

Skyrme-force parametrization: Least-squares fit to nuclear ground-state properties

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We investigate systematically the possibilities and the limits of the Skyrme force for reproducing nuclear ground-state properties in a spherical Hartree-Fock calculation. This investigation is performed by means of least-squares fits of the force parameters to the measured binding energy, diffraction radius, and surface width of eight selected nuclei. Particular emphasis is put on the density dependence of the interaction, which turns out to be determined mainly by the surface width. The least-squares fitting procedure yields the best-fit parameters together with uncertainties on them, and it also allows one to estimate the uncertainties of an extrapolation to other fields, e.g., nuclear matter properties. We also study the contribution of random-phase-approximation correlations to the ground-state properties and their influence on the parameters of the effective interaction. Here, we also compare to giant dipole resonance energies.

I. INTRODUCTION

In the description of nuclear ground state properties by Hartree-Fock calculations, enormous progress has been achieved by the introduction of the density-dependent, zero-range Skyrme forces.¹⁻⁴ With the adjustment of a few parameters in the effective force a good description of nuclei throughout the periodic table has been obtained. Meanwhile, there have been many efforts to improve on the parametrization in order to get a better reproduction of observables such as binding energies and rms radii and, in addition, fission barriers or giant resonance energies.⁵⁻⁹ In fact, one has achieved considerable improvement compared to the first parametrizations, Skyrme 1 through Skyrme 6.^{4,10}

In the present paper we do not aim to add just another parametrization to the existing ones; instead we want to investigate systematically the possibilities and the limits of the Skyrme-force parametrization. This is done by means of the least-squares fitting technique, which optimizes the force parameters such that the Hartree-Fock calculations best reproduce the experimentally determined nuclear ground-state properties as, e.g., binding energies, radii, and surface width. We restrict the investigation to ground state properties for two reasons: First, we want to study in an exhaustive manner the possibilities of the interaction and a number of possible variations in the theoretical approach; for this purpose it is necessary to keep the calculations simple and fast. Second, when fitting to a variety of nuclei (in particular to chains of isotopes) one hopes to take into account some response features of the nuclear system, namely the response to the addition of single nucleons; we will look (after the fit) at

some dynamical nuclear properties in order to learn to what extent this hope is justified. For the same reason, we also include in a further exploratory step giant resonances and ground state correlations (GSC) which we estimate by a sum-rule approach.

Many investigations of the Skyrme force take recourse to nuclear matter properties because there are some simple analytic relations between the force parameters and these properties. However, nuclear matter is not accessible to measurement. We adopt a complementary point of view: We extrapolate to the nuclear matter parameters, as they result from the forces which we fit to experimentally known ground state data, and, using the standard rules of error propagation, we can also estimate the uncertainties of this extrapolation.

The paper is organized as follows. In Sec. II we briefly review the Skyrme force parametrization. In Sec. III we discuss the physical meaning of an effective force and the range where it is expected to be applicable. In Sec. IV we briefly describe the sum-rule approach to giant resonances and ground-state correlations. In Sec. V we outline the fitting technique and the choice of experimental input data. The results are discussed in Sec. VI; Sec. VII summarizes our conclusions and gives an outlook to further improvements.

II. THE SKYRME FORCE: THE PARAMETRIZATION AND POSSIBLE REFINEMENTS

The Skyrme force is an effective force which parametrizes the G matrix for nuclear Hartree-Fock calculations by a zero-range, density- and momentum-dependent ansatz of the form

$$\begin{aligned}
 V_{\text{Skyrme}} = & t_0(1+x_0P_x)\delta(\mathbf{r}_i-\mathbf{r}_j) + \frac{1}{2}t_1(1+x_1P_x)[\mathbf{p}_{12}^2\delta(\mathbf{r}_i-\mathbf{r}_j) + \delta(\mathbf{r}_i-\mathbf{r}_j)\mathbf{p}_{12}^2] \\
 & + t_2(1+x_2P_x)\mathbf{p}_{12}\cdot\delta(\mathbf{r}_i-\mathbf{r}_j)\mathbf{p}_{12} + \frac{1}{6}t_3(1+x_3P_x)\rho^\alpha \left[\frac{\mathbf{r}_i+\mathbf{r}_j}{2} \right] \delta(\mathbf{r}_i-\mathbf{r}_j) \\
 & + it_4\mathbf{p}_{12}\delta(\mathbf{r}_i-\mathbf{r}_j)\{[\sigma(1)+\sigma(2)]\times\mathbf{p}_{12}\} + V_{\text{Coul,dir}} + V_{\text{Coul,exch}} \quad (2.1)
 \end{aligned}$$

where $\mathbf{p}_{12} = \mathbf{p}_i - \mathbf{p}_j$, and P_x is the coordinate exchange operator. A force of this sort was proposed as early as 1959 by Skyrme,¹ but the first satisfactory parametrization did not appear before 1972;⁴ in this paper the authors used, explicitly or tacitly, a form restricted to $x_1 = x_2 = 0$, $x_3 = 1$, and $\alpha = 1$. Later modifications abandoned one or the other of these restrictions, aiming at more flexibility in the force⁵⁻⁹ in order to better reproduce the experimental data.

The ansatz (2.1) can be derived from a Brückner G matrix by the density-matrix expansion technique.^{3,11} In this expansion one can produce an arbitrary number of terms. Too restricted a choice will not give enough flexibility to reproduce the data. On the other hand, with too many terms it is extremely difficult to find out which parameter is responsible for which physical effect. The choice (2.1) with $x_1 = x_2 = 0$ seems to be just adequate for fitting the bulk properties of the ground states, and we will use this form in the following. For more ambitious requirements

it may be necessary to let x_1 and x_2 be different from zero and also to employ further terms, e.g., to allow for a density dependence in the \mathbf{p}_{12}^2 terms.^{9,12}

In order to get some insight into the physical meaning of the different parameters we look at the Hartree-Fock (HF) Hamiltonian resulting from the force (2.1). It reads

$$\hat{H}_{\text{HF}} = \hat{\mathbf{p}} \frac{1}{2m^*} \hat{\mathbf{p}} + U_{\text{HF}} + (\nabla W_{\text{ls}} \times \hat{\mathbf{p}}) \cdot \boldsymbol{\sigma}, \quad (2.2a)$$

where the effective mass m^* is

$$\left(\frac{1}{m^*} \right)_q = \frac{1}{m} + \frac{1}{4} [t_1(1 + \frac{1}{2}x_1) + t_2(1 + \frac{1}{2}x_2)] - \frac{1}{4} [t_1(\frac{1}{2} + x_1) - t_2(\frac{1}{2} + x_2)], \quad (2.2b)$$

the potential is

$$\begin{aligned} (U_{\text{HF}})_q &= t_0(1 + \frac{1}{2}x_0)\rho - t_0(\frac{1}{2} + x_0)\rho_q + \frac{1}{6}t_3\rho^\alpha [(1 + \frac{1}{2}x_3)\rho^2 - (\frac{1}{2} + x_3)(\rho_p^2 + \rho_n^2)] \\ &+ \frac{\alpha}{12}t_3\rho^{\alpha-1} [(1 + \frac{1}{2}x_3)\rho^2 - (\frac{1}{2} + x_3)(\rho_p^2 + \rho_n^2)] + \frac{1}{4} [t_1(1 + \frac{1}{2}x_1) + t_2(1 + \frac{1}{2}x_2)]\tau \\ &- \frac{1}{4} [t_1(\frac{1}{2} + x_1) - t_2(\frac{1}{2} + x_2)]\tau_q - \frac{1}{8} [3t_1(1 + \frac{1}{2}x_1) - t_2(1 + \frac{1}{2}x_2)]\Delta\rho \\ &+ \frac{1}{8} [3t_1(\frac{1}{2} + x_1) + t_2(\frac{1}{2} + x_2)]\Delta\rho_q - \frac{1}{2}t_4(\nabla \cdot \mathbf{J} + \nabla \cdot \mathbf{J}_q), \end{aligned} \quad (2.2c)$$

and the spin-orbit potential is given by

$$W_{\text{ls}} = \frac{1}{8}(t_1 - t_2)J_q - \frac{1}{8}(x_1 t_1 + x_2 t_2)J + \frac{1}{2}t_4(\nabla\rho + \nabla\rho_q). \quad (2.2d)$$

Here, q denotes the protons or neutrons, and ρ , τ , and J are the matter, kinetic energy, and spin-orbit densities, respectively.

From these expressions we can draw inferences about the way the various parameters act. The t_3 term introduces a density-dependent repulsion which essentially guarantees the saturation of the force in the central region of the nucleus.

The $\hat{\mathbf{p}}_{12}^2$ components in the force have two effects: They essentially determine the effective mass m^* and they give rise to a "surface wave" $\Delta\rho$ in the potential. The m^* is responsible for the level spacing, and thus for the energies of the giant resonances. The $\Delta\rho$ has some influence on the oscillations of the charge distribution.³² The four combinations t_0 , $t_1(1 + \frac{1}{2}x_1) + t_2(1 + \frac{1}{2}x_2)$, $t_1(\frac{1}{2} + x_1) - t_2(\frac{1}{2} + x_2)$, $3t_1(1 + \frac{1}{2}x_1) - t_2(1 + \frac{1}{2}x_2)$, and $3t_1(\frac{1}{2} + x_1) + t_2(\frac{1}{2} + x_2)$ would allow one to adjust these effects separately. If, however, x_1 and x_2 are chosen to be zero, these two effects, level spacing and charge oscillations, necessarily are coupled. Nonvanishing exchange parameters x_1 and x_2 allow the adjustment of the contributions from protons and neutrons separately. Therefore, they provide a powerful handle on the nuclear density distribution in heavier nuclei, where protons and neutrons oscillate in opposite phase (e.g., Tondeur⁸ has adjusted the

full charge density distributions of several nuclei including ²⁰⁸Pb by using extremely large values for x_1 and x_2). But, in this paper we will not pursue these possibilities any further since a determination of x_1 and x_2 by mere ground state properties is very cumbersome. In the following we will always assume $x_1 = x_2 = 0$.

Up to now we have defined what we mean by the term "Skyrme force." However, there are several additional points that need to be specified. These further options which are subject to choice in Skyrme-Hartree-Fock calculations are the following:

(1) In the Hartree-Fock spin-orbit potential Eq. (2.2d) there is a term proportional to $t_1 - t_2$, namely

$$\frac{1}{8}(t_1 - t_2)J_q. \quad (2.3)$$

This term is sometimes discarded [this can be done consistently by adding a rather involved tensor force to V_{Skyrme} (Ref. 10)], sometimes it is retained, and it is often hard to find out which option has been used in a particular calculation.

(2) The exchange part of the Coulomb force is approximated by the energy functional¹⁰

$$\langle V_{\text{Coul,exch}} \rangle = -\frac{3}{4}e^2 \left(\frac{3}{\pi} \right)^{1/3} \int d^3r \rho^{4/3}. \quad (2.4)$$

In some calculations this exchange part is taken into account, in others it is not.

