

Constraints on Skyrme Force Parameterizations

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Abstract. Since its first use in Hartree-Fock calculations in 1972, the Skyrme Force, which includes around ten free parameters to be fitted to data, has undergone many such fitting procedures to different sets of data. To date there have been more than 200 parameter sets published. Since the Skyrme force can be thought of as an expansion of an in principle exact density functional, the Skyrme force has sufficient degrees of freedom that the different parameter sets can differ from each other quite extensively in how they reproduce the properties of nuclei. We give a selected history of the fitting of Skyrme forces, then explore some recent work on systematically testing each parameterisation against experimentally-derived nuclear matter properties, and discuss the ability of the (few) parameter sets which pass all constraints to reproduce data in finite nuclei.

1 Introduction

In the 1950s Skyrme put forward an effective nuclear interaction that was intended to capture the key features of an in-medium interaction [1]. He argued that a suitable and simple form for the two-body part of the interaction was a contact interaction in space, combined with a function depending on the relative wavenumber, $\mathbf{k} = \frac{1}{2}i(\nabla_1 - \nabla_2)$;

$$t_{12} = \delta(\mathbf{r}_1 - \mathbf{r}_2)t(\mathbf{k}', \mathbf{k}). \quad (1)$$

Here, \mathbf{k}' means the operator \mathbf{k} placed to the left of the delta function. The form for t_{12} is given as

$$\begin{aligned} t(\mathbf{k}', \mathbf{k}) &= t_0(1 + x_0P^\sigma) + \frac{1}{2}t_1(1 + x_1P^\sigma)(\mathbf{k}'^2 + \mathbf{k}^2) \\ &+ t_2(1 + x_2(P^\sigma - \frac{4}{5}))\mathbf{k}' \cdot \mathbf{k} \\ &+ \frac{1}{2}T(\boldsymbol{\sigma}_1 \cdot \mathbf{k}\boldsymbol{\sigma}_2 \cdot \mathbf{k} - \frac{1}{3}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\mathbf{k}^2 + \text{conj.}) \\ &+ \frac{1}{2}U(\boldsymbol{\sigma}_1 \cdot \mathbf{k}'\boldsymbol{\sigma}_2 \cdot \mathbf{k} - \frac{1}{3}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\mathbf{k}' \cdot \mathbf{k} + \text{conj.}) \\ &+ V(i(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{k}' \times \mathbf{k}). \end{aligned} \quad (2)$$

Here, t_0 , t_1 and t_2 are adjustable parameters for the strength of the contact and momentum-dependent terms, respectively, x_0 , x_1 and x_2 are dimensionless parameters controlling the spin-dependence of each term, T and U are strength parameters for a tensor force and V is the spin-orbit strength. This form was posited as a general form up to second order in power of the relative wavenumber.

This two-body interaction is supplemented with a three-body force, intended to simulate all many-body effects, of the form

$$t_{123} = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_3 - \mathbf{r}_1) \quad (3)$$

with a single adjustable strength parameter t_3 .

Furthermore, in his original paper, Skyrme considered higher-order terms. A term which acts in D-waves of the form $t_D [\mathbf{k}^2 \mathbf{k}'^2 - (\mathbf{k} \cdot \mathbf{k}')^2]$, and a four body contact term $t_4 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_3 - \mathbf{r}_1) \delta(\mathbf{r}_4 - \mathbf{r}_1)$, in which t_D and t_4 are adjustable strengths.

This form of the interaction results in 12 adjustable parameters, and we wish to give something of a (brief) historic overview of how these are usually adjusted, why there are around 250 (to date) parameter sets, give an overview of some recent stringent constraints on nuclear matter properties, and then show some new results of the behaviour of these parameter sets in finite nuclei. The remaining sections of this paper present these themes in order.

2 Adjustment of Skyrme Parameters

In the original analysis of Skyrme [1], the Fermi gas Hamiltonian expectation value for spin- and isospin-symmetric nuclear matter was worked out, and used as a constraint based on the results of the semi-empirical mass formula, along with the expected nuclear matter density. Similarly an expression was obtained for the symmetry energy in the semi-empirical mass formula. Surface properties were approximated with a tanh form for the density taken from the Thomas-Fermi approximation, and single particle properties derived from a quadratic potential well, giving expressions for the energies of the topmost nucleons in the well. Assuming oscillator wave functions, a shell-model picture of light nuclei was also used to give a series of relations linking the parameters of the force. In this fitting procedure, it was assumed that $t_D = t_4 = T = U = 0$. The t_D and t_4 terms were analysed separately, with the conclusion that, based on the observables chosen, both t_4 and t_D were essentially undetermined, though the benefits of a finite value for t_D were indicated.

