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SKYRME FORCE AND THE MASS FORMULA

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Abstract: Coefficients of the mass formula related to the property of the nuclear surface are calculated from the Skyrme forces SII, SIII and SV defined by the Orsay group. Comparing with Myers' mass formula parameters, it is found that the effective stiffness Q for separation of the neutron and proton surfaces is too large by a factor of about two for SIII. The discrepancy can also be stated by saying that the surface symmetry energy calculated from SIII is too small, and related to this is a too thin neutron skin for $N > Z$ nuclei. The SV force gives a much too small value for Q. The SII force, with a repulsive term somewhere intermediate between SIII and SV gives a better value for Q. The strong density dependence of SIII is needed, however, to give good single-particle spectra (or the effective mass large enough). The SIII force has a density dependence between unlike nucleons only (between neutrons and protons). In this paper we modify the Skyrme force so as to allow for a density dependence also between like nucleons. A many-body theoretical justification for this modification is given in the paper. The mass formula parameter Q is reproduced with our new force maintaining a sufficiently strong density dependence. The neutron skin thickness is increased and the ^{40}Ca-^{48}Ca isotope shift of the charge radius is also well reproduced with this new force. A change of the density dependence from a linear to a one-third power dependence improves the agreement with the compressibility, and also affects the neutron-proton distributions in the surface.

1. Introduction

There are two methods for the theoretical study of nuclear properties: binding energies, deformations, fission, etc.

The most extensively applied method uses the mass formula. The parametrization of Myers and Swiatecki [1]), based on the nuclear droplet model, is chosen by detailed theoretical considerations and nine parameters are adjusted to give a least-squares fit to some 1800 data on binding energies and fission barriers. The droplet model is derived from a macroscopic theory. It has been found necessary, however, to incorporate the effects of nuclear shell structure, which is of microscopic origin. This is done via the Nilsson model [2]) and the Strutinsky averaging procedure [3]). This method has had apparent success for example in the prediction of the double-humped fission barrier.

The other method is purely microscopic, starting with an effective nucleon-nucleon interaction. This interaction is sometimes calculated from a free nucleon-nucleon interaction using the Brueckner many-body theory. Some adjustment of the calculated effective interaction (the reaction matrix) is then usually required to fit the

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binding energies of nuclei. These calculations are often rather complex and the agreement with experimental data is mostly disappointingly poor in relation to the computational effort that is required [4]).

Ground-state and macroscopic properties of nuclei are however *not* to be expected to depend on the detailed structure of the interaction. For example, in the calculation of the total energy of a closed shell nucleus one averages over angular momentum states and over the momentum dependence (nonlocality) of the interaction. This suggests that one should expect some success by using some averaged and simplified force for that calculation. Several such forces have been used in the literature [5-8]). They are more or less closely related to our theoretical understanding of such an effective force as derived by the many-body theory (Brueckner theory). Usually these forces are parametrized to fit some nuclear properties like binding energies, radii, etc. One should notice the analogy of the development of this microscopic theory with the theory of the macroscopic mass formula. In the former there is a parametrization on the microscopic level which can be guided by our (unfortunately incomplete) knowledge of the effective force. In the latter the parametrization is on the macroscopic level and it is guided by the theory of the droplet model.

It would of course be desirable to fit the parameters of the microscopic theory, i.e. those of the two-body interaction by a least-squares fit to the 1800 or so data used for the mass formula. This is not possible in practice (although it might be so in the future). Instead one has to be content with an adjustment of the parameters to fit a fewer number of data. Such a fit is usually done in conjunction with a calculation of mass formula coefficients such as volume and symmetry energy, saturation density and compressibility. One usually finds a fair agreement with these mass formula coefficients. Sometimes one even determines some of the parameters of the interaction by adjusting them to reproduce mass formula coefficients.

Among the several forces, the Skyrme force [5]) has become very popular in recent years, and its success and limitations are becoming increasingly known. Its popularity might be mainly connected with its simplicity. It has also received some touch of realism from the work of Negele and Vautherin [9]) who compare the Skyrme Hamiltonian with that of the Negele interaction [10]). The simplicity of the Skyrme force stems largely from the expansion of both the range and the nonlocality of the force to second order in momentum space. This simplifies the calculation (especially of deformed nuclei) as the force is then for practical purposes a δ-function force. For comparison, the force used by Köhler [8]) expands only the nonlocality but not the range.

The microscopic approach is in principle more fundamental and should be more powerful as one does then not need to impose any shell corrections as these are (hopefully) already included in the model. In order for the microscopic method to successfully compete with the macroscopic method in practical work, it is necessary however to make an equally good fit to the many experimental data. It would be technically next to impossible to do such a fit for the two-body parameters at this time because of the excessive computing time that would be required.

An alternative procedure would be to choose the two-body parameters so as to reproduce directly, not the experimental data, but the mass formula parameters derived from these data. We could for example adjust the interaction to give the mass formula volume, symmetry and surface energies as well as saturation density and compressibility. This would determine the five parameters (neglecting the spin-orbit term) of the Skyrme interaction. This would not guarantee however a good fit to actual nuclei for two reasons. The first reason is that the mass formula (of Myers and Swiatecki) contains nine adjustable parameters so that although we have fitted five, there are another four. We would not expect for example our force to reproduce the surface-symmetry energy after the adjustment of the five parameters as described above.

