8, (b) Ref .9.

4. INTRINSEC MULTIPOLE MOMENTS

The nuclear charge intrinsic quadrupole and hexadecapole moments are defined by the expectation values

$$Q_0^C = 2 \langle \Phi_0 | \hat{Q}_0^2 | \Phi_0 \rangle \quad (11)$$

and

$$H_0^C = \langle \Phi_0 | \hat{Q}_0^4 | \Phi_0 \rangle, \quad (12)$$

where $|\Phi_0\rangle$ is the Hartree-Fock ground state, the operators having the well-known forms

$$\hat{Q}_0^2 = \frac{1}{e} \sum_{i=1}^Z \sqrt{\frac{4\pi}{5}} e_i r_i^2 Y_{20}(\Omega_i) \quad (13)$$

and

$$\hat{Q}_0^4 = \frac{1}{e} \sum_{i=1}^Z \sqrt{\frac{4\pi}{9}} e_i r_i^4 Y_{40}(\Omega_i) \quad (14)$$

Assuming that the proton and neutron wave function are equal, plus the fact that $N=Z$, we can write

$$Q_0^C = (1 + \alpha_p + \alpha_n) \frac{8\pi}{5} \int_0^\infty \rho_2^C(r) r^4 dr \quad (15)$$

$$H_0^C = (1 + \alpha_p + \alpha_n) \frac{4\pi}{9} \int_0^\infty \rho_4^C(r) r^6 dr. \quad (16)$$

The nuclear charge distribution densities are the ones including the corrections mentioned before. The proton and neutron effective charge corrections, α_p and α_n , were taken as 0.5. One sees that Q_0^C (H_0^C) measures the quadrupole (hexadecapole) deformation of the nuclear charge distribution. Depending of the sign of Q_0^C being positive or negative, the deformation will be prolate or oblate, respectively.

The quadrupole moments are in Table II; the best comparison with the experimental data was reached by Vautherin, with the VB-II set of parameters, also by Zofka and Ripka and this work. Our values of the hexadecapole moments in Table III are too low by a factor of two compared to the experimental ones.

Table II - Electric quadrupole moments (in fm²) calculated by various authors. In the case of S³² and Ar³⁶, experiment does not provide their signs.

Q_0^2	Exp.	VB-I	VB-II	MDI-I	ZR	This Work
Ne ²⁰	58 ± 3 ^(a)	34.	46.	45.	49.8	47.9
Mg ²⁴	69 ± 3 ^(a)	50.	60.	50.	68.6	58.9
Si ²⁸	-64 ± 3 ^(a)	-26	-60		-72.2	-67.8
S ³²	47 ± 3 ^(b)	28.	52.	36.	-63.8	46.8
Ar ³⁶	54 ± 6 ^(b)	-36	-48	-50	-52.0	-48.4

(a) Ref.10, (b) Ref. 4.

Table III - Electric hexadecapole moments (in fm²) calculated by various authors.

H_0^2	Exp. ^(a)	Theor.
Ne ²⁰	249 ± 27	127.
Mg ²⁴	48 ± 16	-14.
Si ²⁸	205 ± 33	105.
S ³²		-72.
Ar ³⁶		90.

(a) Ref. 10.

5. ELECTRON-NUCLEUS SCATTERING FORM FACTORS

In the Born approximation, the elastic and inelastic form factors are given by the following expressions:

$$F_{e1}^2(k) = \frac{4\pi}{Z^2} \left| \int_0^\infty j_0(kr) \rho_0^C(r) r^2 dr \right|^2 \quad (17)$$

and

$$F_{0 \rightarrow J}^2(k) = \frac{4\pi}{(2J+1)^2} \frac{(1+\alpha_p + \alpha_n)^2}{Z^2} \frac{C_J^2}{C_0^2} \cdot \left| \int_0^\infty j_J(kr) \rho_J^C(r) r^2 dr \right|^2 \quad (18)$$

The momentum transfer is hk ; the target nucleus has Z protons, the ground state spin is zero and J is the angular momentum of its final excited state; these excited states are projected from the HF wave function, the C_J 's being their normalization constant.

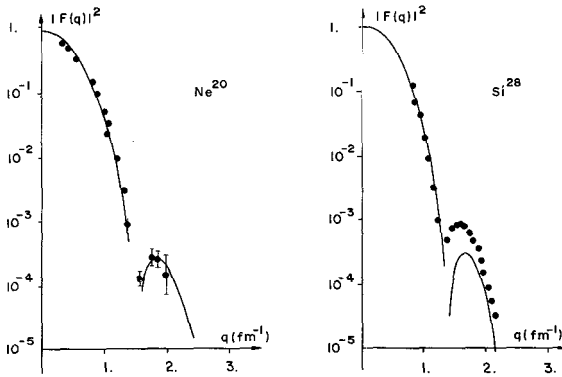


Fig.2a- Elastic scattering form factors for Ne^{20} and Si^{28} . The points represent experimental values.

