A new Skyrme interaction with improved spin-isospin properties

X. Roca-Maza\textsuperscript{1}, G. Colò\textsuperscript{1,2}, and H. Sagawa\textsuperscript{3,4}

\textsuperscript{1} INFN, sezione di Milano, via Celoria 16, I-20133 Milano, Italy
\textsuperscript{2} Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, I-20133 Milano, Italy
\textsuperscript{3} Center for Mathematics and Physics, University of Aizu, Aizu-Wakamatsu, Fukushima 965-8560, Japan
\textsuperscript{4} Nishina Center, Wako, Saitama 351-0198, Japan

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The Skyrme Hartree-Fock (HF) approach is one of the successful techniques for the study of the ground state properties of nuclei and, if supplemented by a proper description of nuclear superfluidity (e.g., within the Hartree-Fock-Bogoliubov scheme), it can be applied throughout the whole periodic table\textsuperscript{1}. The small amplitude limit of time-dependent HF calculations, or Random Phase Approximation (RPA), has allowed to describe many kinds of nuclear collective motion\textsuperscript{2}. The versatility of the Skyrme ansatz allows its use in more elaborated theoretical frameworks that include higher-order nuclear correlations - like the Generator Coordinate Method\textsuperscript{3}, or the Particle-Vibration Coupling approach\textsuperscript{4}.

Despite the existence of drawbacks and open issues, the Skyrme-HF approach enables an effective description of the nuclear many-body problem in terms of a local energy density functional. Problems concerning specific terms of this functional need to be understood and eventually solved (cf. also Ref.\textsuperscript{5}). One of these problems, and the focus of the present work, is the accurate determination of the spin-isospin properties of the nuclear effective interaction and of the associated functional. Such a determination should lead to accurate predictions of the properties of GTR, that are among the clearest manifestations of nuclear collective motion\textsuperscript{6}. Gamow-Teller (GT) transitions determine weak-interaction rates between fp-shell nuclei that play an essential role in the core-collapse dynamics of massive stars leading to supernova explosion\textsuperscript{7,8} (in this neutron-rich environment, neutrino-induced nucleosynthesis may take place via GT processes\textsuperscript{9}). Accurate GT matrix elements are necessary for the study of double-β decay\textsuperscript{10}, and may be useful in the calibration of detectors aiming to measure electron-neutrinos coming from the Sun\textsuperscript{11}.

The earliest attempt to give a quantitative description of the GTR data was provided by the Skyrme SGII interaction\textsuperscript{12}. However, two component spin-orbit contributions to the nuclear Hamiltonian density – Eq. (6.1) in Ref.\textsuperscript{13} – were not introduced. Later on, using the full Skyrme Hamiltonian density, a functional suitable for the predictions of finite nuclei and charge-exchange resonances was proposed: namely SkO'\textsuperscript{14}. Relativistic mean-field and relativistic HF calculations of the GTR have also become available meanwhile\textsuperscript{15,16}. In a recent and detailed study on the GTR and the spin-isospin Landau-Migdal parameter (G\textsubscript{0}) using several Skyrme sets\textsuperscript{17}, Bender et al. have concluded that this spin-isospin coupling is not the only important quantity in determining the strength and excitation energy of the GTR in nuclei. Actually, the authors state that spin-orbit splittings together with the residual spin-isospin interaction influences the above mentioned quantities.

The GT transition strength (R\textsubscript{GT±}) is mediated by the operator \( \sum_{i=1}^{A} \hat{\sigma}(i) \tau_{\pm}(i) \), where A is the mass number and \( \hat{\sigma} \) and \( \tau_{\pm} \) are the spin and isospin Pauli matrices, respectively. The contributions to R\textsubscript{GT±} come from nucleon transitions that change the spin and isospin of the parent quantum state and the residual interaction between them is repulsive. The dominant transitions will be those between spin-orbit partner levels. In this respect, most of the Skyrme interactions overestimate the experimental spin-orbit splittings in heavy nuclei\textsuperscript{18}.