There is also another reason why we would not obtain a good fit to actual nuclei. In the derivation of the mass formula expression from the droplet model, a truncation is made of a series expansion, implying that certain coefficients are set equal to zero. We would probably not find these coefficients to be exactly zero if we calculated them from our force, but if the mass formula makes sense at all we would find them to be small.

In conclusion, we would request of our two-body force that it at least approximately (but not necessarily exactly) reproduces the mass formula parameters that are determined by a least-squares fit to experimental data. This is admittedly not a very precise statement. It would probably mean that one should expect an agreement to within a few percent or so. Any major discrepancies should be investigated and the force (or the mass formula!?) modified accordingly.

The Skyrme force was mentioned above as one of the forces that has been explored in some detail. The "best" version within the standard parametrization of this force was found by the Orsay group to be the SIII force [11]). The SIII reproduces single-particle spectra reasonably well and also binding energies of some closed shell nuclei. Some of the mass formula coefficients have been calculated with this force previously [11]). In this investigation we also calculate some of the other parameters especially the surface and surface-symmetry energies. These were obtained from self-consistent field (Hartree-Fock) calculations on a semi-infinite system. The method has been described in earlier publications [12]).

2. The mass formula

We are comparing the results of calculations with the Skyrme force to the mass formula of Myers and Swiatecki. A brief review of their results follows. For a spherical nucleus with N-neutrons and Z-protons ($A = N+Z$) the expression for the energy is

$$E(N, Z) = [-a_1 + J\delta^2 - \tfrac{1}{2}K\bar{\varepsilon}^2 + \tfrac{1}{2}M\delta^4]A + [a_2 + \tfrac{9}{4}J^2/Q\delta^2]A^{\frac{2}{3}} + \text{curvature corr.} + \text{Coul. energy}. \quad (1)$$

The curvature correction is probably small and is neglected by Myers, who sets the parameter $a_3 \equiv 0$. There are six parameters; a_1, J, K, M, a_2 and Q. The parameter $\bar{\varepsilon}$ is the average (over the nuclear volume) shift in density from its normal nuclear matter value. This shift results from a compression of the nucleus due to the surface energy a_2, and an expansion due to the Coulomb force, giving

$$\bar{\varepsilon} = [-2a_2A^{-\frac{1}{3}} + L\bar{\delta}^2 + c_1Z^2A^{-\frac{4}{3}}]/K. \tag{2}$$

The parameter L originates from an expansion of the energy e of nuclear matter in ε and δ (asymmetry):

$$e = -a_1 + J\delta^2 + \tfrac{1}{2}K\varepsilon^2 - L\varepsilon\delta^2 + \tfrac{1}{2}M\delta^4. \tag{3}$$

The parameter c_1 is related to the average nucleon distance in nuclear matter r_0 by $c_1 = \frac{3}{5}e^2/r_0$.

In eq. (1) the average asymmetry $\bar{\delta}$ is

$$\bar{\delta} = [I + \tfrac{3}{16}(c_1/Q)ZA^{-\frac{4}{3}}]/[1 + \tfrac{9}{4}(J/Q)A^{-\frac{1}{3}}], \tag{4}$$

where

$$I = (N-Z)/(N+Z). \tag{5}$$

It should be noted that the minus sign in front of the compressibility K in eq. (1) is correct (and not a misprint). It may seem in contradiction with the corresponding plus sign in eq. (3). The term in eq. (1) actually represents the sum of two terms, one coming from the bulk $\frac{1}{2}K\bar{\varepsilon}^2$ and the other from the surface $-K\bar{\varepsilon}^2$.

In the mass formula (1) we also wish to point out the coefficient

$$a_{ss} = \tfrac{9}{4}J^2/Q, \tag{6}$$

often referred to as the surface-symmetry energy.

One important consequence of Myers' analysis is the implication that it is more fundamental to choose Q as a parameter instead of a_{ss}. These parameters are however related by eq. (6). In an analysis of the equilibrium condition in a nucleus Myers found that his original eleven coefficients could be reduced to nine by expressing them in terms of Q. This parameter Q describes the stiffness against the pulling apart of neutrons and protons in the surface. This coefficient is therefore closely related to the neutron skin thickness which is given by

$$t = \tfrac{1}{2}r_0J/Q\bar{\delta}. \tag{7}$$

Myers adjusts the eight parameters of his mass formula by a least-squares fit to some 1800 nuclear masses. The result is shown in table 1. Not all of the parameters can be well determined by this fit. Myers therefore fixes some of them to values determined from his Thomas-Fermi calculations with the Seyler-Blanchard force [13]). These values are indicated in table 1.