In slightly more than a decade after Skyrme's paper, the first self-consistent Hartree-Fock calculations with Skyrme's interaction were made, by Vautherin and Brink [2]. They took Skyrme's interaction, with $t_D = t_4 = T = U = x_1 = x_2 = 0$ and made a readjustment of the parameters, finding those given by Skyrme unsuitable for heavy nuclei. They began by adjusting t_0 , t_1 , t_2 and t_3 to the binding energy and density of nuclear matter, and the binding energy and

radius of ^{16}O as calculated with oscillator wave functions. The parameter x_0 was adjusted to give the nuclear matter symmetry energy of order 30 MeV, and the spin-orbit strength was adjusted to fit the experimental $1p$ splitting in ^{16}O . Hartree-Fock calculations of ^{16}O and ^{208}Pb were then made and the parameters further adjusted to improve the fits. They then examined the resulting parameters for their ability to reproduce other magic nuclei, and comment that “we have been able to find several sets of parameters giving a good description of closed shell nuclei in Hartree-Fock calculations.”

They presented two parameter sets, dubbed “I” and “II” (now, usually referred to as SI and SII) and demonstrated results for nuclei and observables not included in the fit, including single particle energies in ^{208}Pb , which were markedly different between the two forces.

Though they did not include the tensor terms, with parameters T and U in (2), they commented that it would have an effect on the spin-orbit splittings. They also omitted the contribution from the momentum-dependent terms that appears in the spin-orbit potential (presumably because of the computational complexity - they did calculate the first-order effect in perturbation theory). This has remained a theme of parameter set fits, in which terms that should arise from the Skyrme interaction are omitted in Hartree-Fock calculations, and one needs to know which choice was made when fitting to be consistent.

Stancu, Brink and Flocard examined the tensor terms later in the 1970's, along with the previously-ignored momentum-dependent contribution to the spin-orbit potential [3]. Though they found significant effects on the single-particle levels, the procedure of adding these terms to existing fitted parameter sets and looking at only the single-particle energies of doubly-magic nuclei, did not provide enough improvement in observables to make them a standard part of future Skyrme fits.

Following Vautherin and Brink, Beiner, *et al.* [4] performed an extensive analysis of the fitting procedure, using the reduced parameterization of Vautherin and Brink, and arguing that the tensor terms could be made to cancel the momentum-dependent contribution to the spin-orbit field, and both could be consistently ignored. This left them six parameters to fit (t_0, t_1, t_2, t_3, x_0 and W). They made a series of four fits, to a range of doubly- and singly-magic nuclei with wide range of mass and isospin asymmetry. They did not include nuclear matter properties in the fit. Each has a deliberately rather different value of the t_3 parameter, chosen to study the effect of the three-body force, with the other parameters fitted to give good results in the selection of nuclei. Their fits include the curious SV force, which has $t_3 = 0.0 \text{ Mev}\cdot\text{fm}^6$. They computed a large range of variables; single-particle energies, densities, radii, isotope shifts, nuclear matter properties and correlations between them, as one was systematically adjusted. The detailed results are too extensive to reproduce here, though they summarised their conclusions with the phrase in their abstract “The parameters ... are determined by requiring that they accurately reproduce the total binding energies and charge radii of magic nuclei in spherical self-consistent cal-

culations. It is shown that many parameter sets can satisfy these requirements.”

There followed many different parameter fits with different strategies. Some of these revisited parts of the original force which were not usually active, such as the tensor terms, and other explored extensions to the force. A widely-used extension came from Reinhard and Flocard [5] (and at the same time, a similar form from Sharma *et al.* [6]), which generalised the isospin-dependence of the spin-orbit force so that it could be written, in the form of the Hamiltonian density as

$$\epsilon_{ls} = \int d^3r \left\{ b_4 \rho \nabla \mathcal{J} + \sum_{q \in \{p,n\}} b'_4 \rho_q \nabla \mathcal{J}_q \right\}. \quad (4)$$

where ρ is the total particle density, and \mathcal{J} the spin-orbit current. The choice $b_4 = b'_4 = V$ yields the original Skyrme form (2), while $b'_4 = 0$ gives an isospin-dependence like the Relativistic Mean Field approach [7]. Enforcing neither of these conditions gives yet more freedom in the fit. A key part of the motivation of this change was to improve the reproduction of isotope shifts, particularly that of the kink in lead isotopes through the $N = 126$ shell gap. Several fits appeared in Ref. [5], which were made to a selection of ground state binding energies, radii, thicknesses, spin-orbit splittings and isotope shifts (but not nuclear matter). This extended form of the spin-orbit force has subsequently been widely, but not universally used in parameter fitting.