(3) The center-of-mass correction is performed in most papers by using the so-called diagonal correction leading to an effective mass⁴

$$m_{\text{eff}} = m \left[1 - \frac{1}{A} \right]. \quad (2.5a)$$

This procedure might be a useful one in a mere ground-state calculation. But it leads to incorrect collective mass parameters for translation, rotation, vibration, and fission. A more consistent center-of-mass correction is achieved by retaining the free nucleon mass, but subtracting after the Hartree-Fock calculation the translational zero-point-motion energy

$$Z_{\text{trans}} = \frac{\langle \hat{p}_{\text{c.m.}}^2 \rangle}{2Am}, \quad (2.5b)$$

where $\hat{p}_{\text{c.m.}}$ is the center-of-mass momentum operator. This choice is consistent with the zero-point-energy (ZPE) correction in nuclear collective calculations^{13,14} and with the approximate estimate of ground-state correlations in the random-phase approximation (RPA) (Refs. 15 and 16) and therefore should be preferred. The difference between the two options (2.5a) and (2.5b) becomes particularly important in light nuclei.

(4) In the evaluation of the nuclear charge density one normally includes as a first relativistic correction the contribution from the spin-orbit current³⁹

$$\delta\rho_{\text{ls}} = \frac{-1}{r^2} \frac{d}{dr} (r\rho_{\text{LS}}(r)) \quad (2.6)$$

[for details of $\rho_{\text{LS}}(r)$ see Ref. 39].

With two choices for each of the four items we are left with 2^4 options. Of course, each of these options yields different results in a practical calculation, and therefore they must be specified explicitly together with the parameter set used for the Skyrme force. In Sec. V we shall give a brief account of a number of forces currently in use and the most appropriate options to be used with each of them.

A Hartree-Fock calculation is directly applicable only for magic nuclei. In the case of nonmagic nuclei one has to extend it to a Hartree-Fock-Bogoliubov calculation. Since the Skyrme force, in general, does not have good pairing properties, we introduce in addition a schematic pairing force where the gap is given by $\Delta = 11.2/A^{1/2}$ MeV.

III. THE CONCEPT OF AN EFFECTIVE FORCE

The nucleus is a rather complicated many-body system which cannot be described *ab initio* by a mere Hartree-Fock calculation. The problem of the strong short-range correlations requires more elaborate theories like the Brückner theory,¹⁷ the Jastrow method,¹⁸ or the $\exp(S)$ formalism.¹⁹ All these theories embrace the Hartree-Fock equations for the evaluations of the single-particle basis. However, in those Hartree-Fock calculations one has to insert an effective interaction which stems from the solution of the short-range two-body correlations. The generation of an effective force can be explained schematically in the following way: We split the correlated wave function $|\Psi\rangle$ into a Slater determinant $|\Phi_{\text{HF}}\rangle$ and a factor F_{corr}

$$|\Psi\rangle = F_{\text{corr}} |\Phi_{\text{HF}}\rangle, \quad (3.1)$$

where F_{corr} is an operator accounting for the (unknown) correlations. The energy expectation value can be re-grouped

$$\begin{aligned} \langle \Psi | V | \Psi \rangle &= \langle \Phi_{\text{HF}} | F_{\text{corr}}^+ V F_{\text{corr}} | \Phi_{\text{HF}} \rangle \\ &= \langle \Phi_{\text{HF}} | V_{\text{eff}} | \Phi_{\text{HF}} \rangle, \end{aligned} \quad (3.2)$$

defining the effective force for the Hartree-Fock calculation as

$$V_{\text{eff}} = F_{\text{corr}}^+ V F_{\text{corr}} \quad (3.3)$$

and (as pointed out in the preceding section) the Skyrme force is thought to be a reasonable parametrization of such an effective force.

If one determines the free parameters of this force ansatz directly by a fit to measured data with a Hartree-Fock calculation, one has circumvented the enormous problems related to the evaluation of the correlations F_{corr} . On the other hand, one has to pay a price for this simplification: For any observable \hat{A} one should construct analogously an effective operator

$$\hat{A}_{\text{eff}} = F_{\text{corr}}^+ \hat{A} F_{\text{corr}} \quad (3.4)$$

(where \hat{A} may stand for the charge density, the form factor, the rms radius, etc.). Unfortunately we cannot evaluate the transformation (3.4) since we do not know F_{corr} . Therefore an effective force is used together with the normal operators. This procedure should be acceptable for those observables which are not much affected by F_{corr} . We expect that the low momentum components of the form factor can be evaluated reliably without the transformation (3.4), since F_{corr} describes short-range correlations and perhaps mesonic degrees of freedom, both of which become more important only at higher momentum transfers. This means that the calculation using an effective force but only a normal operator should reproduce the bulk properties like radii and surface widths. However, it is not advisable to put too much emphasis on higher Fourier components, say, above the Fermi momentum unless one has some estimate for F_{corr} [the spin-orbit contribution to the density, Eq. (2.6), may be looked at as a first step in this direction].

Besides this problem of effective operators for observables it is important to keep in mind that up to now we have defined the Skyrme force as an effective force for Hartree-Fock calculations and that any application outside this range requires a reconsideration of this effective force. In fact, most applications of Skyrme forces exceed the range of mere Hartree-Fock (or Hartree-Fock-Bogoliubov) calculations. The force is widely used in mean-field calculations of nuclear collective motion (like constrained Hartree-Fock, time-dependent Hartree-Fock, etc.) and also for calculating giant-resonance properties (in a sum-rule approximation or in RPA). Of course, one can declare the Skyrme force as the effective force for Hartree-Fock plus mean field calculations or for Hartree-Fock plus RPA, but then one has at least to readjust the parameters. The important point, however, is that each excitation consistently requires its corresponding ground

state correlations and the Skyrme force is then to be defined as the effective force for the description of the ground state which is calculated in Hartree-Fock plus those correlations which result from the excitations taken into account.

The low-lying collective surface modes, which are described by the mean-field theories, have large zero-point vibrations in the region of the nuclear surface; therefore they lead to smoother density distributions and to larger surface widths in soft nuclei, but they have only little effect on the binding energy. In magic nuclei their contribution is negligible in any respect.²⁰ Therefore, for applications to low energy and large amplitude dynamics (fission, fusion, etc.) it may be justified to use a Skyrme force which has been fitted to measured properties of a few magic nuclei in a mere Hartree-Fock calculation, where eventually some barrier properties are also taken into account.⁷

However, a calculation of the giant-resonance excitations, which are particular RPA modes, must take into account the corresponding RPA ground-state correlations in order to be consistent. These correlations do have a strong impact on the binding energies and moderate influence on the bulk properties of the charge distribution density.¹⁶ Therefore, an extended use of Skyrme forces in RPA calculations (or a sum-rule or fluid dynamical approach to it²¹⁻²³) requires a redetermination by a calculation with RPA-correlated ground states. In the present paper we concentrate mainly on the first sort of usage, namely the Skyrme force as an effective force for nuclear Hartree-Fock calculations (and large-amplitude mean field dynamics).

IV. SUM-RULE APPROXIMATION TO GIANT RESONANCES AND GROUND-STATE CORRELATIONS

In order to estimate RPA properties we evaluate giant resonances within a sum-rule approximation as outlined in Ref. 21 and complemented by some features from Ref. 22. For the $L=0$ and $L=2$ modes the model employs the scaling approximation; for the isovector $L=1$ mode we use the Goldhaber-Teller model (c.m. motion of protons versus neutrons). The latter is known to yield resonance energies which are too high, a deficiency which is tolerable at the present exploratory stage of the investigation.

When considering excitation properties one has to be aware that each excitation mode introduces its corresponding correlation into the ground state. Thus, the collective multipole modes which we estimate by sum-rule approximations have to be complemented by long-range ground-state correlations which ensure that the multipole width $\langle \Psi_0 | \hat{Q}^2 | \Psi_0 \rangle$ will be consistent with the $B(EL)$ strength $|\langle \Psi_0 | \hat{Q} | \Psi_{\text{exc}} \rangle|^2$. By means of the RPA operator algebra or by using the generator coordinate method one can derive simple estimates of the effect of ground-state correlations on observables.^{16,20,24} For the form factor we use

$$\langle \hat{F} \rangle_{\text{corr}} = \langle \hat{F} \rangle_{\text{HF}} + \sum_{\text{giant resonances}} (2L+1) \frac{(\lambda_{\text{HF}} - \lambda)^2}{\lambda \lambda_{\text{HF}}^2} \times \langle [\hat{P}, [\hat{F}, \hat{P}]] \rangle, \quad (4.1a)$$

with

$$\lambda = \langle \hat{Q}^2 \rangle_{\text{corr}}, \quad \lambda_{\text{HF}} = \langle \hat{Q}^2 \rangle_{\text{HF}}, \quad (4.1b)$$

where \hat{Q} is the multipole operator related to each giant resonance and $\hat{P} \propto [\hat{H}, \hat{Q}]$ is the corresponding momentum. For the energy we have to take into account that the Skyrme force is an effective force modeling a Brückner G matrix. Thus we have to subtract from the correlation energy the collective contribution from the lowest order ladder diagram.¹⁶ This leads to the effective correlation energy

$$E_{\text{corr}} = E_{\text{HF}} - \sum_{\text{giant resonances}} (2L+1) \hbar\omega \frac{(\lambda_{\text{HF}} - \lambda)^2}{4\lambda_{\text{HF}}\lambda} \times \frac{(\lambda_{\text{HF}} - \lambda)(3\lambda_{\text{HF}} + \lambda)}{4\lambda_{\text{HF}}^2}, \quad (4.2)$$

where the λ and λ_{HF} are given by Eq. (4.1b) and $\hbar\omega$ is the energy of the giant resonance.

V. DETERMINATION OF THE FREE PARAMETERS BY A DIRECT FIT TO MEASURED DATA

A physical hypothesis is tested by a comparison to measured data. A quantitative judgment on the adequacy of the hypothesis, the model, can be based on the variable χ^2 , which is given by the sum of the deviations squared between model prediction and measured value:

$$\chi^2 = \sum_n (M_n^{\text{exp}} - M_n^{\text{th}})^2 / \Delta M_n^2. \quad (5.1)$$

Here, $\{M_n\}$ is a set of observables to be chosen appropriately, and M_n^{exp} and M_n^{th} are their measured and predicted values, respectively. The weights ΔM with which each observable enters into χ^2 in principle should be the statistical errors in M_n^{exp} , and systematic errors as well in M_n^{exp} as in M_n^{th} should be dealt with separately. However, we do not expect our theoretical ansatz to reproduce the data within their very small statistical experimental errors. In principle, this would mean that we have to reject the model. However, it is our aim to explore the limits and, possibly, to find hints for improvements, and therefore we proceed in a more pragmatic way by choosing the uncertainties such that the different observables contribute roughly unity per data point to χ^2 (the corresponding values are given in Table I). The value of χ^2 itself therefore is somewhat arbitrary; however, tendencies when comparing different sets of data or parameters should give important insight into the ability of the model.