TABLE 1
Mass formula coefficients

		Myers and Swiatecki [b]	SIII	SII	SV	SKa	SKb
vol. energy	a_1	15.986	15.87	16.00	16.06	16.00	16.00
surf. energy	a_2	20.76	19.6	19.8	19.6	19.8	19.8
curv. corr.	a_3	0 [a]					
symm. energy	J	36.5	28.2	34.2	32.72	32.9	33.8
eff. stiffness	Q	17 [b]	38(49)	26(39)	9(29)	21(27)	17(24)
compressibility	K	240	356	342	306	263	263
dens. dep. asymmetry	L	100 [a]	95	153	194	161	180
asymmetry	M	0 [a]	0.83	1.10	1.70		
av. dist.	r_0	1.175	1.18	1.17	1.15	1.15	1.15
eff. mass	m^*/m		0.76	0.58	0.38	0.61	0.61

[a]) Set to values from Thomas-Fermi calculations [13]).
[b]) Yields, eq. (6), $a_{ss} = 176$ MeV.

3. Calculations with the Skyrme force

In this paper we choose to calculate mass formula parameters from some of the previously used Skyrme forces. Our results urge us to make some changes as described below to improve the agreement with the mass formula and with calculations with realistic forces.

The Skyrme force and the corresponding Hartree-Fock equations have been described in detail in the literature [5, 9, 11, 14]). It is usually written in terms of a two-body and three-body part or as a density-dependent part:

$$v_2(\boldsymbol{r}-\boldsymbol{r}') = t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}')+\tfrac{1}{2}t_1[k'^2\delta(\boldsymbol{r}-\boldsymbol{r}') + \delta(\boldsymbol{r}-\boldsymbol{r}')k^2]+t_2\boldsymbol{k}'\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}+iW\boldsymbol{k}'\delta(\boldsymbol{r}-\boldsymbol{r}')(\boldsymbol{\sigma}\times\boldsymbol{k}), \quad (8)$$

where $\boldsymbol{k} = (\nabla_r - \nabla_{r'})/2i$ is the relative momentum operator acting on the wave functions on the right. The parameters of v_2 are t_0, t_1, t_2, x_0 and W.

The density-dependent part we write as

$$v_3(\boldsymbol{r}_1, \boldsymbol{r}_2) = \tfrac{1}{6}t_3(1+x_3P_\sigma)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\rho^\alpha(\tfrac{1}{2}(\boldsymbol{r}_1+\boldsymbol{r}_2)). \quad (9)$$

The parameters of v_3 for the Skyrme force is actually only t_3 while $x_3 = 1$ and $\alpha = 1$, resulting from a zero-range three-body interaction,

$$v_3(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = t_3\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta(\boldsymbol{r}_2-\boldsymbol{r}_3). \quad (10)$$

The mass formula parameters a, J, K, M and r_0 have been calculated previously [11]) for several versions of the Skyrme force. In table 1 the parameter L is also shown,

which is found from the infinite nuclear matter system by varying the density and asymmetry simultaneously. In addition we have made self-consistent ("Hartree-Fock") calculations on the semi-infinite system for different values of I.

The methods of this calculation has been described previously and applied to different forces [12]). The application of the method to the Skyrme force is straightforward.

TABLE 2
Force parameters

Model	t_0	t_1	t_2	t_3	α	x_0	x_3	w
SIII	−1128.75	395.0	−95.0	14000.0	1	0.45	1.0	120.0
SII	−1169.9	586.6	−27.1	9331.1	1	0.34	1.0	105.0
SV	−1248.29	970.56	107.22	0		−0.17		150.0
SKa	−1602.78	570.88	−67.70	8000.0	$\frac{1}{3}$	−0.02	−0.286	125.0
SKb	−1602.78	570.88	−67.70	8000.0	$\frac{1}{3}$	−0.165	−0.286	125.0

The calculations with $I = 0$ yield directly the surface energy a_2, as shown in table 1. The force parameters are given in table 2. The nucleon and surface energy densities are shown in figs. 1a and 1b. The calculations with $I = 0.1$ and $I = 0.2$ are shown in fig. 2. Plotted in fig. 2 is $a_2(\delta)$ where δ is the bulk asymmetry, and the curves connect the points for the specific force that is marked. The slope of each curve yields the surface-symmetry energy a_{ss}, from which Q can be calculated using eq. (6). The curves are however not quite straight lines, as assumed by the truncation of the mass formula expansion. The coefficient a_{ss} is therefore calculated at each of the two points of δ from

$$a_{ss}(\delta) = (a_2(\delta) - a_2(0))/\delta^2. \tag{11}$$

The resulting two values of a_{ss} are marked by the respective curves. The value of Q is calculated from eq. (6), using the point corresponding to $I = 0.1$, and is shown in table 1.

There is an alternative way to calculate Q. The calculation on the surface also gives the neutron skin thickness (being a function of I or δ). Therefore Q can also be calculated from eq. (7). The values of Q that are calculated this way are shown in table 1 within parenthesis. There is a substantial disagreement between the Q-values calculated in these two different ways, showing that the assumptions leading to eqs. (6) and (7) do not hold exactly for the Skyrme force. The reason for the discrepancy may be connected with the nonlinearity of the $a_2(\delta^2)$ curve and/or with the neutron-proton ratio in the surface.

Inspection of table 1 reveals some substantial differences between the mass formula parameters and the corresponding coefficients calculated from the Skyrme forces SII, III and V. Binding energies are shown in table 3.

One important difference is in the compressibility K. The mass formula gives 240 MeV while the Skyrme forces SII, III and V give 342, 356 and 306 MeV, respectively.