Experimentally, the GTR exhausts only about 60-70% of the well known Ikeda Sum Rule (ISR) given by \( \int [R_{GT^{-}}(E) - R_{GT^{+}}(E)]dE = 3(N - Z) \). To explain this well-known quenching problem, it has been proposed that the effects of the second-order configuration mixing, namely 2-particle 2-hole (2p-2h) correlations, or of the coupling with the \( \Delta \) - hole excitation, have to be taken into account. The experimental analysis of \( ^{90}\text{Zr} \)\textsuperscript{19} seems to indicate that most of the quenching (around 2/3) has to be attributed to 2p-2h coupling while the
role played by the $\Delta$ isobar is much smaller.

In our work, we present a new non-relativistic functional of the Skyrme type that include the central tensor terms ($J^2$-terms) and two spin-orbit parameters. It is named SAMi for S-kyrme A-izu Mi-lano. The new functional is as accurate as previous Skyrme models in the description of uniform nuclear matter properties around saturation and of masses and charge radii of double-magic nuclei. It is also precise in the description of the nuclear symmetry energy at normal densities towards reasonable values. Table I provides references for these data and pseudo-data with the corresponding adopted errors, partial contributions to the $\chi^2$, and the number of data points ($n_{data}$) used in the fit. The main differences between the SLy functional and the present protocol are the fitting of the above mentioned spin-orbit splittings, the fact that we fix the spin and spin-isospin Landau-Migdal parameters, and the larger adopted errors for the equation of state of pure neutron matter. This protocol is justified by the fact that pseudo-data are used as a guide and, therefore, it should not impact on the fitted interaction more than experimental data. The minimization of the $\chi^2$ has been performed by means of a variable metric method included in the MINUIT package of Ref. [21].

The parameters and saturation properties of the new interaction are shown in Table II. The estimation of the standard deviation associated to each of them is also displayed. In what follows, the new SAMi functional is compared to available experimental data and other theoretical predictions for ground and excited state properties. First of all, we show in Fig. 1 the results for the symmetric and pure neutron matter Equations of State (EoS) as predicted by the benchmark microscopic calculations used in the fit [24], three-state-of-the-art Brueckner-Hartree-Fock (BHF) calculations [28–30], the SAMi functional, and SLy5 — also fitted to reproduce the neutron matter EoS of Ref. [21]. The agreement of the SAMi functional with these calculations of nuclear matter based on realistic nucleon-nucleon (NN) forces is remarkable. The deviation of the SAMi EoS of pure neutron matter from the fitted microscopic curve (red circles) is essentially due to the relatively large error (20%) adopted in the $\chi^2$ definition in order not to spoil the additional constraints set on the isovector channel of the effective interaction. In addition, we have checked

**Table I: Data and pseudo-data $O_i$, adopted errors for the fit $\Delta O_i$, as well as partial and total number of data points and contributions to the $\chi^2$.**

| $O_i$ | $\Delta O_i$ | $\chi_{\text{partial}}$ | $n_{\text{data}}$ | Ref. |
|-------|---------------|--------------------------|-------------------|------|
| $B$   | 1.00 MeV      | 32.45                    | 5                 | [20] |
| $r_c$ | 0.01 fm       | 13.38                    | 4                 | [21] |
| $\Delta E_{SO}$ | 0.04×$O_i$ | 19.02                    | 2                 | [22] |
| $e_n(\rho)$ | 0.20×$O_i$ | 12.60                    | 11                | [23] |
| $\chi^2$ |            | 77.45 / 22 = 3.52       |                   |      |

baryon density $\rho$ between 0.07 fm$^{-3}$ and 0.4 fm$^{-3}$ that have been helpful in driving the magnitude ($J$) and slope ($L$) of the nuclear symmetry energy at normal densities towards reasonable values.
that the SAMi EoS is stable against spin and spin-isospin instabilities up to a baryon density of 4.1\(\rho_\infty\) and 5.3\(\rho_\infty\), respectively, i.e., well above the region important for the description of finite nuclei and enough for the study of uniform neutron-rich matter in neutron stars. Furthermore, we are aware that particle-number projection techniques lead to instabilities when functionals with non-integer power of the density are employed. At the same time, the adopted density dependence (\(\rho^\alpha\) with \(\alpha\) smaller than one) seems to be the only way to have reasonable values of the nuclear incompressibility and of the GMR energies within the Skyrme functional. As a future perspective, all practitioners of local, Skyrme type, EDFs may need to deal with the problem of reproducing reasonable monopole energies on the one side and making particle number restoration doable on the other side. This is beyond the purpose of the current work.