The present problem is the description of nuclear ground state properties by a Hartree-Fock-Bogoliubov calculation based on a Skyrme-type force. The hypothesis contains a number of unknown parameters p_i which, in this case, are the force parameters $t_0 - t_4$, x_0 , x_3 , and a . The quantity χ^2 depends on the values of these parameters through $M_n^{\text{th}}(p_1, p_2, \dots, p_N)$ (which results from inserting the parameters into the Skyrme-Hartree-Fock-Bogoliubov calculation). One looks for the best-fit parameter set $p_i^{(0)}$ which minimizes χ^2 . The problem of finding the minimum is a technical one; it will turn out to

TABLE I. Experimental data used in this investigation. The binding energies are from Ref. 33, diffraction radii and surface width are taken from Ref. 26 ($R^{(1)}$ in Table I and $\sigma^{(1)}$ in Table III), the spin-orbit splitting is taken as in Ref. 4, and giant dipole resonance energies are from Ref. 28. The last column shows the uncertainties on these data which we assume throughout this paper.

	^{16}O	^{40}Ca	^{48}Ca	^{58}Ni	^{90}Zr	^{116}Sn	^{124}Sn	^{208}Pb	ΔM
$-E_b$ (MeV)	127.6	342.1	416.0	506.5	783.9	988.7	1050.0	1636.4	0.2%
R_d (fm)	2.777	3.845	3.964	4.356	5.040	5.537	5.640	6.806	0.5%
σ (fm)	0.839	0.978	0.881	0.911	0.957	0.947	0.908	0.900	1.5%
ϵ_p (MeV)	6.3								0.1 MeV
ϵ_n (MeV)	6.1								0.1 MeV
E_{11} (MeV)					16.8	15.7	15.2	13.5	0.3 MeV

be quite difficult and to consume much computer time in the case under investigation here; however, with some care it can be solved with well-known techniques.²⁵

The χ^2 -minimizing procedure not only yields the best-fit parameter set, it also gives information on the uncertainties and on the correlations of the parameters.

If the model describes the full physics, then the resulting parameter values would be independent of the particular observables taken into consideration; different sets would lead to the same parameter values, which, however, are determined with different precision. However, the effective interaction is only an approximation to the problem and we can only expect it to be more or less appropriate for the description of selected observables; therefore, the resulting parameter values will depend upon the selection of observables in the fitting procedure. Our confidence in the model, i.e., in its predictive power, will increase the more different available information about the nuclei can be described by it.

It remains for us to specify a proper set of observables. In the present case, we mainly consider Skyrme-Hartree-Fock-Bogoliubov calculations; thus the observables in χ^2 can only be those for ground-state properties (in Sec. VIC we also report on the inclusion of the giant dipole resonance). Among these, the most prominent ones are the binding energy

$$E_b = \langle \Phi_{\text{HF}} | \hat{H} | \Phi_{\text{HF}} \rangle \quad (5.2)$$

and the nuclear extension. To represent the nuclear extension we choose the diffraction radius R_d of the nuclear charge distribution. The R_d is defined by the first zero $q_0^{(1)}$ in the form factor $F(q)$ for elastic electron scattering by²⁶

$$R_d = 4.739/q_0^{(1)}, \quad (5.3a)$$

with

$$F(q_0^{(1)}) = 0. \quad (5.3b)$$

The next important information on the nuclear charge distribution is the surface width σ which is obtained from the form factor at its second maximum,²⁶

$$\sigma^2 = \frac{2}{q_m^2} \ln \frac{3j_1(q_m R_d)}{q_m R_d F(q_m)}, \quad (5.4)$$

where q_m is given by

$$F(q_m) = 2 \cdot \text{form factor maximum}. \quad (5.5)$$

The form parameters R_d and σ are determined by the

low- q behavior of the form factor; therefore, they are rather insensitive to the neglect of short-range correlations and mesonic currents. As a result, we feel that they constitute, together with the binding energy, a set of appropriate observables within the framework of Skyrme-Hartree-Fock. In addition, we take into account the l - s splitting, $\delta\epsilon_{n,p}$, of the $1p$ level in ^{16}O in order to roughly fix the l - s parameter t_4 (here, the indices n and p refer to neutron and proton, respectively).

The choice of the observables is to be completed by the choice of nuclei to be included in the fit. For technical reasons we restrict ourselves to spherical Hartree-Fock calculations for which very fast codes exist.²⁷ For physical reasons we restrict ourselves mainly to nuclei with stiff surface vibrations where we expect ground-state correlations from the low-lying surface modes to be negligible (a force determined in this way should also be useful for fission/fusion calculations). These requirements lead us to choose eight more or less magic nuclei, namely ^{16}O , $^{40,48}\text{Ca}$, ^{58}Ni , ^{90}Zr , $^{116,124}\text{Sn}$, and ^{208}Pb . With the pairs $^{40,48}\text{Ca}$ and $^{116,124}\text{Sn}$ our data set also contains information about isotopic trends.

The values for E_b are taken from Ref. 33, those for R_d and σ from Ref. 26. The data for our standard set of nuclei are given in Table I.

In one case we also look at an enlarged set of nuclei where in addition to the above standard set we include the following nuclei: ^{40}Ar , $^{42,44}\text{Ca}$, $^{46,48}\text{Ti}$, ^{52}Cr , ^{56}Fe , ^{62}Ni , ^{66}Zn , ^{88}Sr , ^{92}Zr , ^{96}Mo , ^{118}Sn , and ^{206}Pb . We do not give their data explicitly here; they may be found in the references cited above.

As mentioned above, the minimization of χ^2 also allows one to determine the uncertainty Δp_i of the minimizing parameter values $p_i^{(0)}$. These uncertainties correspond to the range of the parameter values which still yield $\chi^2 \leq \chi_{\text{min}}^2 + 1$. We shall see that the parameters are strongly correlated such that for the full information the full error matrix must be taken into account. Since this matrix also depends upon the selection of data under consideration, it is useless to always communicate the full matrices. Instead we only give the correlated and uncorrelated errors corresponding to an increase in χ^2 by unity if the other parameters are kept fixed (uncorrelated) or if they are fitted anew (correlated). The correlated errors on the parameters are larger by up to two orders of magnitude, demonstrating the strong correlations of the parameters. We discuss the error correlation for one example in Sec. VID.

TABLE II. The parameters of Skyrme interactions currently in use. Apart from $T3$, all parametrizations are used in calculations with $\hbar^2/2m = 20.7525 \text{ MeV fm}^2$ for protons and neutrons; for $T3$, 20.750 MeV fm^2 has been taken for protons and 20.722 MeV fm^2 for neutrons.

Force	t_0	t_1	t_2	t_3	t_4	x_0	x_1	x_2	x_3	α
Skyrme 1	-1057.3	235.9	-100.0	14463.5	120	0.56	0.0	0.0	1.000	1.0
Skyrme 2	-1169.9	585.6	-27.1	9331.1	105	0.34	0.0	0.0	1.000	1.0
Skyrme 3	-1128.75	395.0	-95.0	14000.0	120	0.45	0.0	0.0	1.000	1.0
Skyrme 4	-1205.6	765.0	35.0	5000.0	150	0.05	0.0	0.0	1.000	1.0
Skyrme 5	-1248.29	970.56	107.22	0.0	150	-0.17	0.0	0.0	1.000	1.0
Skyrme 6	-1101.81	271.67	-138.33	17000.0	115	0.583	0.0	0.0	1.000	1.0
Skyrme a	-1602.78	570.88	-67.70	8000.0	125	-0.020	0.0	0.0	-0.286	$\frac{1}{3}$
Skyrme b	-1602.78	570.88	-67.70	8000.0	125	-0.165	0.0	0.0	-0.286	$\frac{1}{3}$
T	-1788.90	301.50	502.50	12764.0	130	0.353	-2.5	-1.7	0.475	$\frac{1}{3}$
$T3$	-1791.80	298.50	-99.50	12794.0	126	0.138	-1.0	+1.0	0.075	$\frac{1}{3}$
Skyrme M	-2645.0	385.0	-120.0	15595.0	130	0.09	0.0	0.0	0.000	$\frac{1}{6}$
Skyrme M^*	-2645.0	410.0	-135.0	15595.0	130	0.09	0.0	0.0	0.000	$\frac{1}{6}$

A particular advantage of the χ^2 -minimizing procedure is the availability of the full error matrix. It can also be used to estimate the uncertainties of an extrapolation, i.e., a prediction of values of observables which have not been included in the fit. We shall give the results for the extrapolation to nuclear matter properties with the uncertainties calculated from the full error matrix.

VI. RESULTS

A. Parametrizations currently in use

In this subsection we first want to review the χ^2 properties of the Skyrme forces currently in use. The parameters of the interactions are given in Table II.

As pointed out in Sec. II, a Skyrme force is completely defined only if the several options regarding how to handle necessary corrections are specified. For the many parametrizations currently in use, we have performed calculations with all options discussed above. We calculated with ($LS=1$) and without ($LS=0$) the ls contribution to U_{HF} , Eq. (2.3); with ($EX=1$) and without ($EX=0$) the Coulomb exchange force, Eq. (2.4); with the center-of-mass correction in the effective-mass scheme ($ZP=0$) or as the zero-point energy subtraction ($ZP=1$); and with ($SO=1$) and without ($SO=0$) the ls contribution to the form factor. In Table III we show for each interaction the resulting χ^2 using that LS/EX combination which gives minimum χ^2 . Shortcomings and advantages of the different interactions can be recognized from the χ^2 of the single data sets. In all cases we find better results if we include the ls contribution to the form factor ($SO=1$). Concerning the other three options, we found minimal χ^2 for those options which had been used in the original papers, except for the Skyrme 1 force. There we also show the calculation with $ZP=1$ since this option yields better energies than the conventional one. For the case of the widely used Skyrme 3 force we also show a number of dif-

ferent options in order to demonstrate their influence. With the options investigated here we possibly have not enumerated all variants presently in use. In particular, different handlings of the pairing force are in use, whereas we use the constant-gap approach $\Delta = 11.2/A^{1/2} \text{ MeV}$ throughout this investigation.

In future refinements of the present investigation we will also aim at describing giant resonance properties and the finer details of the charge distribution. Therefore, in Table III we also show for the different interactions the predicted values for several further characteristic properties of ^{208}Pb . We show the energies E_{00} of the isoscalar breathing mode and E_{11} of the isovector giant dipole resonance and also the amplitude $\Delta\rho$ of the fluctuations of the charge distribution, $\Delta\rho = \rho(r=1.8 \text{ fm}) - \rho(r=0 \text{ fm})$. Without going into details we only note the following observations which express partially well-known facts:

- (i) The breathing mode energy increases with increasing α , being too high in particular for the Skyrme interactions 1–6.
- (ii) Even the energy ordering between E_{00} and E_{11} differs for the different parametrizations.
- (iii) Apart from the Tondeur interactions T and $T3$ (cf. Table II), which have been fitted in particular to measured charge densities, all interactions yield amplitudes $\Delta\rho$ which are too large.