Several parameterizations have taken information from the Equation of State away from saturation density into account. In particular, the “Lyon” Skyrmes of Chabanat *et al.* [8, 9]. In the first paper [8] they explicitly give the chi-squared function to which they fit, including a term ¹

$$\sum_{i=1}^{11} \left(\frac{E_{\text{skyrme}}(Y_p = 0; i) - E_{\text{AV14+UVII}}(i)}{\Delta E_i} \right) \quad (5)$$

indicating 11 points at which the Skyrme equation of state for symmetric nuclear matter was fitted to points calculated with realistic interactions - The Argonne V14 two-body force, augmented with a three-body force [10]. In common with most papers describing new forces, exact details of how the χ^2 function was minimized is not given. Such information is valuable as the χ^2 function is a nonlinear function of the force parameters, with possibly many local minima, as evinced by the statement above from Beiner *et al.* [4], and which can be seen in practical calculations. At least having the exact χ^2 with weights for each observable is useful.

Other common fit strategies include the work of Goriely, Pearson and others on producing a global fit to all known nuclear masses [11–14], which have achieved global mass fits with a root-mean-squared error on masses of the order of a few hundred keV.

¹We have corrected the presumed typographical error “UV14” in the referenced paper to read “AV14” here.

It would require a full review article to describe the fit processes and the properties of all existing Skyrme fits in the literature. We have attempted to indicate, though, some of the many strategies, and observables, that are used in the process. In addition, the exact form of the Skyrme force has changed over the years (indeed [14], for example, uses density-dependent extensions to the t_1 and t_2 terms in the original Skyrme force), so that several variants, each with the same overall spirit, exist.

3 Applying Constraints to Existing Parameters

While one may take each Skyrme parameterisation on its merits and attempt to apply each to its own area of strength, there is a sense in which the philosophy of the Skyrme force is that it should be applicable to all nuclei and to many observables. At least, this should be the case if the basic form is correct and sufficiently complete, and the parameters have been fitted in the right way. Indeed, the UNEDF project¹ is seeking to produce a parameter set on this basis [15]. It is therefore reasonable to take the whole body of Skyrme parameterizations and subject them to constraints to find a subset of forces which are able to satisfy a chosen set of observables. A recent paper [16], following up a previous study [17], undertakes this task, using an extensive set of nuclear matter properties, derived from observables. These constraints included the incompressibility, and its first derivative, as constrained by giant monopole resonance observations, the relationship between pressure and density, as deduced by heavy ion collisions, the universal behaviour of dilute neutron matter, the symmetry energy from the liquid drop model, pygmy dipole resonances and heavy ion collision data, along with the first derivative of the symmetry energy. Values of nuclear matter quantities were taken at different densities, including the equation of state over a range, as with the *Lyon* force example above. The symmetry energy was taken at saturation and at half-saturation density, to account for nuclear surface properties. Constraints on the Landau parameters were taken into account to ensure at least some instabilities were accounted for. No constraints were made on spin-polarised matter [18], beyond general constraints on the Landau parameters. A short list of 16 parameter sets, from the 240 considered, passed the macroscopic nuclear matter constraints, with 5 of those also passing the microscopic constraints. We discuss those five sets here as a prelude to evaluate how well they work in finite nuclei, given that they alone pass an extensive series of nuclear matter tests.

The five forces are SKRA [19], KDE0v1 [20], NRAPR [21], LNS [22], and SQMC700 [23]. SKRA, dating from 2000, was fitted to the equation of state of symmetric nuclear matter up to about $\rho = 0.45 \text{ fm}^{-3}$ as calculated via Bruckner Hartree-Fock with the Reid Soft Core potential, with relativistic and three body corrections. It was also fitted to ground state properties of some doubly magic nuclei.