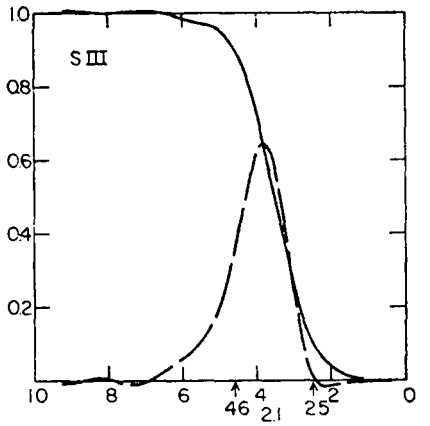

Fig. 1a. Full curve shows nucleon density, normalized to interior density, calculated with the SIII force. The 10% to 90% surface thickness, 2.1 fm, is indicated. The broken curve shows the surface-energy density [see ref. [12])].

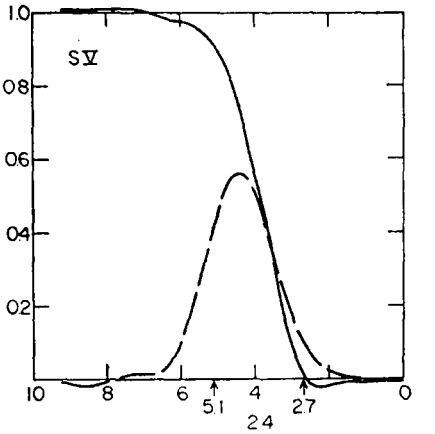

Fig. 1b. Same as fig. 1a for the SV force.

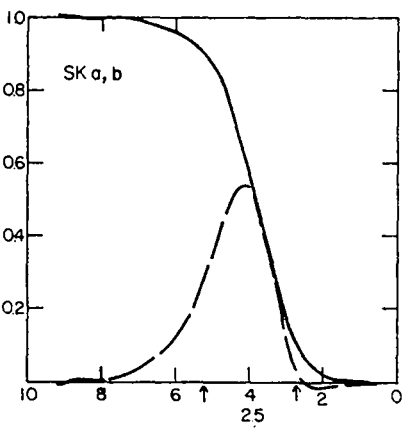

Fig. 1c. Same as fig. 1a for the SKa, b forces.

This failure of the force can be remedied by changing the density dependence of the force, making the repulsion build up more gently with increasing density.

Another important difference is in the symmetry energy, both in the bulk J and in the surface Q. The difference pertaining to the surface is also seen in fig. 2. One sees that the slope of the SIII curve is less than one-third of that of the mass formula, while the slope of the SV curve especially for small values of I is much too large. The SII curve shows a somewhat too small slope. As shown by eq. (7), the stiffness against separation of the neutron and proton surfaces, i.e. Q, is directly related to the neutron skin thickness t (table 4). Consequently t is much smaller for ^{208}Pb (0.125 fm) with

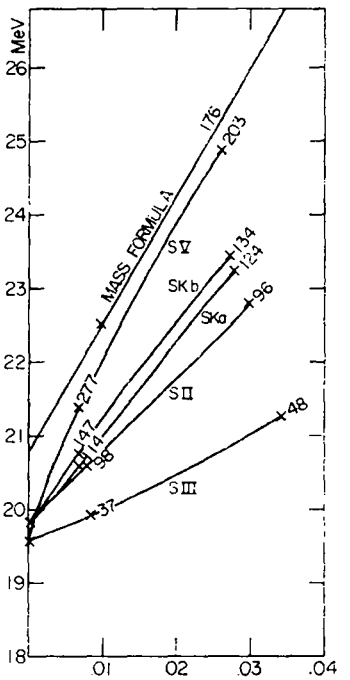

Fig. 2. Plots of surface energy a_2 versus the square of the bulk symmetry energy I.

TABLE 3
Binding energies (MeV)

	B_{exp}	ΔB_0				
		SIII	SII	SV	SKa	SKb
^{40}Ca	342.06	−0.18	−5.60	0.93	0.11	0.11
^{48}Ca	416.01	2.20	−13.45	2.25	0.98	1.29
^{208}Pb	1636.49	0.12	−68.6	0.55	−0.73	0.23

SIII than it is for SV where $t = 0.230$ fm. The difference in t for the different forces is also shown in figs. 3a and b where the neutron and proton semi-infinite surfaces are plotted for SIII and SV respectively with $\delta = 0.2$. The average surface locations (defined as $Z_i = N_i/\rho_{0i}$, where ρ_{0i} is the bulk neutron or proton density and N_i the number of neutrons or protons in the surface) are indicated by arrows.

We thus see that the neutron skin thickness increases with a decreasing value of t_3. The decrease in t_3 is accompanied by a decrease in effective mass or increase in non-locality of the shell-model potential. Negele has shown how the nonlocality of the field influences the neutron skin thickness, as confirmed by the results presented here [15]).

If one compares the calculated values of the mass formula coefficients for SIII and SV with the Myers parameters, the SV model appears slightly in favor. The value of L is larger but it must be remembered that the mass formula value, $L = 100$, was set at this value. It would of course be desirable to know the result of a determination of the mass formula parameters with $L \approx 200$. There is however a marked improvement in both Q and J and also in K in going from SIII to SV, i.e. when t_3 is decreased from 14 000 to zero.