B. Fit using Hartree-Fock ground states

It is our aim to determine the free parameters of the effective interaction in a Hartree-Fock calculation by a direct and exhausting fit to measured ground-state properties. Since these calculations are very time consuming we can perform the analysis only for a few of the options mentioned above. Since the ls contribution to U_{HF} directly follows from the force ansatz (2.1), we retain this term throughout this investigation ($LS=1$). We also include

TABLE III. The ability of the different Skyrme interactions to describe the data (force T from Ref. 8). The numbers EX , LS , ZP , and SO indicate calculation with (1) or without (0) the corresponding term in the calculation (see the text). The columns labeled χ_i^2 indicate the contribution to χ^2 from the data set i . The last three columns show, for the case of ^{208}Pb , the calculated giant resonance energies for the (0,0) and (1,1) mode and the amplitude of the oscillation on the charge distribution; the corresponding experimental numbers are shown in the last line [we have determined the value for $\Delta\rho$ from a model-independent analysis of all available elastic electron scattering cross sections (Ref. 26)].

Force	EX	LS	ZP	SO	χ_E^2	χ_R^2	χ_σ^2	χ_b^2	^{208}Pb		
									E_{00} (MeV)	E_{11} (MeV)	$\Delta\rho^*100$ ($e\text{ fm}^{-3}$)
Skyrme 1	0	1	0	1	562	18	466	109	18.8	16.7	-0.51
	0	1	1	1	171	31	415	41	18.7	16.7	-0.50
Skyrme 2	1	0	0	1	760	113	47	134	17.7	18.7	-0.72
Skyrme 3	1	0	0	1	29	246	140	12	18.3	16.8	-0.60
	1	0	1	1	967	283	121	50	18.2	16.8	-0.60
	1	0	1	0	967	281	163	50	18.2	16.8	-0.63
	1	1	0	1	84	255	128	15	18.2	16.8	-0.60
	0	0	0	0	912	263	131	15	18.2	16.8	-0.60
	0	1	0	0	1227	272	120	19	18.1	16.8	-0.60
Skyrme 4	1	0	0	1	129	39	114	582	17.6	18.9	-0.96
Skyrme 5	1	0	0	1	353	42	126	738	17.0	19.5	-1.16
Skyrme 6	1	0	0	1	21	359	267	59	18.5	15.8	-0.49
Skyrme A	1	0	0	1	71	35	63	5	15.7	16.7	-0.71
Skyrme B	1	1	0	1	376	53	98	7	15.8	15.1	-0.86
T	1	0	0	1	176	16	21	14	15.1	14.4	-0.22
$T3$	1	1	0	1	21	17	17	8	14.9	13.4	-0.65
Skyrme M	0	0	0	1	150	16	34	21	14.3	15.3	-0.56
Skyrme M^*	1	0	0	1	45	25	61	7	14.4	15.2	-0.56
Experiment									13.4 ^a	13.5 ^b	-0.20

^aReference 34.

^bReference 28.

the Coulomb-exchange term (2.4) in all cases ($EX=1$) and we always take into account the ls -current contribution to the form factor ($SO=1$). The center-of-mass correction, however, will be used with each of the two choices, i.e., with a correction via the effective mass from Eq. (2.5a) ($ZP=0$) and with the correction by subtracting ZPE according to Eq. (2.5b) ($ZP=1$). In addition to preselecting these options, we kept the exchange parameters fixed in the mass term at $x_1=0$ and $x_2=0$. In order to learn about the importance of the different nuclear properties for the fit, we perform the analysis with different data sets. We first fit the parameters to binding energy E_b , diffraction radius R_d , and spin-orbit splitting $\delta\epsilon_{n,p}(^{16}\text{O})$, and then, in addition to these data also to the surface width σ . Thus, we consider the four cases fit E , fit E_σ , fit Z , and fit Z_σ ; here, E and Z stand for correcting with the effective mass (E) or with the ZPE subtraction (Z), and the index σ indicates inclusion of σ in the fit.

It is our intention not just to produce another set of Skyrme parameters but, instead, to give some insight into the behavior of the fit, its trends and limitations. To this end it would be interesting to see the full dependence of χ^2 on the parameters. However, we cannot draw an eight-dimensional function; we are limited to cuts through the parameter space. A particularly critical and interesting parameter is α , the power in the density-dependent term. We find that this parameter cannot be determined directly

in our fitting routine; we therefore vary it by hand, i.e., for given α we fit the remaining parameters $t_0, t_1, t_2, t_3, t_4, x_0$, and x_3 by minimizing χ^2 . Thus having the cut along the α axis anyway, we present in the following a number of details of the analysis, as a function of α :

(i) the dependence of χ^2 on α and the contribution of the different observables to χ^2 (Fig. 1);

(ii) the deviation between theory and experiment for the different observables and for each fit nucleus separately, dependent on α (Fig. 2);

(iii) the particular relationship between σ and α (Fig. 3);

(iv) the dependence of the Skyrme force parameters on α (Fig. 4);

(v) the extrapolation to nuclear matter properties (Figs. 8 and 9);

(vi) an extensive comparison of measured values with calculated ones for one best-fit parameter set and for many chains of isotopes (Fig. 10).

In Fig. 1 we plot the total χ^2 as a function of α , and also the contributions to χ^2 from the different observables (apart from χ_b^2 , which is practically independent of α and the same for all fits). Each point corresponds to an actual fit with the corresponding α kept fixed; the density of points in α had to be chosen so high in order not to lose track of the minimum χ^2 . From fit E we learn that the reproduction of the energies is independent of α , whereas χ_R^2 , representing the information about the nuclear extension, produces a flat minimum determining α as

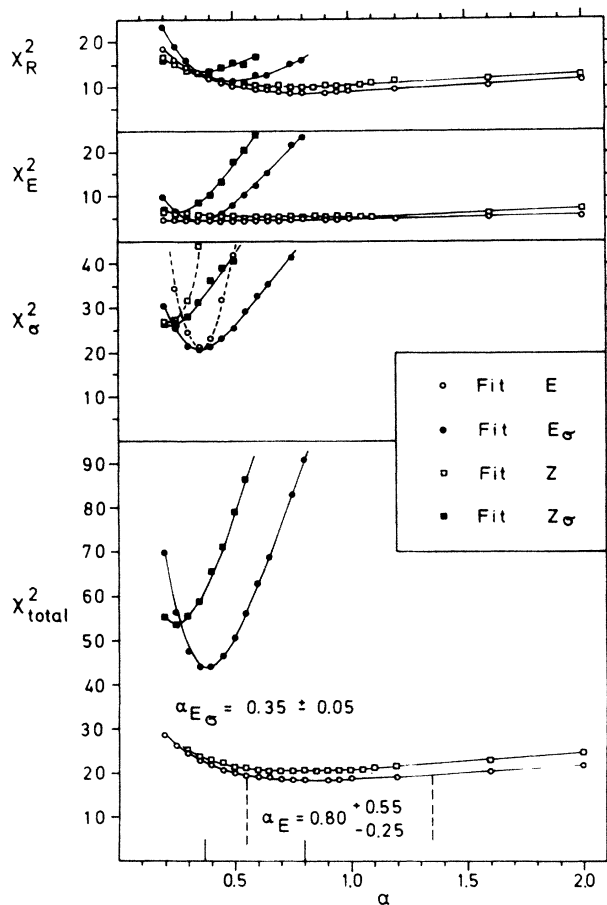


FIG. 1. The total χ^2 as a function of the density parameter α and the contribution of the different observables to χ^2 . Fits E are performed with zero point correction via the effective mass, fits Z with a subtraction according to Eq. (2.5b); the index σ refers to the inclusion of the surface width in the fit. Dashed curve in χ^2_σ : calculated with the best-fit parameters from the fit without σ . For fits E and E_σ there is indicated α_0 (where χ^2_{tot} has a minimum) together with its uncertainty corresponding to an increase in χ^2_{tot} by unity.

$\alpha_E = 0.80^{+0.55}_{-0.25}$. Calculating the surface width σ and the corresponding χ^2_σ with the best-fit parameters from fit E for each α shows that the calculated widths compare best with the measured values for $\alpha = 0.35$. This remains true when σ is also included in the fit (fit E_σ). Thus the full χ^2 for fit E_σ finds its minimum at $\alpha_{E_\sigma} = 0.35 \pm 0.05$. It is interesting to note that there is only a minimal change in the best-fit parameter values for $\alpha \approx 0.35$, where the surface widths were already described best by the fit E (cf. Figs. 1 and 4). This result is the signature of a close relationship between σ and α which we demonstrate in detail in Figs. 2 and 3, and which we will discuss also in Sec. VI E.

The results are very similar for fits Z and Z_σ , where we use the ZPE correction (2.5b) instead of the effective mass (2.5a). In this case χ^2 is a little larger, particularly when σ is included, and here the minimum is shifted to even smaller values of α (for numbers cf. Table VI).

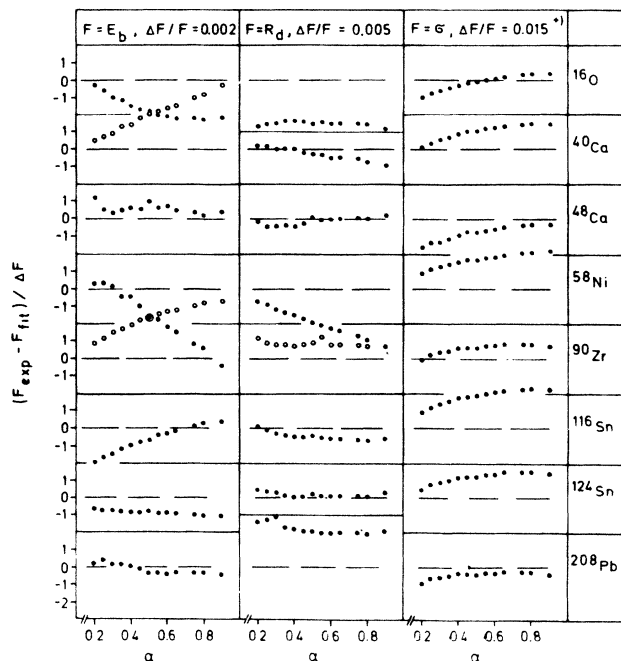


FIG. 2. Difference between measured and calculated observables F (R_d , E_b , and σ) normalized to the adopted uncertainty in F . (Where the curves for two adjacent nuclei intersect the values for the lower nucleus are plotted as open circles.) The plus sign indicates that the scale for $F = \sigma$ is to be multiplied by 2.

