Misfits in Skyrme-Hartree-Fock

J. Erler\textsuperscript{1}, P. Klüpfel\textsuperscript{1}, P.-G. Reinhard\textsuperscript{1}

\textsuperscript{1} Institut für Theoretische Physik, Universität Erlangen, D-91058, Erlangen, Germany

Abstract. We address very briefly five critical points in the context of the Skyrme-Hartree-Fock (SHF) scheme: 1) the impossibility to consider it as an interaction, 2) a possible inconsistency of correlation corrections as, e.g., the center-of-mass correction, 3) problems to describe the giant dipole resonance (GDR) simultaneously in light and heavy nuclei, 4) deficiencies in the extrapolation of binding energies to super-heavy elements (SHE), and 5) a yet inappropriate trend in fission life-times when going to the heaviest SHE. While the first two points have more a formal bias, the other three points have practical implications and wait for solution.

PACS numbers: 21.10.Dr; 21.30.Fe; 21.60.Jz; 24.30.Cz; 24.75.+i

1. Introduction

This manuscript addresses a couple of open problems in the Skyrme-Hartree-Fock (SHF) scheme. Before coming to these puzzling details, we want to emphasize the enormous merits of SHF. The SHF energy functional manages to establish a reliable description of nuclear properties all over the chart of isotopes (except perhaps the lightest ones) with an adjustment of only a dozen universal parameters, for reviews see e.g. \cite{1,2}. The enormous success of SHF implies the temptation to ask for more details and it is mostly here where we encounter the present limitations of SHF. The aim of this contribution is to identify problems in order to solve them later on in a common effort of the nuclear physics community. We will in the following address five points: the interpretation as “force”, the consistency of ground state correlations, the giant dipole resonance in light nuclei, extrapolation of binding energies to super-heavy elements (SHE), and fission of SHE. The first two points are of formal nature, the last three more phenomenological.

\textsuperscript{\S} To whom correspondence should be addressed (jochen.erler@physik.uni-erlangen.de)
2. Formal inconsistencies

2.1. The concept of a “force”

One often thinks in terms of a “Skyrme-force”, to be more precise a Skyrme interaction, whose most touchy ingredient is the density dependent term

\[ \hat{V}_3(r_1, r_2) = \frac{t_3}{6} \delta(r_1 - r_2) \rho^3(r_1) \left( 1 + x_3 \hat{\Pi}_\sigma \right), \quad \rho(r) = \langle \Phi | \rho(r) | \Phi \rangle, \quad (1) \]

where \( \hat{\Pi}_\sigma \) is the spin-exchange operator. We argue that this is a most dubious object. It is not a “stand alone” interaction operator, but depends on a mean-field state |\( \Phi \rangle \) from which the density \( \rho(r) \) is taken. Non-integer values of \( \alpha \) immediately hinder an identification with an \( N \)-body force. The simplest case is \( \alpha = 1 \) and one is tempted to interpret the interaction then as a three body force. Let us consider this case and also ignore the spin-exchange term by setting \( x_3 = 0 \) for simplicity. If the operator (1) was a true interaction operator, one should be able to produce an equivalent expression in terms of Fermion operators as

\[ \hat{V}_3^{(\text{FO})} = \sum_{\alpha_1 \alpha_2 \alpha_3} V_{\alpha_1 \alpha_2 \alpha_3 \beta_1 \beta_2 \beta_3} \hat{a}_{\alpha_1}^\dagger \hat{a}_{\alpha_2}^\dagger \hat{a}_{\alpha_3} \hat{a}_{\beta_1} \hat{a}_{\beta_2} \hat{a}_{\beta_3}. \quad (2) \]

The ground-state expectation value of such a \( \hat{V}_3^{(\text{FO})} \) reads

\[ \langle \Phi | \hat{V}_3^{(\text{FO})} | \Phi \rangle = \sum_{nmk} V_{nmk,\overline{nmk}}, \quad (3) \]

where \( \overline{nmk} \) stands for anti-symmetrization of all three states \( nmk \). However, the expectation value of the effective interaction (1) for \( \alpha = 1 \) reads

\[ \langle \Phi | \hat{V}_3 | \Phi \rangle \propto \sum_{nmk,\overline{nmk}}^N \int d^3r \left[ 2 \rho_n r_n \rho_m r_m - \rho_n \theta_{nmrm} \rho_m \theta_{nm} \right] \varphi_k \varphi_k \]

\[ \equiv \sum_{nmk} V_{nmk,\overline{nmk}}. \quad (4) \]

Note that the state \( k \) is not included in the anti-symmetrization. Thus the whole expression can never be written in the form (3) and the Skyrme ansatz (1) cannot be interpreted as an interaction.