TABLE 4
Skin thickness (fm)

Model	Radii	^{40}Ca	^{48}Ca	^{208}Pb	Surface $\delta = 0.2$
SIII	r_m	3.39	3.55	5.60	
	r_p	3.41	3.47	5.39	
	$r_n - r_p$	−0.043	0.138	0.125	0.20
SKa	r_m	3.40	3.56	5.59	
	r_p	3.43	3.45	5.46	
	$r_n - r_p$	−0.046	0.182	0.212	0.37
SKb	r_m	3.40	3.56	5.60	
	r_p	3.43	3.45	5.46	
	$r_n - r_p$	−0.046	0.184	0.24	0.40
	r_c(p)	3.500	3.523	5.513	
	r_c(n+p)	3.483	3.500	5.496	
	$r_c(L \cdot S)$		3.486		
exp.	r_c	3.49	3.48	5.50	

From the above observation and remarks it would seem that SV is the best model. There is however also the question of shell fluctuations. The mass formula describes the smoothed energy as a function of nucleon number. The smoothing is obtained by imposing a shell correction [16]). In the microscopic model the shell corrections are built into the theory. Correct shell fluctuations implies here "good" agreement with single-particle energies, defined as removal or addition energies. Stated otherwise, one requests the "correct" effective mass. From this point of view the model SIII is clearly to be preferred. It has been observed previously that a density-dependent interaction is necessary to obtain good agreement with single-particle energies [5-10]).

In the next section we show how the density-dependent Skyrme force can be modified so as to maintain good agreement with single-particle spectra but improve the agreement with mass formula parameters. Moreover, the modifications that lead to an improvement agree with results from calculation of the density-dependent force from a realistic interaction.

4. Modified Skyrme force

The modifications that we present in this paper involve the repulsive density-dependent term. In the Skyrme force the term v_3 in eq. (9) with $x_3 = 1$ implies a density dependence only between unlike particles, i.e., between neutrons and protons only. It implies a relatively stronger n-p attraction in the nuclear surface than in the bulk of the nucleon where the density is higher. The consequence of this is the relatively large value of Q and the relatively thin neutron skin for model SIII, as shown in tables 1 and 4. The increased n-p attraction at the low density in the surface agrees with a qualitative argument: At low density, nuclear matter calculations give an increased n-p attraction because of the tensor force. A detailed analysis however of the effective density dependence reveals some interesting results.

Such an analysis is shown in ref. [17]). We refer especially to figs. 1, 2, 4 and 5 of this reference. The qualitative argument given above is illustrated by fig. 1. This figure shows that the unlike interactions have a relatively much stronger density dependence. From fig. 2 one also finds, however, that the quadratic approximation to the momentum dependence increases the effective density dependence. In figs. 4 and 5 one finds indeed that the density dependence for *like* interactions may not be negligible [see also table 1 of ref. [17])].

The modification of the Skyrme force suggested by these results is to include one more parameter in this force, allowing also a density dependence between like nucleons. This is achieved by letting $x_3 \neq 1$ in expression (9) for v_3. This modification should be compared with the MDI of Moszkowski and Ehlers [18]) which corresponds to $x_3 = 0$.

Without doing any calculations it is rather evident that by this modification one can achieve a smaller effective stiffness Q for separation of the neutron and proton surfaces, as the x_3 parameter directly effects the ratio of the like to the unlike force in the surface compared to the same ratio in the bulk of the nucleus.

Another modification is also suggested by fig. 4 of ref. [17]). The density dependence of the Skyrme force is linear in the density ρ. The results of ref. [17]) (fig. 4) show an almost linear dependence on k_F, i.e. $\alpha = \frac{1}{3}$ instead of $\alpha = 1$ in eq. (9). It would be expected that such a modification would also affect the stiffness parameter Q because the ratio of the like to the unlike force would then also be modified in the surface.

The value $\alpha = \frac{1}{3}$ compares with $\alpha = \frac{2}{3}$ used in other work [8, 18]). In addition, fig. 5 of ref. [17]) shows a quite strong increase in the quadratically momentum dependent term for $k_F < 0.8$ fm^{-1}. The Skyrme force in its present parametrization (9) does not allow for such a density dependence. One may probably correct for this by increasing α somewhat. We have in this paper however chosen $\alpha = \frac{1}{3}$.

Choosing $\alpha = \frac{1}{3}$, the force parameters were adjusted to give $a_1 = 16.0$ MeV for the volume energy and to give the experimental binding and radius of ^{40}Ca. The parameter t_3 was chosen to give a single-particle spectrum close to that of SIII, see figs. 4a–c.

One might consider calculating the ratio between unlike and like interactions from the "realistic" calculations of fig. 4, ref. [17]). One then finds $x_3 \approx 0.4$. Adjusting x_0 to give the right binding of ^{208}Pb one finds $x_0 = 0.187$. The symmetry energy calculated with this force is $J = 31.3$ MeV and the surface energy is 19.8 MeV.