We display in Table III the SAMi results for binding energies, charge radii and proton spin-orbit splittings of all measured doubly-magic spherical nuclei. The description of a large set of Skyrme interactions is, within the same spirit, the experimental data on the GDR has clearly improved the results obtained with SGII interaction for the description of the strength distribution (calculated within RPA in the cases of the GMR and GDR in \(^{208}\text{Pb}\)). The results are compared with experimental data and with the predictions of SLy5. The operators used in the GMR and GDR cases are, respectively, \(\sum_{i=1}^A r_i^2\) and \(Z/A \sum_{n=1}^N r_n - N/A \sum_{p=1}^P r_p\). The experimental centroid energy of the GMR has allowed to constrain the nuclear matter incompressibility at the value \(K_\infty = 240 \pm 20\) MeV, by means of an analysis of a large set of Skyrme interactions. Within the same spirit, the experimental data on the GDR has allowed to determine the nuclear symmetry energy at a sub-saturation density \(S(\rho=0.1 \text{ fm}^{-3}) = 24.1\pm 0.8\) MeV. The SAMi interaction predicts compatible values, namely \(K_\infty = 245\) MeV and \(S(\rho=0.1 \text{ fm}^{-3}) = 22\) MeV. Consistently, the giant resonance centroid energy predicted by SAMi agrees well with the experimental findings: \(E_{\text{cAMi}}^{\text{GMR}} = 14.48\) MeV should be compared with \(E_{\text{cexp}}^{\text{GMR}} = 14.24 \pm 0.11\) MeV [35], exhausting both almost 100% of the Energy Weighted Sum Rule (EWSR) between \(E_x = 8 - 22\) MeV, and \(E_{\text{cAMi}}^{\text{GDR}} = 13.95\) MeV should be compared with \(E_{\text{cexp}}^{\text{GDR}} = 13.25 \pm 0.10\) MeV [36] (exhausting both around 95% of the EWSR between \(E_x = 9 - 20\) MeV).

The strength distributions of the GTR are displayed in Fig. 2. HF+RPA results obtained with the forces SAMi, SGII, SLy5 and SkO’ are compared with experiment. In the upper panel of Fig. 3, we show the experimental data of Ref. [37] as well as the prediction of the SAMi, SGII and SkO’ functionals for \(^{48}\text{Ca}\). In this case the SLy5 result is not shown because RPA produce instabilities. The nice agreement of the SAMi prediction in the excitation energy, \(E_x^{\text{exp}} = 10.5\) MeV and \(E_x^{\text{SAMi}} = 10.2\) MeV for the high-energy peak and \(E_x^{\text{exp}} = 3.0\) MeV and \(E_x^{\text{SAMi}} = 2.0\) MeV for the low-energy peak, and the % of the ISR exhausted by the main peak between 5 and 17 MeV, around 46% in the experiment and 71% in the calculation, is noticeable (in keeping with the fact that RPA does not include 2p-2h couplings). The prediction of the SAMi interaction in the case of \(^{90}\text{Zr}\) (middle panel of Fig. 3) is even better than in the case of \(^{48}\text{Ca}\). Despite of the accuracy of SGII, SLy5 and SkO’ in describing other properties of nuclei, they do not perform as well as our new proposed functional. The excitation energy and % of the ISR exhausted by the high- and low-energy peaks in the experimental data [19, 38] (in the calculation done with the SAMi functional) are, respectively, \(E_x^{\text{exp}} = 15.8 \pm 0.5\) MeV and 71% in the calculation, is noticeable (in keeping with the fact that RPA does not include 2p-2h couplings).
FIG. 2: Strength function at the relevant excitation energies in $^{208}$Pb as predicted by SLy5 [13] and the SAMi interaction for GMR (left panel) and GDR (right panel). A Lorentzian smearing parameter equal to 1 MeV is used. Experimental data for the centroid energies is also shown: $E_c$(GMR) = 14.24±0.11 MeV [43] and $E_c$(GDR) = 13.25 ± 0.10 MeV [38].

FIG. 3: GT strength distributions in $^{48}$Ca (upper panel), $^{90}$Zr (middle panel) and $^{208}$Pb (lower panel) as measured in the experiment [19,37–40] and predicted by SLy5, SkO’, SGII and SAMi forces.