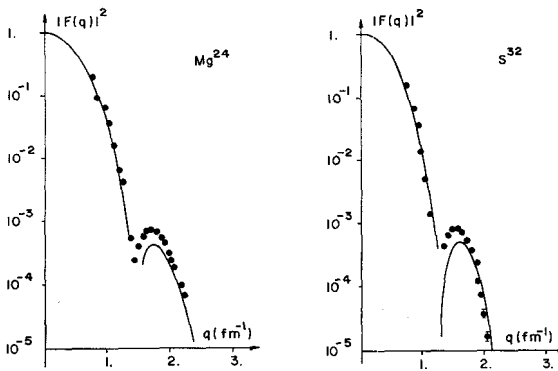


Fig.2b - Elastic scattering form factors for Mg^{24} and S^{32} . The points represent experimental values.

We show the elastic form factors in Figs. 2a, 2b.

The experimental points for Mg^{24} , Si^{28} and S^{32} are from Ref. (9); for Ne^{20} they are from Ref.(11). The curves reproduce quite well the experimental points before the diffraction minimum. This region of low momentum transfer corresponds to the nuclear surface, which is, therefore, well described by our wave functions, justifying the good values obtained for the nuclear charge radii. After the first minimum, the curves have a peak localized below the experimental points, except for Ne^{20} . Ripka found similar results, which may not be due to the Born Approximation, as Ford, Braley and Bar-Touv¹² also obtained this behaviour employing a better approximation. This region corresponds to high nuclear densities and the discrepancies are attributed to the fact that the Hartree-Fock wave functions do not contain short range correlations. It has been verified¹³ that, when Jastrow correlations are introduced in the nuclear wave functions, the form factor second peak value increases.

The form factors corresponding to the inelastic scattering, with a $0^+ \rightarrow 2^+$ nuclear transition, are shown in Figs. 3a, 3b.

The experimental points were taken from the same references as in the elastic case. This form factor depends on the charge quadrupole density shown in Figs. 1a, 1b. Some authors¹² suggest that one should increase the number of the shell model basis states in order to improve the results. In our case, it seems that only the $1s-0d$ states were enough to account for Si^{28} . The other nuclei may have a bigger quadrupolar deformation, thus requiring more single particle states.

In Figure 4, we show the $0^+ \rightarrow 4^+$ transition form factors only for Ne^{20} and Si^{28} , which are not in good agreement with the experimental points. There are no data available for the other nuclei we studied.

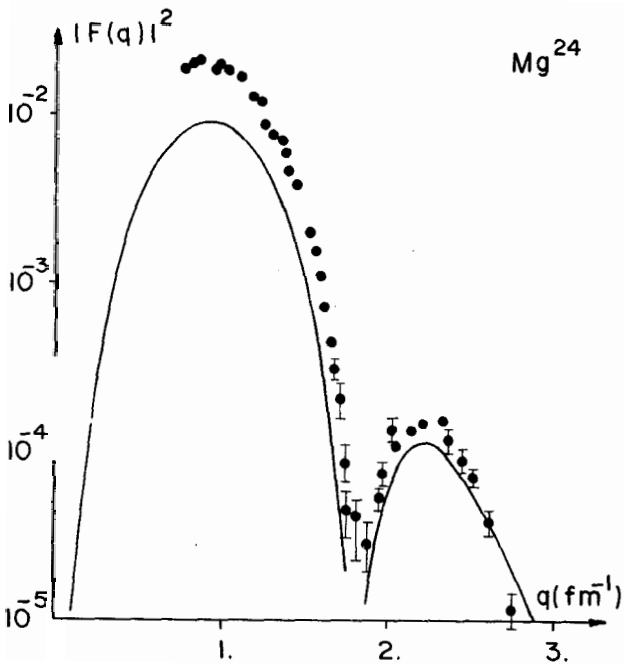
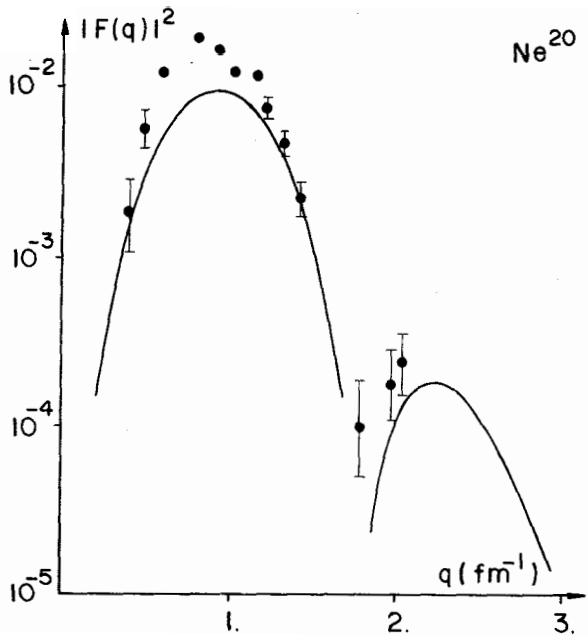