The stiffness $Q \approx 22.3$ MeV. Although this is an improvement over model SIII, this value of x_3 is still not compatible with the mass formula parameters. Although this x_3 was chosen from the realistic calculations it might not still be the most realistic value. The reason is that the parametrization of our model neglects several effects such as density dependence of the quadratic terms [see fig. 5 of ref. [17])] or, probably more important, the dependence on initial energies.

By letting x_3 instead be an adjustable parameter and choosing its value to reproduce Q, we find $x_3 = -0.286$. This defines the model SKa. The parameters of model SKa are shown in table 2 and the mass formula coefficients calculated with this force are shown in table 1. The value $\alpha = \frac{1}{3}$ rather than $\alpha = 1$ leads to a decrease of K from 356 to 263 in better agreement with the mass formula values $K = 240$. There is also, as expected, a decrease in Q from 38 to 21 MeV, to be compared with the mass formula $Q = 17$ MeV. This improvement in Q is also accompanied by a slight improvement in J. Fig. 1 shows the surface. Associated with these improvements is an increase of the neutron skin thickness which for ^{208}Pb, with the SIII force, was 0.125 fm but with the SKa force is 0.212 fm, as shown in table 4.

There is a corresponding increase in the neutron skin thickness for the semi-infinite surface with $\delta = 0.2$ from 0.20 to 0.37 fm as shown in table 4. The charge radius calculated from the proton point-charge distribution r_p is also shown in table 3. The ^{40}Ca-^{48}Ca isotope shift of r_p is from 3.41 to 3.47 fm for the SIII force. This is too large a shift to be explained by any of the corrections suggested [19]). As is known, experiment gives a 0.01 fm smaller charge radius for ^{48}Ca than for ^{40}Ca. The model SKa has a weaker n-p attraction in the surface than has the SIII force. It is therefore to be expected that as the $f_{\frac{1}{2}}$ neutrons are added to ^{40}Ca there will be relatively less "pulling out" of the protons when calculating with the SKa force. This is also seen in table 4 where there is an isotope shift in r_p from 3.43 to 3.45 fm, i.e. of 0.02 fm compared to 0.06 fm for SIII. The effect of the charge distribution of the neutron and the proton is calculated below for our next model SKb.

Other calculations not included here show that the improvement in Q and J are actually due not only to the new value of the parameter x_3 but also to the decrease in α from 1 to $\frac{1}{3}$. This refers even more to the improvement in the isotope shift of the radius. The functional dependence on the density is therefore very important in explaining the effects we are concerned with here.

In the model SKa we assumed both the like and the unlike interactions to depend upon the total nucleon density. There is no *a priori* justification for any of these interactions to have this dependence. The interaction between neutrons should depend rather on the neutron density, and that between protons on the proton density. Calculations of the reaction matrix from a realistic nucleon potential have shown, however,

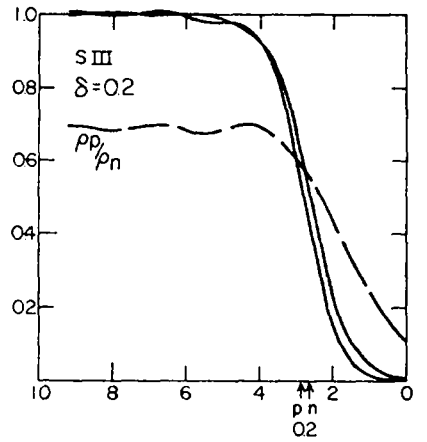

Fig. 3a. Full curves show neutron and proton densities normalized to interior densities. Broken curve shows ratio of proton and neutron densities. Arrows indicate average neutron and proton surfaces.

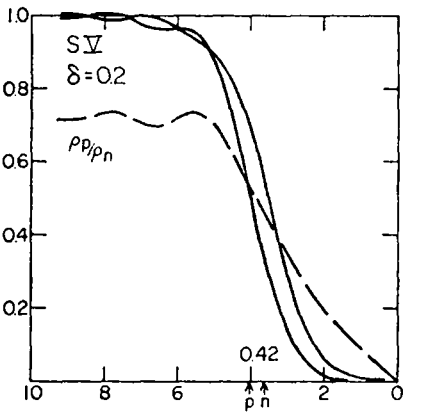

Fig. 3b. Same as fig. 3a for the SV force.

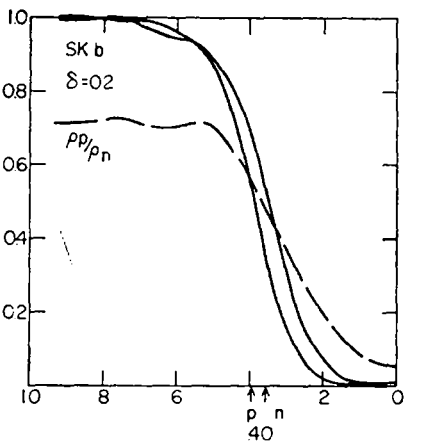

Fig. 3c. Same as fig. 3a for the SKb force.

that the n-p interaction is almost exactly a function only of the total density and not a function of the two densities separately [20]).