Overall, the fits E fit the data a bit better than the fits Z . However, it depends on the application in view of what option one finally prefers. For instance, in a calculation of potential energy surfaces for fusion/fission or for low-energy anharmonic vibrations, we would take fit Z_σ since, first, a proper description of the surface is important to obtain good fission barriers, and, second, the ZPE correction is more natural in that case than the application of an effective mass.

In Fig. 2 we plot, for each of the single observables F taken into account in the fit, the difference between the theoretical and experimental value, normalized to the un-

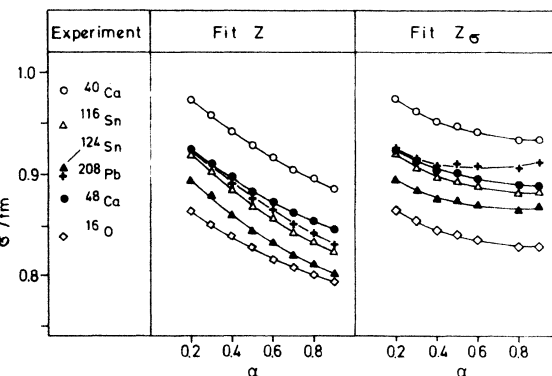


FIG. 3. Surface width σ as a function of α calculated for the fits Z (center) and Z_σ (right) for the nuclei indicated. The measured values are shown on the left side.

certainty of the data, i.e., $\chi = (F_{\text{exp}} - F_{\text{fit}}) / \Delta F$. While the energies and radii show, for each nucleus, an individual behavior as a function of α , the surface widths of all nuclei decrease systematically with increasing α . This is shown again in Fig. 3. Note that the dependence of σ on α is quantitatively different for the fits with and without σ , respectively (fit Z vs fit Z_σ): when σ is included in the fit it depends less on α . This is achieved at the cost of other observables. In Sec. VIE we discuss the α dependence of σ within the model of semi-infinite nuclear matter.

In Fig. 4 we show the resulting best fit parameters, again as a function of α and for the different fits. One clearly recognizes correlations between the parameters and the value of α . Plotting is not precise enough to communicate the force parameters since the uncorrelated errors for each of them are very small. Therefore, in Table IV we give the best-fit parameter sets for the four fits together with the correlated and uncorrelated errors. The full error information would be contained in the full error matrix, but it is impossible to present all these 8×8 matrices here. Concerning the uncertainties in the parameters, we add only two remarks:

(i) The correlated errors are often larger by two orders of magnitude than the uncorrelated ones; this indicates that the parameters are strongly correlated, and this correlation makes the fits numerically difficult and finally the whole investigation extremely time consuming.

(ii) One can try to construct less correlated parameter sets by building proper combinations of the Skyrme parameters. Indeed, in any particular fit one can project out the well- and the poorly-determined parameter combinations, but we did not find general rules which allowed us to reduce the number of free parameters in the fit by fixing beforehand the poorly-determined combinations at some approximate value. We present one particular example in Sec. VID.

We have not shown χ^2_{ls} in any of the graphs since it depends only very weakly on α . However, one peculiar observation concerning the l_s splitting in ^{16}O is worth mentioning: We observe throughout all fits (actually, we have performed many more than the ones presented here) without any exception that the calculated l_s splitting for protons is smaller than that for the neutrons, whereas the measured input data are just the other way round—the present form of the interaction is not able to reproduce this input data. The contribution from the Coulomb interaction can account only for roughly 20 keV, which is too small to invert the result. Therefore we must take the result $\delta\epsilon_p < \delta\epsilon_n$ in ^{16}O as a typical feature of this kind of calculation. This sheds some doubt on whether it is appropriate to identify the calculated l_s splitting in the inert ^{16}O nucleus with the experimental input data given in Table I [it may be that one should identify the calculated $\delta\epsilon_{p,n}$ with the centroid energy of all levels with the appropriate quantum numbers, which, for example, shifts

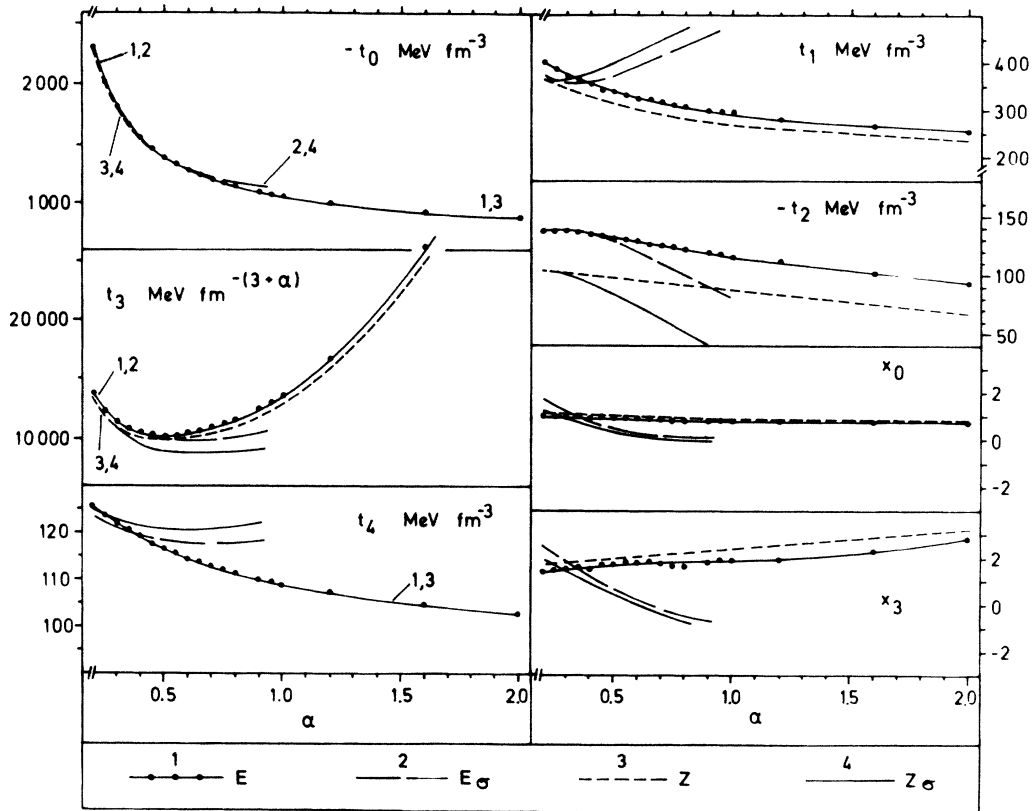


FIG. 4. Best-fit parameters as a function of α for the fits E , E_σ , Z , and Z_σ . For errors on the parameters see Table IV.

TABLE IV. Best-fit parameters for fits E , E_σ , Z , Z_σ , R_σ , and G_σ (for the meaning of the different fits see the text). The numbers in parentheses are the correlated (upper line) and uncorrelated (lower line) statistical errors. The fit Z_σ^* is performed under identical conditions as Z_σ but for the extended set of nuclei. For further details see Sec. V F.

Fit	α	t_0	t_1	t_2	t_3	t_4	x_0	x_3
E	0.80	-1140.25 (8.8) (0.14)	309.61 (30) (0.2)	-122.22 (7) (0.2)	11608.1 (410) (4)	111.45 (2.2) (0.9)	0.7979 (0.26) (0.008)	1.632 (0.72) (0.02)
E_σ	0.35	-1664.05 (10) (0.14)	358.83 (15) (0.3)	-137.22 (5) (0.2)	10931.5 (240) (2)	120.14 (1.8) (0.9)	1.0770 (0.25) (0.005)	1.6918 (0.46) (0.009)
Z	0.80	-1137.57 (7.2) (0.13)	284.67 (23) (0.2)	-92.73 (6) (0.2)	11269.5 (344) (4)	111.95 (1.9) (0.9)	0.9260 (0.20) (0.007)	2.1561 (0.56) (0.02)
Z_σ	0.25	-1983.76 (16) (0.14)	362.25 (15) (0.3)	-104.27 (5) (0.2)	11861.4 (253) (1)	123.69 (1.9) (0.9)	1.1717 (0.32) (0.004)	1.7620 (0.54) (0.007)
Z_σ^*	0.25	-1987.64 (5) (0.09)	380.92 (7) (0.2)	-109.88 (2) (0.1)	11837.7 (76) (1)	126.13 (1.5) (0.6)	0.8897 (0.16) (0.003)	1.2780 (0.26) (0.006)
R_σ	0.30	-1798.00 (7.5) (0.14)	335.97 (21) (0.3)	-84.81 (4) (0.2)	11083.9 (221) (2)	121.59 (2.4) (0.9)	-0.4036 (0.11) (0.004)	-0.8705 (0.22) (0.007)
G_σ	0.30	-1800.16 (8.8) (0.14)	336.23 (15) (0.3)	-85.74 (3) (0.2)	11113.5 (160) (2)	121.86 (2.2) (0.9)	-0.4862 (0.11) (0.003)	-1.0295 (0.20) (0.006)

$\delta\epsilon_p$ (experiment) to 6.8 MeV (Ref. 37)].

In Table V we compile the χ^2 values for the different fits and for the best-fit α in each case. In general, the χ^2 for the data not included in the fit is considerably larger than in the case where these data are also taken into account. Also shown in Table V are predictions for several characteristic quantities in ^{208}Pb . It is surprising to see that the calculated amplitude of the oscillation on $\rho(r)$ is independent of the details of the fit and, in any case, is too large by roughly a factor of 3. The fits of this subsection without the GSC yield giant dipole resonance energies which are too high. The breathing mode energy is too high in all fits; note that this also holds in the case of fit Z_σ in spite of the small compressibility in this fit.

C. A fit to correlated ground states

If one wants to use the Skyrme force in an RPA calculation one has to also take into account the RPA ground state correlations. For such an application, however, we have to abandon the above parameter sets. Instead one must perform a new fit where the contributions from the RPA correlation to E_b , R_d , and σ are also taken into account. Moreover, it is also desirable to include one or the other giant resonance in the fit. Here, we will only briefly present first results of such a fit in order to demonstrate the importance of these effects.

The ground-state correlations are evaluated in a sum-rule approximation (which is a very fast procedure) such

TABLE V. The ability of the different fits to describe the data expressed in terms of χ_i^2 and the predictive power for several quantities in ^{208}Pb . Numbers in parentheses indicate χ^2 for quantities not included in the fit.