A unique and consistent object is the total energy which turns out to be a functional of the local density \( \rho(r) \) and spin density \( \sigma(r) \), i.e. for \( \alpha = 1 \) and \( x_3 = 0 \)

\[ E_3 = \langle \Phi | \hat{V}_3 | \Phi \rangle = \frac{t_3}{24} \int d^3r \left\{ 2 \rho^3 - \rho \left( \rho_n^2 + \rho_p^2 \right) - \rho \left( \sigma^2_n + \sigma^2_p \right) \right\}. \quad (5) \]

The main use of the interaction (1) is that it serves nicely as a formal generator for that functional. But any other use is dangerous. Let us consider, e.g., the residual interaction in RPA. It is deduced from the energy functional by second functional derivative (3) and reads, e.g., for pure density variations (no spin excitations)

\[ V_3^{(\text{res})} = \frac{\partial^2 E_3}{\partial \rho(r_1) \partial \rho(r_2)} = \frac{t_3}{2} \delta(r_1 - r_2) \rho(r_1). \quad (6) \]
This has a strength factor $t_3/2$ which is different from the $t_3/6$ of the initial interaction (1). Thus the interaction (1) is not consistently reproducible by standard many-body techniques.

Most energy-density functionals are plagued by the self-interaction error [4]. It can be checked simply by considering the case of exactly one particle. Functionals with self interaction then yield still a non-vanishing energy which is, of course, unphysical. The functional (5) yields correctly value zero for the case of one particle and is thus self-interaction free. That nice feature is achieved by derivation from the interaction (1). It ought to be mentioned, however, that a derivation from an interaction is not a necessary condition for constructing self-interaction free energy functionals.

We thus have seen from two different aspects that the notion of a Skyrme “force” is misleading. The cleanest view of Skyrme-Hartree-Fock is to derive it from an energy-density functional. On the other hand, deriving the functional (5) from the effective interaction (1) avoids the self-interaction error and provides the spin terms which otherwise would be much undetermined. It is a matter of phenomenology to check whether the thus imposed spin terms in the nuclear energy density functional are supported by phenomenological data.

2.2. Fragmentation and collective correlations

The ground state of a nucleus is usually computed with a correction of the center-of-mass energy. The motivation is that the mean-field state violates translational invariance and that one needs to consider an “intrinsic” state which is obtained by center-of-mass projection. This projection can be simplified by many-body techniques (second order Gaussian-Overlap-Approximation [5]) to

$$E_{\text{cm}} = \frac{\langle \Phi | \hat{P}_{\text{cm}}^2 | \Phi \rangle}{2mA} \approx 30 \text{ MeV } A^{-1/3} .$$

Both forms (the operator expectation value or the simple estimate) are widely used and both include the total nucleon number $A$. Now consider fusion of two nuclei. Initially, we have a c.m. energy (7) for each nucleus $A_1$ and $A_2$, but finally only one for the total $A$, i.e.

$$E_{\text{cm}}^{(\text{in})} = E_{\text{cm}}(A_1) + E_{\text{cm}}(A_2) \leftrightarrow E_{\text{cm}}^{(\text{fus})} = E_{\text{cm}}(A_1 + A_2) .$$