¹<http://www.unedf.org>

KDE0v1, from 2005, fitted to an extensive set of data for finite nuclei, including breathing mode energies as well as ground state properties, and some limited nuclear matter data (the critical density, along with a veto on forces giving negative pressure below $3\rho_0$, and a sign condition on a Landau parameter). A unique aspect to the KDE0v1 force is that the minimization of the χ^2 function took place via a simulated annealing algorithm, with a check that the discovered solution was indeed a minimum. Since the χ^2 function has many minima, the result of the algorithm can give different answers depending on the starting point. Indeed, this is found and alternate sets are given depending on the starting vector. Only one of the resultant solutions actually satisfied all the nuclear matter tests.

NRAPR, from 2005, was fitted to the equation of state of Akmal, Pandharipande and Ravenhall (APR) [24] for symmetric nuclear matter and pure neutron matter up to a density of $3\rho_0/2$, with a fit also of the effective mass to that of APR, and an adjustment of the spin-orbit parameter to improve binding energies in ^{208}Pb , ^{90}Zr and ^{40}Ca .

LNS, from 2006, included constraints on the parameters to fit effective masses from Bruckner Hartree-Fock calculations. Then sets of acceptable parameters which also fit the equation of state at different densities and isospin asymmetries. Then constraints on the G_0 Landau parameter and surface properties are used to select a set. Finally, some adjustment is made to improve the fit to finite nuclei.

The last force to pass the constraints, QMC700, from 2006, has a slightly different functional form to standard Skyrme forces in the density-dependence. It is derived as a non-relativistic expansion of a quark-level description of nuclei.

In summary, the forces that passed all the constraints do not appear to have a lot in common, except perhaps that three of them took a more than average weight in their fit from the nuclear matter equation of state at a range of densities, and sometimes isospin asymmetries. That, at least, should be part of the reason why the forces passed the nuclear matter constraints used in the recent paper [16]. We now proceed to examine the properties of these force, which give very similar results in a wide range of nuclear matter calculations, to see if this similarity will automatically transfer to finite nuclei.

4 Results in Finite Nuclei

As a first check of the ability of the shortlist of forces to reproduce finite nuclei, we check binding energies of ^{16}O , ^{34}Si , ^{40}Ca , ^{48}Ca , ^{48}Ni , ^{56}Ni , ^{68}Ni , ^{78}Ni , ^{100}Sn , ^{114}Sn , ^{132}Sn , ^{146}Gd and ^{208}Pb . The results for all the subset of forces, except QMC700 (because it is not quite a standard Skyrme force) are shown in Figure 1. SkI4 is included as an extant Skyrme force of good quality for comparison. The results for each force are connected by lines to help show the general trends, and the independent variable is chosen as \sqrt{NZ} in order to scale the plot nicely, given that each point falls at (semi-)magic values of N or Z.

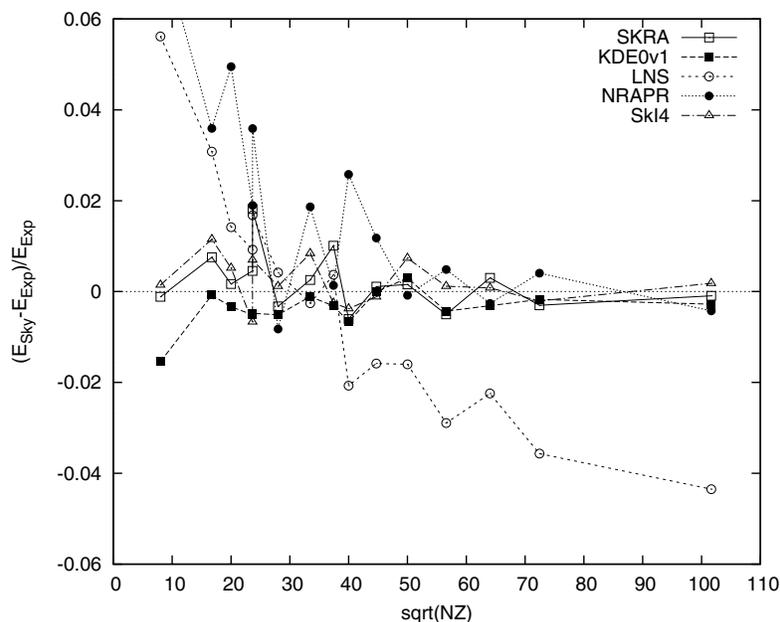


Figure 1. Comparison to experimental data of quality of fit to binding energies of doubly- and singly- magic nuclei