The above considerations leads to the model interaction that we consider more realistic; the model SKb. In this model we allow the interactions between n-n, p-p, and n-p nucleons to depend on three different densities, namely the neutron, proton and total density respectively. The parameters were determined as before after setting $t_3 = 8000$ and $x_3 = -0.286$ as in model SKa. The value of x_0 is then found to be -0.165 while the other parameters are the same as for SKa (see table 2). Table 3 shows that now $Q = 17$ MeV equal to the mass formula value, while the symmetry energy J increased slightly to 33.8 MeV. Table 4 shows that there are only minor

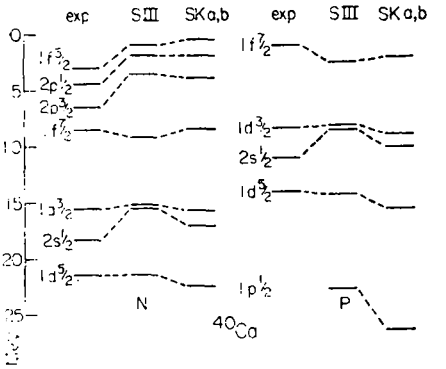

Fig. 4a. Single-particle energies for ^{40}Ca calculated with SIII and SKa, b.

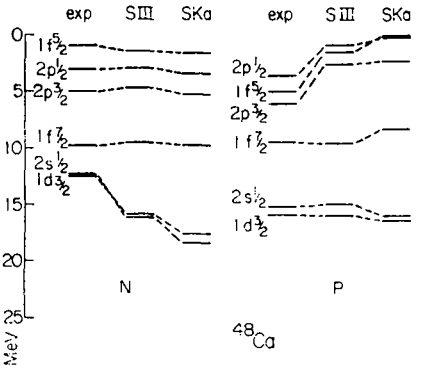

Fig. 4b. Single-particle energies for ^{48}Ca calculated with SIII and SKa. SKb gives a spectrum almost identical to SKa.

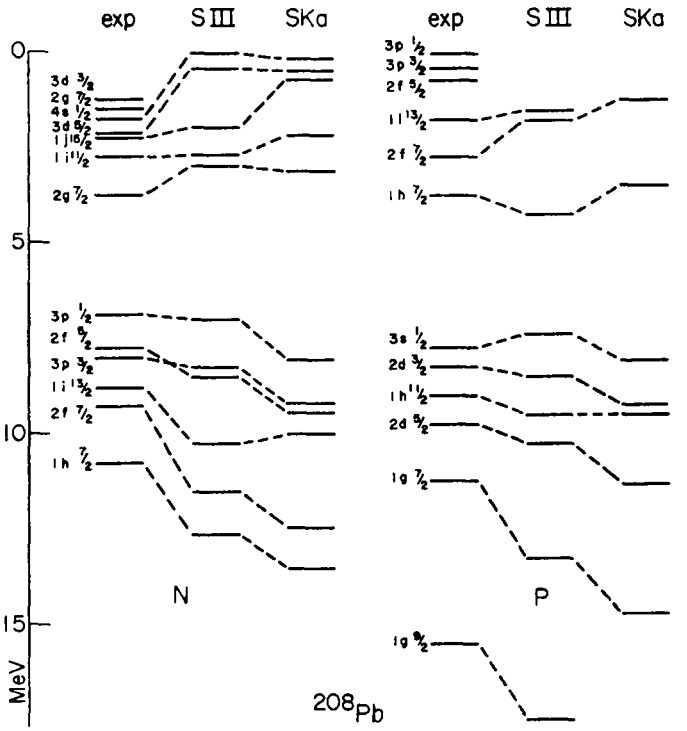

Fig. 4c. Single-particle energies for ^{208}Pb calculated with SIII and SKa. SKb gives a spectrum almost identical to SKa.

changes in the radii and neutron skin thickness. For model SKb, table 4 also shows, for ^{40}Ca and ^{48}Ca, the charge radius after folding in the charge distribution of the proton r_c(p), and also the charge distribution of the neutron r_c(n+p). After these corrections, the charge radius of ^{40}Ca is 3.483 fm and that of ^{48}Ca is 3.500 fm, com-

pared with the experimental values 3.49 and 3.48 fm, respectively. In our calculations the charge form factor of the neutrons in ^{40}Ca and ^{48}Ca were found to decrease the radii by 0.017 and 0.020 fm respectively. The decrease due to the extra $f_{\frac{7}{2}}$ neutrons in ^{48}Ca thus contributed 0.006 fm to this decrease compared to 0.007 fm in ref. [19]). According to ref. [19]), the decrease of 0.014 fm in ^{48}Ca is due to the spin-orbit interaction thus further reducing the ^{48}Ca radius to 3.486 fm. There is therefore after these corrections, a difference of 0.01 fm between the calculated and experimental isotope shifts. This may be explained by the admixture of higher order states. For $\delta = 0$, the model SKb gives a surface identical to SKa (fig. 1c). The surface for $\delta = 0.2$ is shown in fig. 3c.

5. Concluding remarks

In our opinion the modifications of the Skyrme interaction that are proposed in this paper lead to significant improvements. It should be observed that the improvement is not only in one but in several respects: compressibility, symmetry energy (both the bulk and surface), neutron skin thickness and radial isotope shift.