Fig.3a - $0^+ \rightarrow 2^+$ inelastic scattering form factors for Ne^{20} and Mg^{24} . Experimental values are shown for comparison.

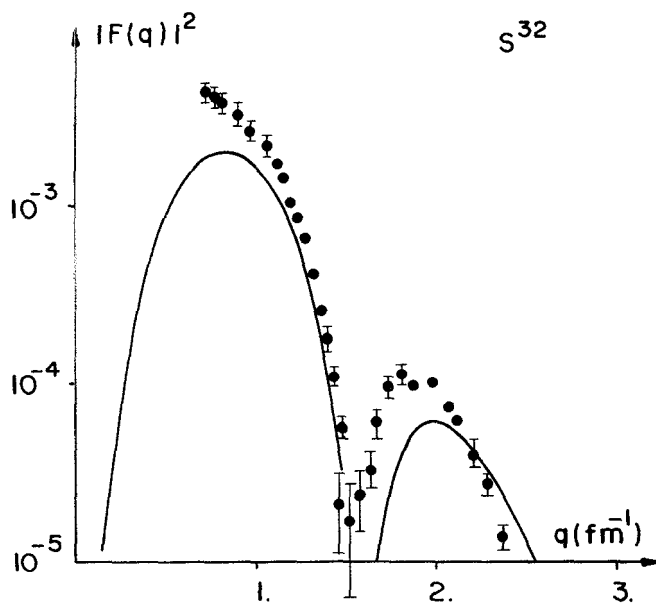
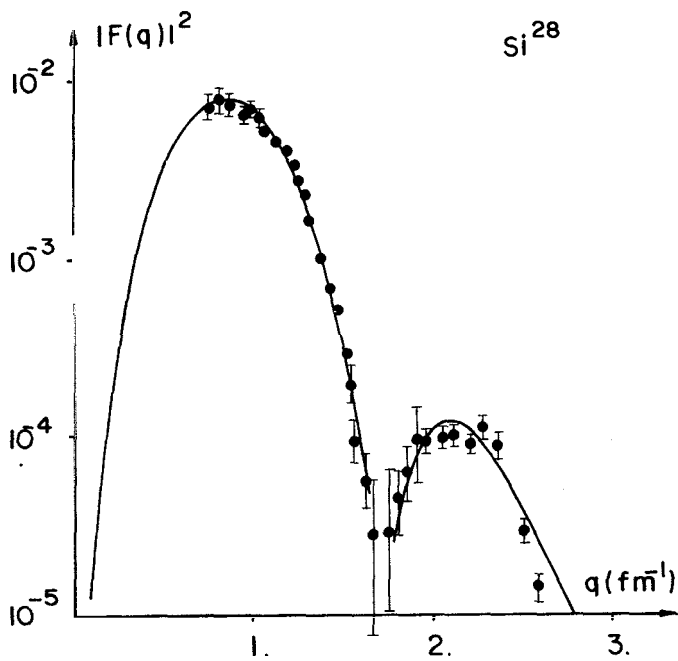


Fig.3b - $0^+ \rightarrow 2^+$ inelastic scattering form factors for Si^{28} and S^{32} . Experimental values are also shown.