It can be seen that there is considerable variation in the quality of the reproduction of binding energies. LNS, for example, shows a systematically skewed mass-dependence, with light nuclei overbound and heavy nuclei underbound, though the authors of the original LNS force have provided an update with better reproduction of binding energies [25]. NRAPR shows a similar overbinding of light nuclei, though matches heavy nuclei quite reasonably. NRAPR and KDE0v1 have a quality similar to SkI4. One can conclude that it is not sufficient to pass the set of tests in Ref. [16] to give a best-quality reproduction of binding energies. On the other hand, it is clearly possible to both pass the nuclear matter constraints, and give a good reproduction of binding energies. The two forces which are able to do so have quite different fitting strategies; One (SKRA) concentrates on fitting an equation of state, with adjustment to finite nuclei, whereas the other (KDE0v1) concentrated on a wide range of finite nuclear parameters, including breathing mode energies.

For the same set of nuclei, results for charge radii are given in Figure 2. The radii are shown scaled by $A^{-1/3}$ to make discrepancies between the data and calculated values more apparent. Since data are not available for the full set of nuclei in our study (some of which are very exotic), the experimental data is not subtracted from the calculated values, as for the energies in Figure 1. The experimental data are taken from a compilation using a variety of experimen-

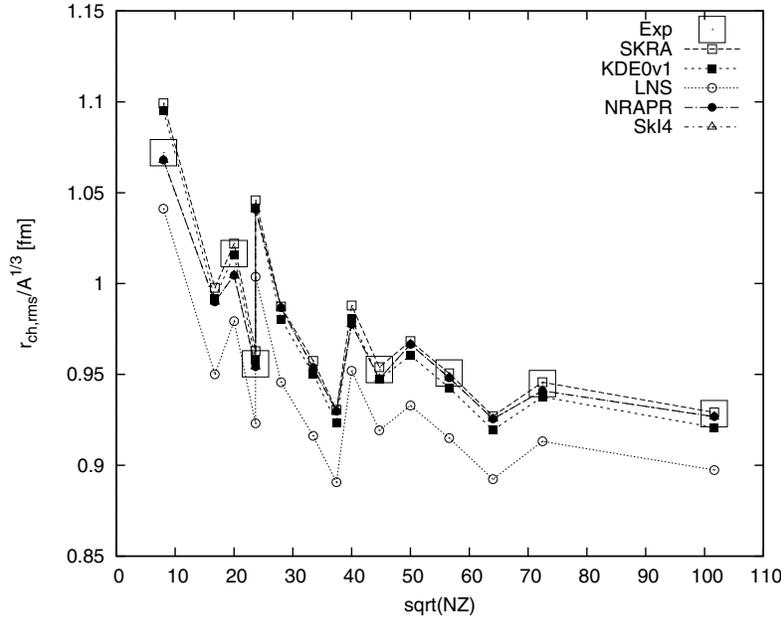


Figure 2. Charge radii for the selected forces and nuclei, compared with experimental data

tal methods [26] and to aid understanding of the Figure, the experimental data points are for ^{16}O , ^{40}Ca , ^{48}Ca , ^{90}Zr , ^{114}Sn , ^{146}Gd and ^{208}Pb .

Again, LNS has a systematic deviation from the experimental data, though it does follow the general trend, but always underestimating the radii. The other shortlisted forces do quite well, with NRAPR performing best, perhaps surprisingly, given its variable performance with mass number for binding energies.

We have performed further studies reported elsewhere, looking more at isotope shifts [27], which are more of a shell effect than the observables we have considered here, and in particular at the lead isotope shift.

5 Conclusion

We have presented a short and selective summary of the history of fitting Skyrme forces, and of a recent paper which seeks to test each parameterisation for its ability to pass a series of nuclear matter constraints. It is found that parameter sets can pass the constraints while either giving good results for binding energies in finite nuclei, or not giving good results. For charge radii, the parameterizations generally performed better than for energies, but curiously those that performed least well showed different isotopic dependence than the energies. One may conclude that passing nuclear matter constraints per se is not sufficient to

give a globally good parameterisation, or that the constraints are not correct. In the spirit of the Skyrme interaction, in which one might hope that a sufficiently complete expansion will describe all data, the Skyrme force will need to be extended with higher order terms before finite nuclei and nuclear matter will be fitted on the same basis.

Acknowledgements

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