Fit	χ_E^2	χ_R^2	χ_σ^2	χ_k^2	χ_{11}^2	^{208}Pb		
						E_{00} (MeV)	E_{11} (MeV)	$\Delta\rho$ ($e\text{ fm}^{-3}$)
E	5.0	8.7	(156)	4.9	(740)	18.2	17.7	-0.56
E_σ	4.4	13.7	20.7	5.1	(790)	16.0	17.9	-0.60
Z	5.7	9.9	(264)	4.9	(1070)	18.4	18.4	-0.60
Z_σ	6.2	16.0	26.2	5.2	(955)	15.3	18.2	-0.62
R_σ	24.1	7.8	26.1	5.4	(4.6)	15.1	14.0	-0.62
G_σ	24.8	8.4	25.4	5.4	2.2	15.1	13.8	-0.62

that it can be implemented in the fit.¹⁶ A fit to ground state properties only is performed with the option of fit Z_σ , i.e., $LS=1$, $EX=1$, $SO=1$, and $ZP=1$; we call it fit R_σ . In a further fit we also include the dipole giant resonance energies (evaluated in the sum-rule approximation) for ^{90}Zr , $^{116,124}\text{Sn}$, and ^{208}Pb ; this is fit G_σ .

In Fig. 5 we show χ^2 , again as a function of α . With respect to the fit Z_σ performed without accounting for GSC, the minimum is shifted to larger α . The reason for this is that the correlations enlarge the surface width σ , and thus lower Hartree-Fock values are needed, which occur at larger α . In the fits with GSC the radii are better reproduced, but the energies now are much worse, leading to an increase in χ^2_{tot} by 10. On the other hand, these fits yield excellent giant dipole resonance energies, independent of whether or not these are included in the fit (R_σ vs G_σ). This gives us confidence that we are on the right

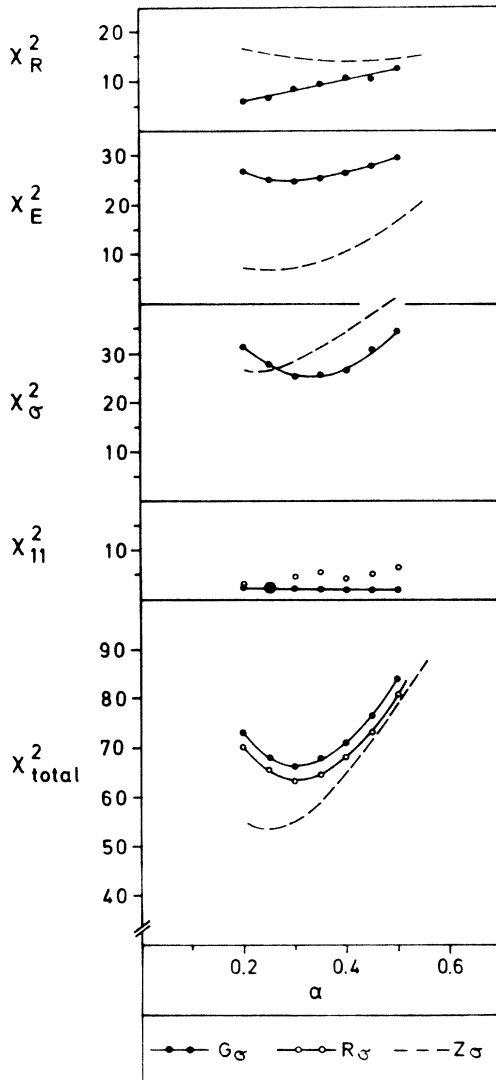


FIG. 5. The total χ^2 as a function of the density parameter α and the contribution from the different observables to χ^2 for fits including ground-state correlations. The contribution χ^2_{11} for Z_σ is about 1000 (cf. Table V) and thus far out of the scale of this graph.

track, and one must now look for other improvements which also allow us to readjust the binding energies. The parameters of these fits are also compiled in Table III. In Fig. 6 we compare them to the fit Z_σ : Including the GSC has an important impact, in particular on x_0 and x_3 which now become negative. A calculation of the GSC with the pure Hartree-Fock fit Z_σ gives much larger correlations than with fits R_σ and G_σ . Thus, the inclusion of ground state correlations in the fit reduces their influence. This demonstrates that one should not calculate correlations with an interaction which is fitted without accounting for correlations. The other way, just omitting the GSC and using fit R_σ or G_σ in a pure Hartree-Fock calculation, is less critical; but in any case, the GSC have effects on the observables which are large with respect to the achieved quality of the fits.

D. Parameter correlations

As mentioned before, it is impossible to document the involved error correlations between the parameters. Therefore, in Fig. 7 we only show as an example the correlation between the exchange parameters x_0 and x_3 in the fits Z and G_σ . The eigenvectors of the error matrix constitute orthogonal and error-uncorrelated parameter combinations. In Fig. 7 we show the well-determined combination $X=ax_0-bx_3$ and the orthogonal, poorly determined $Y=bx_0+ax_3$. We also show the coefficients a and b which depend on α .

The findings in the case of fit Z can be understood essentially by nuclear matter considerations. The exchange parameters x_0 and x_3 have no influence on symmetric nuclear matter, but they enter into the expression of the volume asymmetry coefficient J (Ref. 30) in the combination

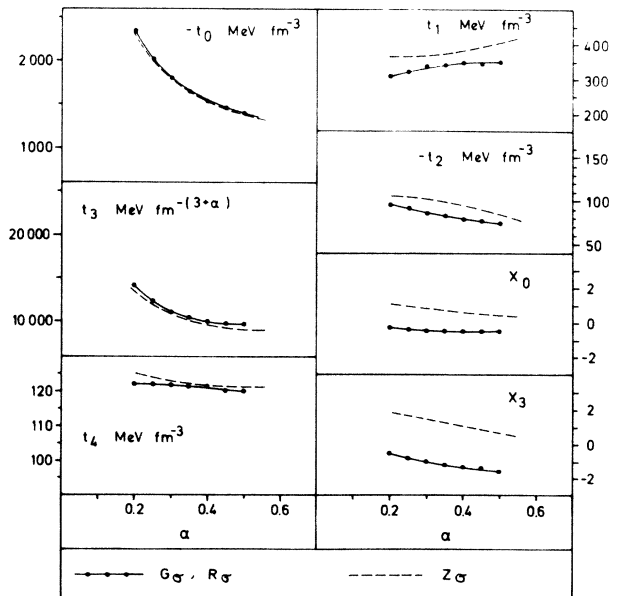


FIG. 6. Best-fit parameters as a function of α for fits Z_σ and G_σ . Parameters for R_σ are roughly identical with those of G_σ .

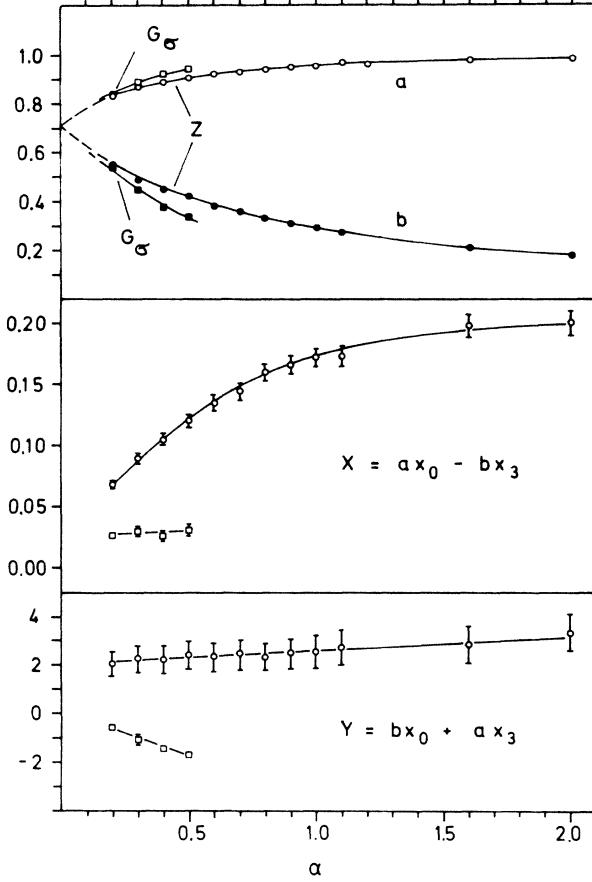


FIG. 7. Correlation between the exchange parameters x_0 and x_3 as a function of α for the fits Z and G_σ . In both cases, the combination $X = ax_0 - bx_3$ is the combination with the smaller error; the orthogonal combination $Y = bx_0 + ax_3$ has the larger error. The coefficients a and b vary with α as shown at the top. The error bars are the statistical errors on the combinations X and Y .

$$X_{nm} = a_{nm}x_0 - b_{nm}x_3, \quad (6.1)$$

with $a_{nm} = -t_0/N$ and $b_{nm} = \frac{1}{6}t_3\rho_{nm}^\alpha/N$, where N guarantees the normalization $a^2 + b^2 = 1$. We expect this combination to be the well-determined one, and in fact this value of a_{nm} agrees within a few percent with the values found for a in the fits and shown in Fig. 7, thus suggesting that x_0 and x_3 enter into the fit dominantly via the asymmetry energy.

When the E_{11} resonance energy (and correlations) are also included in the fit, the resulting values for t_0 , t_3 , and ρ_{nm} yield practically the same values for a_{nm} and b_{nm} as in fit Z . However, the a and b determined from the error matrix are different from those in fit Z , and both combinations, X as well as Y , are equally well determined in fit G_σ . Furthermore, we note that the volume asymmetry coefficient is different in the two fits. From this we learn that, in a fit, a restricted set of data may leave certain parameter combinations undetermined and that nuclear matter parameters may serve as guidance to find those which are well determined; including the appropriate ad-

ditional data removes such uncertainties. The situation is less transparent when more parameters are involved. We did not find a generally applicable recipe to reduce the numbers of parameters in the fits. Nevertheless, we believe that the correlations contain important physical information; therefore they need further study.