MeV and 57% ($E_x^{SAMi} = 15.5$ MeV and 70%) between 12 and 30 MeV and $E_x^{exp} = 9.0 ± 0.5$ MeV and 12% ($E_x^{SAMi} = 7.8$ MeV and 27%) between 3 and 12 MeV. In the lower panel and with unprecedented accuracy in HF+RPA calculations, the SAMi functional perfectly reproduces the excitation energy of the experimental GTR in $^{208}$Pb [33]: $E_x^{exp} = 19.2 ± 0.2$ MeV and $E_x^{SAMi} = 19.3$ MeV. We also compare our results with the predictions of SGII, SLy5 and SkO’ that fail in the description of the GTR in $^{208}$Pb. It is important to notice that, opposite to SLy5, the spin-orbit parameters ($W_0$ and $W_0'$) are not fixed to be equal in the SAMi and SkO’ interactions. Note also that, $G_0$ and $G_0'$ were fixed to be 0.011 and 0.503 in SGII interaction [12] together with $K_\infty$=215 MeV and $J$=26.8 MeV which give reasonable descriptions for other resonances but predict the GT excitation energies in $^{208}$Pb at slightly higher values (21.2 MeV) – partly due to a larger $G_0'$.

In order to assess the robustness of the SAMi functional in the description of other charge-exchange reactions, we have analyzed the Isobaric Analog Resonance (IAR) in $^{90}$Zr and $^{208}$Pb. In this nuclear excitation, modeled by the operator $\sum_{i=1}^A \tau_\pm(i)$, the nucleon transitions change the isospin of the parent quantum state. We have found that the experimental value for the IAR in both, $^{90}$Zr and $^{208}$Pb is very well reproduced by the SAMi functional – within a 1.5% discrepancy with respect to the experiment [38] and the sum rule, $\int[R_{1A}^{}(E) - R_{1A^+}^{}(E)\,dE = (N-Z)$, is perfectly exhausted in our calculations.

Furthermore, experimental and theoretical studies on the Spin Dipole Resonance (SDR) have been recently revitalized due to its connection, via a sum rule, to the neutron skin thickness of nuclei $\langle\Delta r_{np}\rangle_{\mathrm{I}}$ [41] and, therefore, to the density dependence of the nuclear symmetry energy [12,13]. For these reasons, we also present the SAMi predictions for this important charge-exchange excitation in $^{90}$Zr (Fig. 4) and $^{208}$Pb (Fig. 5) as compared with the experiment [39,40]. The operator used for the RPA calculations is $\sum_{i=1}^A \sum_{JM} \tau_\pm(i)r_i^M [Y_L(\hat{r}_i) \otimes \sigma(i)]_{JM}$ and, as it is shown in both figures, it connects single particle states differing by a total angular momentum: $J^z = 0^-, 1^-$ and $2^-$. The sum rule, $\int[R_{SD}^{}(E) - R_{SD^+}^{}(E)\,dE = \frac{\mu^2}{4\pi}(N(r_p^2) - Z(r_n^2))$, is completely exhausted in our calculations, 99.99% in the case of $^{90}$Zr and 100% in the case of $^{208}$Pb. The experimental (calculated) value for the sum rule is 148 ± 12 fm$^2$ [41] (150 fm$^2$) for the case of $^{90}$Zr. The total and multipole decomposition of the experimental [40] (calculated) value for the integral of
The neutron skin thickness of medium and heavy nuclei is known to be strongly correlated with the isospin properties of the nuclear effective interaction \[ J = 2 \]. A recent study \[ 4 \] shows that the \( J = 0^+ \) channel from experiment \[ 41 \] and SAMi predictions when the strength distributions as a function of the excitation energies shown in Figs. 4 and 5 are compared.

Finally, it is noticeable the overall agreement between experiment and SAMi predictions when the strength isospin Landau-Migdal parameters and the proton spin-orbit splittings of different high angular momenta single-particle levels. As a proof, the GTR in \( ^{48}\text{Ca} \) and the GTR, IAR and SDR in \( ^{90}\text{Zr} \) and \( ^{208}\text{Pb} \) are predicted with high accuracy by SAMi without deteriorating the description of other nuclear observables and, therefore, promising its wide applicability in nuclear physics and astrophysics.

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