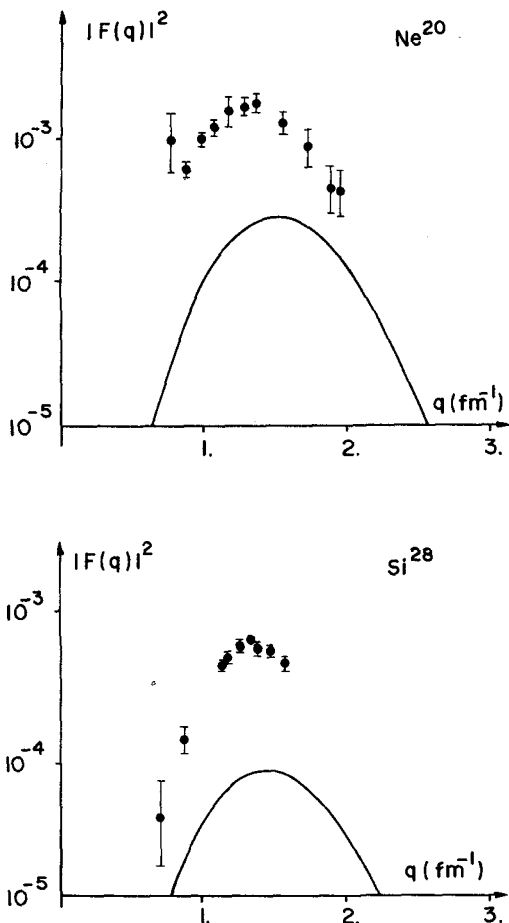


Fig.4 - $0^+ \rightarrow 4^+$ inelastic scattering form factors for Ne^{20} and Si^{28} with experimental values.

6. TRANSITION PROBABILITIES

In the limit of zero momentum transfer, the form factor for the $0^+ \rightarrow J^+$ level excitation is usually¹⁷ related to the corresponding reduced electric transition probability by

$$B(EJ, k \rightarrow 0, 0^+ \rightarrow J^+) = 2^2 \lim_{k \rightarrow 0} \frac{[(2J+1)!!]^2}{k^{2J}} F_{0^+ \rightarrow J^+}^2(k), \quad (19)$$

which, in the case of $J=2$, reduces to

$$B(E2) = \frac{1}{16\pi} \left(\frac{C_2}{C_0} \right)^2 (Q_0^e)^2. \quad (20)$$

In spite of its simplicity the above expression is incomplete when we are dealing with projected states. The correct value must be obtained from the definition¹⁴

$$B(E2) = \frac{1}{5} \sum_M |\langle 2M | \hat{Q}_M^2 | 00 \rangle|^2, \quad (21)$$

where the final and initial states have well defined angular momentum, projected from the HF ground state wave function; \hat{Q}_M^2 is the electric quadrupole one-body operator. The matrix element becomes an expression which is evaluated after inserting a complete set of states, namely, the HF ground-state, the $1p-1h$ states, the $2p-2h$ states, etc. The particle-hole excitations involving two or more particles do not contribute. With the $1p-1h$ terms, the results were shown in Ref. (1). Without the $1p-1h$ terms, i.e., keeping only the H-F ground state in the complete set, it can be shown that the expression (21) will reduce to (20). In Table IV we show the results from each formula and the experimental values.

Table IV - The $B(E2; 0^+ \rightarrow 2^+)$ reduced transition probabilities in units of $e^2 \text{fm}^4$. Our results from expressions (20) and (21) are in the second and third lines, respectively. The values of Ripka are from Ref. (11). In the last line we have the results of Ford, Braley and Bar-Touv, Ref. (12).

	Ne ²⁰	Mg ²⁴	Si ²⁸	S ³²
Exp.	340 ± 40 ^(a)	446 ± 45 ^(b)	346. ± 33 ^(b)	330. ± 50 ^(c)
Eq. (21)	313.	453.	566.	311.
Eq. (20)	167.	243.	331.	131.
Ripka	247.	470.	520.	
FBB	204.	374.	376.	325.

(a) Ref.10, (b) Ref.15, (c) Ref.16.

For Si^{2+} the best theoretical value occurs when the expression (20) is used. This is consistent with the excellent fitting obtained for the $0^+ \rightarrow 2^+$ scattering form factor shown in Figs. 3a, 3b.

7. CONCLUSIONS

The results presented here are quite satisfactory in spite of the approximations we had to make concerning the inert core, as discussed in Ref. (1), plus the fact that the calculation was restricted to the s-d shell states.

The nuclear radii were in good agreement with the experimental values. The harmonic oscillator parameter b was not adjusted to reproduce the best radius. The value of b was fixed for each nucleus, given by the formula of Blomqvist and Molinari, which works well for light nuclei.

The best values for the quadrupole moments were obtained in the case of Si^{28} and S^{32} , the other nuclei presented a 10-20% deviation from experiment. With the usual nucleon effective charge we could not reproduce the hexadecapole moments; this could be attributed to the small subspace we worked with.

The elastic form factor has been well reproduced up to the first minimum, suggesting that, in the HF approximation, the nuclear long range correlations are correctly described by the Skyrme interaction. Except for Si^{28} , we failed to reproduce the inelastic form factors for the $0^+ \rightarrow 2^+$ transition, what is consistent with the quadrupole moments results.

A more complete study of nuclear properties in the HF approximation, with the Skyrme force, should be performed in a larger basis of single particle states, without the inert core hypothesis, but including short range correlations.

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