That is inconsistent and is particularly puzzling in between where one does not know which one of the both rules to apply. The problem was already noted in [6, 7] and an interpolation formula was proposed as an ad-hoc remedy. We want to analyze the case further. Short closer inspection shows that the six initial c.m. degrees-of-freedom merge into three final c.m. degrees-of-freedom, two rotational degrees-of-freedom (for axial symmetry of the final state), and one quadrupole mode. The problem could be resolved by associating (axial) quadrupole and rotational correlations with the compound nucleus. However, this imposes a new problem: we should do the same with the initial two nuclei. This, in turn, provides even more initial degrees-of-freedom (12
instead of 6) which have to merge into further collective modes of the compound system. This loop generates more and more correlating modes and it is not clear where to stop. The problem may be bearable as long as one considers only intact nuclei with fixed particle number. It becomes a big hindrance in any reaction which changes particle number. Thus there is an urgent need to develop a counting of collective correlations which is robust under fission, fusion and fragmentation. For the time being, it is the most consistent procedure to assume that all correlations are already built into the energy-density functional and to discard any correlation correction, even the ones for c.m. or rotational motion. That holds particularly for all TDHF calculations of large amplitude collective motion.

3. Trend of the GDR with mass number

Giant resonances are crucial nuclear excitation modes. They can be described consistently with a given energy functional by using time-dependent density functional theory, in the nuclear context called TDHF, and considering the small amplitude limit thereof. The scheme is called Random-Phase-Approximation (RPA), for details see [3]. Information from giant resonances in heavy nuclei has often been used in the calibration of a Skyrme parameterization, see e.g. [8]. A particular prominent mode is the Giant Dipole Resonance (GDR) which is commonly believed to be well under control with SHF. However, this holds only for heavy nuclei. This is demonstrated in the left panel of figure 2 which compares RPA values for the average energy of the GDR with experimental data. The peak energies are deduced from the dipole strength distributions. We show results for two Skyrme forces (SKM* [8] and SLy6 [9]). We have checked a broad variety of other Skyrme forces and always find the same trend. The discrepancy is obvious: while the GDR for heavy nuclei can be adjusted very well, it is impossible to have simultaneously a reasonable description in small nuclei. The trend is grossly wrong. The experimental data comply fairly well with a trend $E_{\text{GDR}} \propto A^{-1/6}$, but RPA predicts a much different trend with a sizeable admixture of $E_{\text{GDR}} \propto A^{-1/3}$. The right panel of figure 2 shows results of an estimate using the Thomas-Reiche-Kuhn (TRK) sum rule [3, 10]. The peak energy is, of course, overestimated. But the trend $\propto A^{-1/6}$ complies with experiment.
Figure 2. Peak energies of the Giant-Dipole-Resonance (GDR) drawn versus inverse radius $R = 1.16 \text{ fm} \, A^{1/3}$. Heavy nuclei (e.g. Pb) are found at the left side and light nuclei (e.g. O) to the right. The energies are scaled with $A^{1/6}$. Compared are results from two different Skyrme parameterizations and experimental data. Left: Peak energy from a full RPA calculation. Right: Energy from a sum-rule estimate.

The TRK mode is a surface mode (Goldhaber-Teller). The competitor is the volume mode (Steinwedel-Jensen) which produces a trend $\propto A^{-1/3}$ \[10\]. We thus see that the RPA description underestimates the surface contribution and leaves to much bias on the volume. The conjecture is that the present Skyrme forces are still having an inappropriate isovector surface energy. Substantial improvement in that part is needed.

4. Extrapolation to SHE

Skyrme parameterizations are usually determined by a phenomenological adjustment to a given pool of fit data (binding energies, radii, etc., for a chosen set of nuclei). The aim is to obtain a reliable description for all nuclei deep into the regime of exotic ones. The predictive power of a parameterization is to be checked at three levels: 1) the ability to reproduce the fit-data, 2) the performance for interpolation to other nuclei in the range of the fit data, and 3) the reliability of extrapolations to other regions of the nuclear chart (e.g. super-heavy elements) or other observables. It is found that check 1 and check 2 are usually well satisfied while the extrapolation to super-heavy elements (SHE) reveals a systematic deviation. That holds for all modern Skyrme parameterizations. We will discuss this issue in terms of a newly developed fit protocol \[12\]. Reference point is the Skyrme parameterization SV-min which was fitted to a large set of nuclei covering a wide span of mass numbers $A$ as well as long isotopic and isotonic chains. The fit pool selected good “mean-field nuclei”, i.e. nuclei which have negligible effects from collective ground state correlations \[13\], and was confined to spherical systems for reasons of technical simplicity.