E. Nuclear matter properties

We have exploited the information available from actual measurements on nuclei in an exhaustive manner within the framework of the Skyrme-force ansatz and, as a result, obtained a set of parameters with an estimate of their uncertainties. In addition, we have obtained the full error matrix which now allows extrapolation from the available information to unknown quantities with an estimate of their uncertainty. In this subsection we present the result of the extrapolation to properties of symmetric nuclear matter: the density ρ_{nm} , the binding energy per particle E/A , the compressibility K_{nm} , the effective mass m^*/m , and also the Landau parameters f_0, f'_0, g_0 , and g'_0 . The expression for the Landau parameters in terms of the Skyrme force parameters are taken from Refs. 12 and 31. The expressions for the nuclear matter properties are standard (see, e.g., Ref. 30); they establish a relation between the four properties $E/A, \rho_{nm}, K_{nm}$, and m^*/m and the parameters $t_0, 3t_1 + 5t_2, t_3$, and α . For fixed α only three of the nuclear matter properties can be independent; for instance, the compressibility can be written in terms of the others as

$$K_{nm} = -9(1 + \alpha)(E/A)$$

$$+ 10.127 \frac{\hbar^2}{2m} \rho_{nm}^{2/3} [1 + 3\alpha + (m/m^* - 1)(4 - 6\alpha)]. \quad (6.2)$$

This should be kept in mind when looking at Fig. 8, where we show the nuclear matter properties for the fits E, E_σ, Z, Z_σ , and G_σ , again as a function of α . The corresponding numbers are given in Table VI. The clearest result emerges for the nuclear compressibility, which is found to be independent of the peculiarities of the fit and to increase linearly with α . This behavior is evident from Eq. (6.2) if the other nuclear matter properties do not depend on α . However, the other properties do vary with α (cf. Fig. 8), therefore it is finally a surprising result to find that the influence of these variations on K_{nm} cancel, leaving us with a linear dependence on α . Quantitatively, the nuclear matter compressibility is found as $K_{nm} = 182(1 + 1.04\alpha)$ MeV. Therefore, K_{nm} can be deduced once the correct density dependence α is known. Fits without the surface width have $\alpha \approx 0.8$ and they predict values of $K_{nm} \approx 330$ MeV with a large uncertainty. We mention in passing that this result compares surprisingly well with that determined from the same kind of data within the framework of the droplet model.²⁶ Generally accepted are values around 240 MeV; that is just what we deduce from the fits including σ (cf. Table VI). There, the uncertainty in α is reduced considerably. Averaging the different fits we get $K_m = 235 \pm 12$ MeV. Here it will be interesting to also include breathing mode energies as

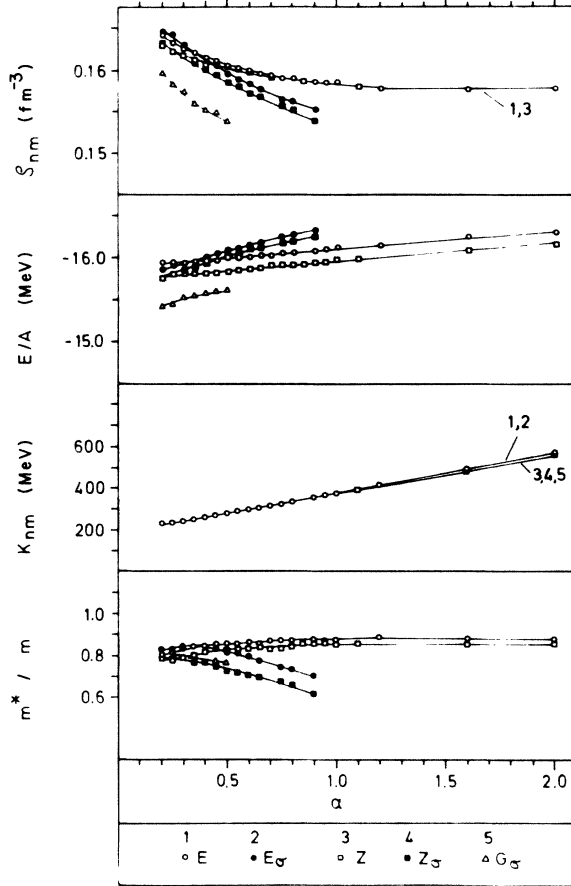


FIG. 8. Nuclear matter parameters calculated with the best-fit parameters of the different fits.

input data, which constitute a good check for the consistency and thus the reliability of the present ansatz.

The extrapolation to the binding energy per particle E/A depends slightly on the inclusion of σ in the fit (0.1 MeV) and on the zero-point-energy correction (0.15 MeV), and to a larger extent on the ground state correlations (0.3 MeV). These numbers give us a feeling for the uncertainty which one encounters when talking about the binding energy in nuclear matter (the uncertainty from error propagation is small compared to these systematics). Fit G_σ tries to account for the largest set of data, but it is just in this fit that the binding energies are not well reproduced. One cannot foresee at this point how the necessary modifications will influence the extrapolation. However, we feel that a quite safe prediction is a value of $E/A = -15.8$ MeV with an uncertainty of 0.4 MeV. Similar remarks hold for the nuclear matter density. So, briefly, we estimate it to be $\rho_{nm} = 0.160 \pm 0.004$ particles per fm^3 . Averaging over the numbers for the effective mass yields $m^*/m = 0.82 \pm 0.07$.

With these findings in mind we look back at the dependence of the nuclear surface width on α . In a model of semi-infinite nuclear matter one can establish a relation between the surface thickness and the nuclear matter properties K_{nm} and m/m^* (Ref. 30)

$$\sigma \propto \left\{ \frac{\hbar^2}{2m} \left[\frac{1}{36} + (m/m^* - 1)/K_{nm} \right] \right\}^{1/2}. \quad (6.3)$$

This equation allows one to relate the α dependence of σ as given in Fig. 3 to the trends of m/m^* and K_{nm} shown in Fig. 8. For all fits K_{nm} increases linearly with α . The m^*/m is rather constant for the fits without σ (E and Z), for which then the observed decrease of σ with increasing α is just due to K_{nm} . In the fits E_σ and Z_σ the m^*/m decreases with α such that $(m/m^* - 1)$ counterweights the variation in K_{nm} ; as a result we are left with a more constant σ . The data predominantly fix the quantity K_{nm} at the linear dependence on α , and only the less determined quantity m/m^* is left to adjust the surface width σ .

Other valuable information is expressed in terms of the Landau parameters. To understand their importance we need only to recall the long standing quarrel about the possible existence of pion condensates, now reduced to the possible existence of precursor effects. Although the Landau parametrization is an effective force for nuclear excitation properties and the Skyrme forces are determined mainly by ground state data, it is interesting to look at the Landau parameters as they can be calculated from the effective-force parameters of the present fits. They are shown in Fig. 9, again as a function of α . Numbers are also given in Table VI. As usual, we present the normal-

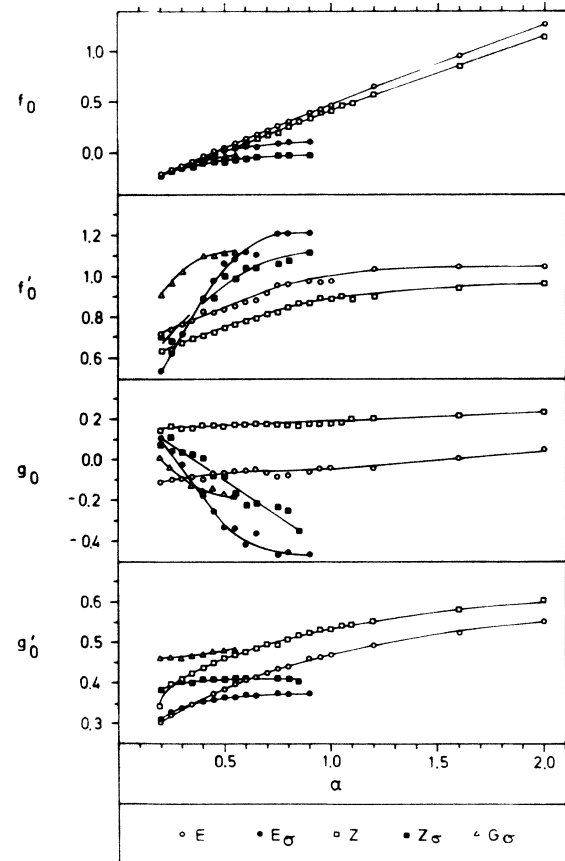


FIG. 9. Landau parameters calculated with the best-fit parameters of the different fits.

TABLE VI. Nuclear matter quantities determined from the different fits. Numbers in parentheses are the uncertainties (upper line, from the error propagation of the seven fitted parameters; lower line, from the uncertainty in α as given in the second column). In the last line we show a set of Landau parameters which is determined from different experimental data (Ref. 38).

Fit	α	E/A	K_{nm}	ρ_{nm}	m^*/m	f_0	f'_0	g_0	g'_0
E	0.80	-16.06 (0.06)	332.6 (1.3)	0.1590 (0.001)	0.868 (0.04)	0.308 (0.05)	0.96 (0.12)	-0.08 (0.13)	0.442 (0.009)
	(+ 0.55) (-0.25)	(+ 0.12) (-0.06)	(+ 100) (-40)	(+ 0.001) (-0.001)	(+ 0.01) (-0.01)	(+ 0.47) (-0.21)	(+ 0.08) (-0.10)	(+ 0.04) (-0.04)	(+ 0.07) (-0.04)
E_σ	0.35	-15.95 (0.05)	247.9 (1.6)	0.1625 (0.001)	0.840 (0.02)	-0.07 (0.02)	0.79 (0.09)	-0.09 (0.08)	0.348 (0.008)
	(0.05)	(0.05)	(10)	(0.001)	(0.00)	(0.05)	(0.09)	(0.08)	(0.007)
Z	0.80	-15.91 (0.05)	329.4 (0.9)	0.1588 (0.001)	0.843 (0.03)	0.259 (0.04)	0.85 (0.08)	0.17 (0.08)	0.509 (0.008)
	(+ 0.55) (-0.25)	(+ 0.12) (-0.06)	(+ 110) (-40)	(+ 0.001) (-0.001)	(+ 0.01) (-0.01)	(+ 0.43) (-0.20)	(+ 0.08) (-0.10)	(+ 0.02) (-0.02)	(+ 0.06) (-0.04)
Z_σ	0.25	-15.81 (0.04)	232.6 (1.9)	0.1627 (0.001)	0.783 (0.02)	-0.187 (0.02)	0.68 (0.09)	0.11 (0.09)	0.395 (0.009)
	(0.05)	(0.05)	(10)	(0.001)	(0.003)	(0.04)	(0.06)	(0.04)	(0.008)
R_σ	0.30	-15.53 (0.04)	236.7 (1.7)	0.1575 (0.001)	0.783 (0.02)	-0.155 (0.02)	0.97 (0.08)	-0.04 (0.08)	0.465 (0.007)
	(0.05)	(0.04)	(10)	(0.001)	(0.01)	(0.04)	(0.05)	(0.04)	(0.003)
G_s	0.30	-15.53 (0.04)	236.6 (1.8)	0.1573 (0.001)	0.785 (0.02)	-0.153 (0.01)	1.02 (0.11)	-0.09 (0.24)	0.464 (0.006)
	(0.05)	(0.04)	(10)	(0.001)	(0.01)	(0.04)	(0.05)	(0.04)	(0.003)
Ref. 38						0.20	1.50	0.55	0.70

ized values, i.e., the values calculated with the formulae in Refs. 12 and 31 multiplied by $2k_F m^*/(\pi\hbar)^2$.

Without inclusion of σ in the fits, the parameter f_0 has a very large uncertainty due to the uncertainty in α . Including σ shifts this parameter to negative values, going further down when the effective-mass scheme is replaced by the zero-point-energy subtraction ($E_\sigma \rightarrow Z_\sigma$). Trusting in the fits with σ and with the ZPE correction leads to $f_0 = -0.17 \pm 0.07$. The situation for g_0 is very unclear; its value seems to be compatible with 0. Averaging over the numbers from all fits we get $f'_0 = 0.85 \pm 0.35$. In each fit g'_0 is quite well behaved; however, the values differ substantially from fit to fit. Including σ reduces the value by 0.1; replacing the effective-mass scheme by the ZPE subtraction increases it by 0.05, and including GSC increases it further by 0.07. On the average we are left with the quite small value $g'_0 = 0.45 \pm 0.06$. We remark without comment that these values do not compare well with the set³⁸ given in the last line of Table VI.

