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Towards the improvement of spin-isospin properties in nuclear energy density functionals

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Abstract. We address the problem of improving existing nuclear Energy Density Functionals (EDFs) in the spin-isospin channel. For that, we propose two different ways. The first one is to carefully take into account in the fitting protocol some of the key ground state properties for an accurate description of the most studied spin-isospin resonances: the Gamow-Teller Resonance (GTR) [1]. The second consists in providing a strategy to build local covariant EDF keeping the main features from their non-local counterparts [2]. The RHF model based on a Lagrangian where heavy mesons carry the nuclear effective interaction have been shown to be successful in the description of spin-isospin resonances [3].

1. Introduction

Density functional theory is a successful approach extensively used in physics, chemistry and material sciences [4]. In nuclear physics, energy density functionals are usually based on effective interactions solved at the Hartree (H) or Hartree-Fock (HF) level, time-dependent (TD) versions of these schemes also exist [5, 6]. The small amplitude limit of the TDH(F) theories reduces to the well known Random Phase Approximation (RPA). Pairing correlations and deformations have been consistently taken into account within these methods. Existent functionals are of very different nature: based on finite-range or zero-range effective interactions, on relativistic or non-relativistic frameworks, assuming coupling constants that changes as a function of the baryon density in nuclei or considering point-coupling—fixed—coupling constants. In addition, very frequently in the literature, not all the operators allowed by the symmetries are included in such a model Hamiltonians or Lagrangians. All these models have been shown to be successful and reach similar accuracy in the description of bulk nuclear properties such as masses, charge radii, deformations or excitation energies in Giant Resonances. Nevertheless, there are different drawbacks to overcome. One of them, briefly reviewed in Sec.2, is the proper characterization of the spin-isospin channel in nuclear energy density functionals.



Here, we propose two different ways to, at least partially, improve current EDFs in such a channel. The first one, explained in Sec.3, takes into account some of the key ground state properties for an accurate description of one of the most studied spin-isospin resonances: the Gamow-Teller Resonance (GTR) [1]. On the other side, recent studies within the relativistic framework show the benefits of including the effects of the exchange (Fock) terms on spin-isospin resonances. The latter models usually based on the exchange of heavy mesons are, however, difficult to extend—e.g. perform full 3D calculations or include the coupling of single-particle degrees of freedom with the vibrational ones—as compared to relativistic Hartree models of the same kind. This is due to the non-locality of the Hartree-Fock potentials. Therefore, to improve current available functionals keeping the calculations as simple as possible, we proposed a way to localize relativistic Hartree-Fock models [2]. Based on the latter, we provide in Sec.4 a possible strategy to fit local and covariant EDF keeping the main features from their non-local counterparts.

2. Current energy density functional predictions on Gamow-Teller Resonances

Theoretical Gamow Teller (GT) transition strengths ($S_{\text{GT}\pm}$) are mediated by the operator $\sum_{i=1}^A \sigma(i)\tau_{\pm}(i)$, where A is the mass number and σ and τ are the spin and isospin Pauli matrices, respectively. For example, in neutron rich nuclei, the dominant transitions to $S_{\text{GT}-}$ will be those involving proton spin-orbit partner levels close to the Fermi surface (see left panel of Fig.1). In this respect, it is clear that an accurate description of spin-orbit splittings will be desirable for an accurate description of the GTR. Indeed, in a detailed study on the GTR and the spin-isospin Landau-Migdal parameter G'_0 using several Skyrme sets [7], Bender et al. 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. As an example, most of the Skyrme functionals overestimate the experimental spin-orbit splittings in heavy nuclei [8]. In addition to this work, an empirical determination of the Landau-Migdal parameters G_0 (spin-channel) and G'_0 can be found in Ref. [9, 10]. The estimated values for these two parameters were based on single-particle energies obtained with a Woods-Saxon potential. Since we aim at using EDFs which usually predict different effective masses, we can just take inspiration from the empirical indications in [9, 10] in a qualitative way. Specifically, the latter means to keep the empirical hierarchy $G'_0 > G_0 > 0$ found. In Ref. [11], Li-Gang Cao et al. show that the mentioned hierarchy is not a very common feature within available Skyrme functionals (cf. Fig.1 in Ref. [11]).