The upper panel of figure 3 summarizes the error in binding energy for SV-min taken over all available nuclei. All energies are computed including collective ground
state correlations. Filled squares indicate the fit nuclei (for which correlations are ignorable), open circles indicate well deformed nuclei (deformation $\beta_2 > 0.2$), and open triangles indicate the majority of vibrationally soft nuclei (vibrational amplitude larger than deformation, large correlations). The figure shows that interpolation (results for nuclei $A < 210$) works nice with errors remaining acceptably small and distributed on both sides of the zero line. But the extrapolation to SHE shows a significant trend to increasing underbinding. The same trend (often worse) is found for other Skyrme forces.

One could try to cure that defect by including data from SHE. This has been done by adding the energy of $^{264}$Hs (a well deformed SHE) to the fit data. This yields a modified parameterization “SV-def” whose distribution of errors on binding is shown in the lower panel of figure 3. The predictions for other SHE (now being an interpolation) has clearly improved. But that is achieved at the price of sacrificing the quality of many other nuclei which are now often overbound. This indicates that there is an intrinsic problem with the form of the Skyrme energy functional which inhibits to span a wider mass range.

5. Fission barriers and half-lives of super-heavy elements

The microscopic description of nuclear fission is a long standing problem which was handled long ago in terms of empirical shell models, see e.g. [14]. The case is extremely demanding for self-consistent mean-field models as all aspects of the effective nuclear
interaction are probed, global parameters of the nuclear liquid drop as well as details of the shell structure. SHF studies of fission are thus still rare, see e.g. [15, 16, 17]. We have recently developed a fully self-consistent description of fission life-times [18] and use it here to work out conflicting trends of fission properties in SHE. We summarize briefly the computational scheme as outlined in [18]: The fission path is generated by quadrupole-constrained SHF whose energy expectation values yield a “raw” collective energy surface. The collective mass and moments of inertia are computed by self-consistent cranking along the states of the path [19]. Approximate projection onto angular momentum zero is performed using the moments of inertia and angular-momentum width. Quantum corrections for the spurious vibrational zero-point energy are applied (using quadrupole mass and width). The collective ground state energy is computed fully quantum mechanically [13]. The tunneling rate at the given ground state energy and the repetition rates are computed by the standard semi-classical formula (known as WKB) using the quantum-corrected potential energy and collective mass; the fission life-time is finally composed from these two rates. All calculations are performed in axial symmetry. Figure 4 summarizes results on fission barriers and lifetimes for a few typical SHE and for a large variety of Skyrme parameterizations. The SHE represent two groups, one at the lower side and another one with much heavier nuclei at the limits of present days available experimental data. The span of predictions from the various Skyrme forces is huge in all cases in spite of the fact that all these parameterizations provide a high-level description of basic nuclear properties. But the variation of predictions is not the problem. One may decide to chose from the manifold of parameterizations just those which provide at the same time good fission properties throughout. But this turns

![Figure 4](image-url)

**Figure 4.** Fission barriers (lower) and half-lives (upper) for a selection of SHE as indicated. Experimental data are compared with results from a variety of different Skyrme parameterizations, SkM*, SkP [20], SkI3 [21], SV-bas and SV-min [12]. The experimental data is taken from [22, 23, 24, 25, 26].
out to be impossible at present. The true problem becomes apparent when looking at the trend from the lighter side (Rf, Sg, Hs) to the heavier elements (Z=112, 114). All parameterizations produce a wrong trend of the predictions from the lower to the upper region. Forces which perform acceptable for Rf, Sg, Hs fail badly for Z=112,114 and vice versa. One may argue that triaxiality, ignored here, could resolve the trend because triaxial deformation may lower some barriers selectively. But that is very unlikely in view of the experience that the triaxial barrier-lowering amounts typically to 1 MeV, at most 2 MeV [27], which does not suffice to bridge the gap here.