Further overall improvements in comparing the symmetry energy to mass formula and isotope shift can be achieved by decreasing the value of x_3. For example, by reducing x_3 of model SKa to -1.25 ($x_0 = -0.4$, and keeping all other parameters the same as SKa) we found $J = 36.1$ and $Q = 17$ MeV with a 0.01 fm reduction in the ^{40}Ca-^{48}Ca isotope shift. (This calculation was made as for SKa neglecting the separate dependences on neutron and proton densities.) This small value of x_3 may not seem realistic but may cover up for effects not included by the model interaction. Other effects suggested by the work of ref. [17]) would for example be a density dependence of t_1 and t_2, and also a dependence on starting energies. There are also several other approximations such as that to the range of the interaction which would contribute to the discrepancies. It seemed for example that an explicit range can lead to better single-particle spectra [8]).

There is however always the question as to what kind of agreement with mass formula parameters and with spectra one should request. In the case of the mass formula, this was discussed in sect. 1. It is for example, not clear if the observed differences are meaningful or not. The mass formula surface energy $a_2 = 20.76$ MeV while all Skyrme forces including the modified ones, are about 1 MeV smaller. The modified Skyrme forces lead to a nuclear matter density that is about 6 % higher than the mass formula predicts. As regards the spectra, there are corrections that are known only roughly or for a few select states [8, 21]).

The Skyrme force contains a three-body contact force (10) that in Hartree-Fock calculations is equivalent to the density-dependent force (9), with $x_3 = 1$ and $\alpha = 1$. The density-dependent force derived here gives $x_3 \approx -0.3$ and $\alpha \approx \frac{1}{3}$, suggesting that a three-body contact force is not realistic. It should be pointed out that our results suggest rather a density-dependent two-body delta interaction of the type considered

by Moszkowski [18]) in his modified delta interaction (MDI) which corresponds to $x_3 = 0$ and $\alpha = 1$.

Our modifications of the Skyrme force affects (apart from the compressibility) the bulk- and surface-symmetry energies. It should be observed that the mass formula values of J and Q were obtained by assuming the validity of the droplet model, as detailed by Myers [1]). If one instead lets the two symmetry energies be completely free parameters in a general mass formula (not derived from the droplet model) it is not possibleto uniquely determine J and Q separately. This non-uniqueness as regards the reproduction of binding energies is actually well illustrated by our single-particle spectra shown in fig. 4. All the models give essentially the same spectra. This implies that they all give nearly the same addition or removal energies, and therefore nearly the same *total* (bulk and surface) symmetry energies. The SIII model has been tested in this respect and was found to give correct total symmetry energies [21]).

To decide which model SKa, SKb or SIII is the better (more realistic) one can therefore not look at binding energies alone. The difference between these models shows primarily in the ratio of neutron and proton densities at the surface, i.e. in neutron skin thickness. There is unfortunately no direct experimental measurement of this quantity. One has instead to rely in some part on calculations done with realistic interactions. It is in fact the reaction matrix of such calculations that we want to approximate by our model interaction (believing that these calculations do indeed represent the actual physical situation), so that it is quite logical to test our model against realistic calculations. Realistic calculations on ^{208}Pb gives a neutron skin thickness of 0.23 fm [ref. [10])], 0.26 fm [ref. [22])] and 0.25 fm [ref. [17])]. [The last result is for $U_p \neq 0$ in the notation of ref. [17]).]

Negele [15]) finds that the tail of his neutron distribution of ^{208}Pb agrees with experimental measurements. As his charge radius also agrees with experiment one has some confidence in a neutron skin thickness of about 0.23 fm.

Higher order (correlation) corrections [22]) bring the skin thickness up to $\approx$ 0.34 fm so there is still some uncertainty about the experimental verification of this quantity. We wish to point out, however, that the calculations with the model interaction should reproduce the skin thickness 0.23 fm because these calculations do not incorporate the correlation corrections. The experimental skin thickness is on the other hand predicted to be 0.34 fm. The ^{40}Ca-^{48}Ca (proton point charge) radial isotope shift is $\approx$ 0.06 fm in ref. [22]) and in Negele and Vautherin's DME $\approx$ 0.1 fm [ref. [24])]. These results are nearly reproduced by choosing $x_3 \approx -0.3$ as in model SKb but not by $x_3 = 1$ as in SIII. We therefore conclude, by this indirect evidence, that SKb is a better representation of the reaction matrix deduced from a realistic interaction. From the evidence that SKb is more realistic than SIII, we can also to some degree support the mass formula values of J and Q in table 1; i.e. we have evidence that the physics underlying the droplet model is on the whole correct. We can conclude this because the SKb that reproduces the n-p densities in the surface also reproduces the values of J and Q obtained by assuming the droplet model.

It should be pointed out however that there are some reservations with this conclusion. We have in mind here not just the actual discrepancies between the mass formula coefficients and the same coefficients calculated by SKb. It is not clear, for reasons discussed in sect. 1, if these observed differences are meaningful or not.

The droplet model assumes a specific relation between neutron and proton distributions in the surface. According to this relation the two values of Q in table 1 calculated from eqs. (6) and (7) should agree. They do not, however, the largest disagreement being for SV. This shows that the droplet model does not completely describe the physics corresponding to these model interactions. It is consoling however, that the smallest discrepancy occurs for the model we consider most realistic, namely model SKa, b.

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