All these extrapolations must be taken with great care. They are performed within a model which does not reproduce the known data for nuclei correctly; in particular the fits E through Z_σ give giant dipole resonance energies which are too high, whereas the fits R_σ and G_σ give not so good binding energies. It is impossible to say by now to which extent the necessary improvements in the model will influence the extrapolation.

F. Fit to an extended set of nuclei

We have repeated fit Z_σ , at $\alpha = 0.25$, with the extended set of data given in Sec. IV; we will call this fit Z_σ^* . The new best-fit parameters differ by less than twice the correlated error from fit Z_σ .

In the additional nuclei, which are less magic than the standard set, the surface width is larger on the average. In view of this the fit is surprisingly stable with respect to an enlargement of the data set. The resulting values for the nuclear matter parameters are also in excellent agreement with the values given in Sec. VI E: $E/A = -15.90 \pm 0.03$ MeV, $K_{nm} = 234.2 \pm 0.9$ MeV, $\rho_{nm} = 0.162 \pm 0.001$ particles per fm^3 , and $m^*/m = 0.776 \pm 0.007$. The Landau parameters essentially remain in the ranges given above.

Enlarging the set of data in the fit reduces the statistical uncertainty of the extracted parameters and deduced quantities. The systematic problems, however, increase. In particular, the treatment of pairing and of correlations has to be improved before far-reaching conclusions can be drawn.

G. Shortcomings

In Fig. 10 we plot the χ for the various observables and for a wide variety of nuclei for fit Z_σ , at $\alpha = 0.25$. This demonstrates that also in such a fit where χ^2 looks quite

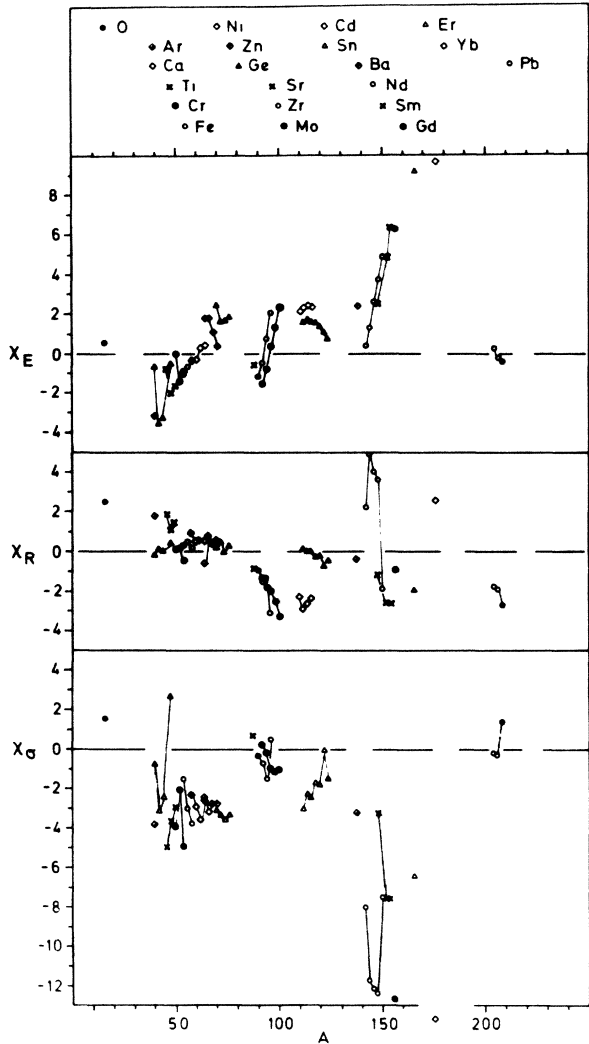


FIG. 10. Trends in the deviation of the calculation from measured values. Top: binding energies; center: radii; bottom: surface widths for nuclei throughout the periodic table, in particular for chains of isotopes. The calculation is performed with the parameters from fit Z_σ , $\alpha=0.25$. Nuclei included in the fit are indicated by full symbols.

reasonable, systematic trends remain in the deviation between calculation and measured values. For the binding energies we see isotopic effects; for the radii an additional overall trend with A . This also holds more or less for the surface width where one certainly must account most carefully for correlations, nuclear deformation being one of them. Systematic trends in χ (rather than stochastic behavior) show that something is still missing in the theory. Further improvements might be expected from a refined treatment of pairing.^{35,36} In addition, the problem with the oscillations on $\rho(r)$ seems to demand inclusion of the exchange parameters x_1 and x_2 . At least up to now, that has been the only way to reduce their amplitude.^{8,32}

The present systematic study has revealed a number of shortcomings and there is no room left to get rid of them by readjustments of the parameter values of the standard

parametrization—by the method used here we have exhausted this possibility. However, there are still several possible refinements within the framework of the present ansatz such that we cannot yet state whether or not we have reached the limits of the effective force ansatz of the Skyrme type as such. The model needs to be refined, presumably by exploiting more of the flexibility in the force ansatz.

VII. CONCLUSIONS

We have investigated the properties of the Skyrme force by applying the method of least squares for fitting the free parameters of the force to measured nuclear data, mainly for the ground state, but in one case also for the excitation energy of the giant dipole resonance. An interpretation of the Skyrme force as an effective interaction for nuclear Hartree-Fock calculations contains two problems: First, the force should be used only for that restricted range of applications where it has been fitted to; second, in order to be consistent an analogous effective operator should be used for the observables (e.g., the form factor or, equivalently, the density distribution). The second problem is essentially avoided by using only those pieces of the form factor which are insensitive to short range correlations and mesonic effects; this is assumed to be the case for the low-momentum components. With respect to the first problem, we must distinguish between a force which is appropriate for mere Hartree-Fock calculations (including constrained Hartree-Fock calculations for evaluating the collective potential-energy surface of anharmonic low-energy modes), and another force which is appropriate for RPA calculations on top of an RPA-correlated ground state. We have studied both concepts in this paper, with an emphasis on the Hartree-Fock case.

As experimental input for the least-squares fit we have taken into account binding energies, diffraction radii, and, optionally, the surface widths of eight nuclei with at least one magic nucleon number; in addition, we have included the $1s$ splitting of the $1p$ level in ^{16}O . These eight nuclei from ^{16}O to ^{208}Pb span a large A range and they contain two isotopic pairs; thus we assume that they provide a sufficiently complete body of information about nuclear ground states. This assumption is confirmed by a fit with an enlarged set of 22 nuclei which did not yield substantially different results. Thus, the Skyrme force ansatz yields indeed a good “interpolation” of nuclear properties from ^{16}O to ^{208}Pb .

Apart from the precise values for the force parameters, it is also necessary to specify further features of the calculations. We include the Coulomb exchange term, we use the $(t_1 - t_2)$ contribution to the spin-orbit force, and we take into account the $1s$ contribution to the form factor. In particular, we investigate two possibilities for correcting for the spurious center-of-mass energy, once by the effective-mass scheme, second by an explicit subtraction (after variation) of the expectation value of the center-of-mass energy. The latter concept is the physically more reasonable one in view of an application to constrained Hartree-Fock and RPA calculations.

We find that the surface width σ is a particularly important ingredient in the fit. Without σ the power of the

density dependence in the force is only weakly determined, being $\alpha=0.80_{-0.25}^{+0.55}$ for the fit without σ . On the other hand, by including σ , we find smaller and better defined values for α , namely $\alpha=0.35\pm 0.05$ with the effective-mass scheme and 0.25 ± 0.05 with the ZPE correction scheme. Since ground state correlations increase the surface width, in a fit including GSC one needs smaller surface widths from the Hartree-Fock calculation itself; this yields a slightly larger α : $\alpha=0.30\pm 0.05$ (with GSC and ZPE). In any case we feel that the fits including σ are more reliable for an application in fusion/fission calculations because a good description of the nuclear surface is important to obtain realistic barriers.

Alternative fits to RPA-correlated ground states and dipole giant resonance energies give different forces compared to the previous fits. In particular, negative exchange parameters x_0 and x_3 are preferred in this case. Thus we have to face the fact that we will need different Skyrme forces for different applications (expressing a different range of "effectiveness"). We mention in passing that we have also worked out a force which is particularly suited for light nuclei up to ^{40}Ca and which we have used successfully for calculating ^{16}O - ^{16}O fusion.²⁹

Nuclear matter parameters are deduced from the fit. We also obtain an estimate for the uncertainty on these parameters. We, so to say, extrapolate from the measured ground-state properties of well-behaved finite nuclei to infinite systems by means of a Skyrme-Hartree-Fock model. The extrapolation to the binding energy and the density of the infinite system is well defined by the data, independent of the different options (with or without σ). The effective mass, however, is a bit more sensitive to the power α and also to account for different data in the fit. The nuclear compressibility exhibits a very clean linear dependence on α and we find that including the surface width σ in the fit allows us to fix the value of K_{nm} very precisely: Fits without σ yield large α and thus large K_{nm} ($\simeq 300$ MeV), whereas fits including σ give low α and thus low K_{nm} ($\simeq 230$ MeV). The influence of σ on the determination of K_{nm} can be understood within the model of semi-infinite nuclear matter. The extrapolation yields the following values: $K_{nm}=235\pm 12$ MeV, $E/A=-15.8\pm 0.4$ MeV, $\rho_{nm}=0.160\pm 0.004$ particles per fm^3 , and $m^*/m=0.82\pm 0.07$. We have also extracted values for the Landau parameters.

The correct treatment of error propagation in the least-

squares fitting procedure allows us to estimate the uncertainties in the parameters and also correlations among them. We find "hard" parameters which are well determined, and "soft" parameters with larger uncertainties. The latter show that there is already some redundancy in the parametrization (at least as long as we do not include more data in the fit). On the other hand, we find that there are systematic deviations between measured and calculated data, demonstrating that the model is not yet flexible enough: There remain definite isotopic trends in the deviations for E_b and R_d and, in addition, an overall trend in the deviation of R_d with mass number A . Thus, we have both too many and not enough parameters at the same time. That is to say we do not yet have the appropriate parametrization. More theoretical understanding of the Skyrme force would be very useful to reduce first the number of free parameters and then add the appropriate additional ones in order to allow a systematic study also of an extended body of data. Corresponding extensions are straightforward¹² and have already been used for improving on the description of charge distributions.^{8,32} The more complex experimental data are described by the model, the more confidence we have in predictions within the framework of this model. However, it may also be that the ansatz has basic physical shortcomings, that it finally fails to describe consistently the whole body of known properties, e.g., including the fine details of the charge distributions and the electric and magnetic moments, etc. The present work must be extended to include more data and a more flexible, eventually also more fundamental, model. Corresponding work is in progress.

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