6. Conclusion

We have worked out briefly five puzzling points in connection with SHF:
1) An interpretation as “force” is inconsistent because the density dependence inhibits an expression of the Skyrme energy as standard quantum-mechanical expectation value.
2) The center-of-mass correction, usually applied, causes conceptual problems in nuclear fusion, fission and fragmentation; parameterizations which are used for such reactions should be adjusted without including the center-of-mass correction.
3) It is presently impossible to find a parameterization which delivers a good description of the giant dipole resonance in all regions of the nuclear chart; it seems that the relation of surface to volume mode is not properly balanced.
4) The extrapolation of binding energies to SHE yields quickly increasing underbinding and a refit including energies of known SHE spoils the quality in the region of stable nuclei; the problem is probably caused by a still inappropriate surface or curvature energy.
5) The experimentally observed trend of fission properties from the Hs region to much heavier SHE is not reproduced by any SHF parameterization.

For all these points, we do not have presently any solution and often we have not even figured out the deeper reasons. This has to be put on the work schedule for future studies.

Acknowledgment

We thank the regional computing center of the university Erlangen-Nürnberg for generous supply of computer time for the demanding calculations. The work was supported by the BMBF under contracts 06 ER 808 and 06 ER 9063.

References

[1] Bender M, Heenen P-H and Reinhard P-G 2003 Rev. Mod. Phys. 75 121
[2] Stone J R and Reinhard P-G 2007 Prog. Part. Nucl. Phys. 58 587
[3] Reinhard P-G and Gambhir Y 1992 Ann. Phys. (Leipzig) 1 598; Reinhard P-G 1992 Ann. Phys. (Leipzig) 1 632
[4] Dreizler R M and Gross E K U 1990 Density Functional Theory: An Approach to the Quantum Many-Body Problem Berlin: Springer
[5] Schmid K W and Reinhard P-G 1991 Nucl. Phys. A 530 283
[6] Berger J-F, Gogny D 1980 Nucl. Phys. A 333 302
[7] Skalski 2007 Phys. Rev. C 76 044603
[8] Bartel J, Quentin P, Brack M, Guet C and Håkansson H-B 1982 Nucl. Phys. A 386 79
[9] Chabanat E, Bonche P, Haensel P, Meyer J and Schaeffer R 1997 Nucl. Phys. A 627 710
[10] Brack M and Stocker W 1983 Nucl. Phys. A 406 413
[11] Audi G, Wapstra A H and Thibault T 2003 Nucl. Phys. A 729 337
[12] Klüpfel P, Reinhard P-G, Bürvenich T J and Maruhn J A 2009 Phys. Rev. C 79 034310
[13] Klüpfel P, Erler J, Reinhard P-G and Maruhn J A 2008 Eur. Phys. J. A 37 343
[14] Brack M, Damgård J, Jensen A S, Pauli H C, Strutinsky V M and Wong C Y 1972 Rev. Mod. Phys. 44 320
[15] Berger J-F, Bitaud L, Decharge J, Girod M and Dietrich K 2001 Nucl. Phys. A 685 1
[16] Bürvenich T, Bender M, Maruhn J A and Reinhard P-G 2004 Phys. Rev. C 69 014307
[17] Warda M, Egido J and Robledo L 2006 Phys. Scr. T 125 226
[18] Schindzielorz N, Erler J, Klüpfel P, Reinhard P-G and Hager G 2009 Int. J. Mod. Phys. E 18 773
[19] Reinhard P-G and Goeke K 1987 Rep. Prog. Phys. 50 1
[20] Dobaczewski J, Flocard H and Treiner J 1984 Nucl. Phys. A 422 103
[21] Reinhard P-G and Flocard H 1995 Nucl. Phys. A 584 467
[22] Hofmann S et al 2001 Eur. Phys. J. A 10 5
[23] Peter J 2004 Eur. Phys. J. A 22 271
[24] Oganessian Y T et al 2004 Phys. Rev. C 70 064609
[25] Gregorich K E et al 2006 Phys. Rev. C 74 044611
[26] Gates J M et al 2008 Phys. Rev. C 77 034603
[27] Ćwiok S, Dobaczewski J, Heenen P-H, Magierski P, and Nazarewicz W 1996 Nucl. Phys. A 611 211