The studies discussed above are based on non-relativistic approaches. Only recently some efforts have been reported on the description of charge-exchange excitations in the relativistic framework (see [12] and references therein). In covariant Hartree calculations, the pion do not contribute because of parity conservation. However, for the calculation of the linear response (RPA) produced by the GT operator, the pion contribution is a crucial ingredient. Therefore, it is needed to introduce the pion term in the residual interaction—where the bare pion coupling constant is commonly adopted ($f_{\pi}^2/4\pi = 0.08$). Because of the derivative type of the pion-nucleon coupling, it is necessary to include the so-called Landau-Migdal (zero-range) term that accounts for the short-range correlations of the nucleon-nucleon interaction (see for example discussion around Eqs. (1) and (2) in Ref. [13]). Following this strategy, one does not find satisfactory results (cf. Fig.3 in Ref. [2]) and, commonly, the strength of the Migdal term is fitted to reproduce the excitation energy of the GTR in ^{208}Pb [12]. A possible solution to avoid the latter fitting staying at the H level is what we proposed in Ref. [2]. The idea is inspired by the good results obtained within the relativistic HF approach for spin-isospin resonances [3]. In the latter case, the terms coming from the isoscalar σ and ω mesons—that generate an isovector contribution via the Fock terms—were able to produce an accurate result for the excitation

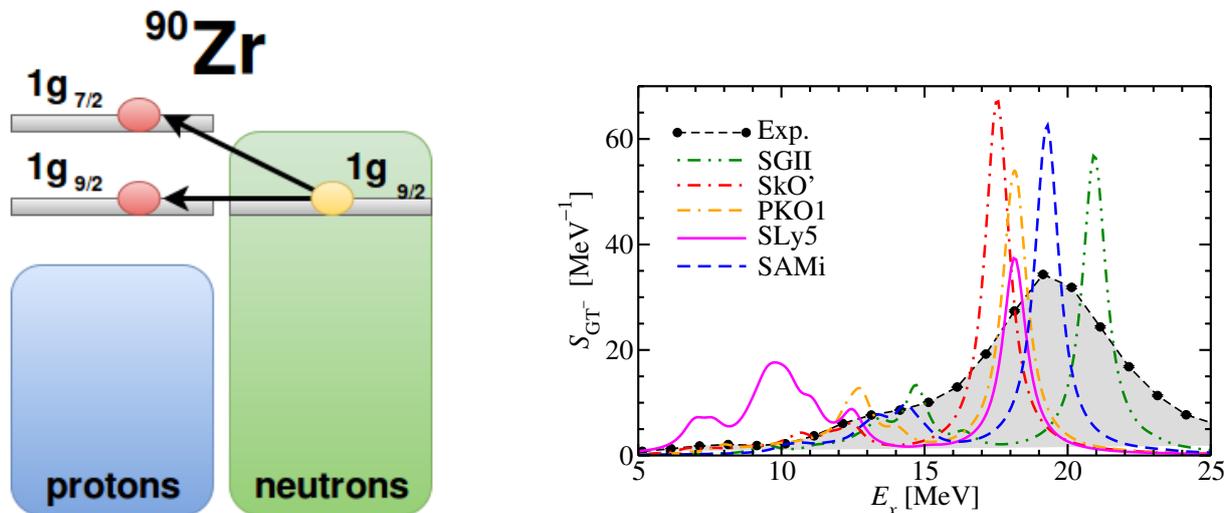


Figure 1. Left panel: schematic picture of dominant single-particle transitions excited by $\sigma\tau_-$ in ^{90}Zr . Right panel: strength of the GTR in ^{208}Pb as a function of the excitation energy. Experimental data [15] and predictions of different EDFs are shown, see the text for the details. A Lorentzian smearing parameter equal to 2 MeV is used in the calculations.

energy of the GTR in different closed-shell nuclei, without recourse of a fitting of the Migdal term [2].

Finally, it is worth mentioning that from the experimental side, the GTR exhausts 60-70% of the well known Ikeda Sum Rule (ISR) given by $\int [S_{\text{GT}^-}(E) - S_{\text{GT}^+}(E)]dE = 3(N - Z)$. To explain this quenching problem, it has been proposed that the effects of the second-order (or multi-order) configuration mixing, namely $2p - 2h$ correlations, have to be taken into account [14]. Since our approach is based on the $1p - 1h$ RPA, we concentrate here on improving the excitation energies of the GTR in some selected doubly magic spherical nuclei. The latter quantity is expected to be accurately reproduced at the adopted approach.

3. A fitting protocol to improve the spin-isospin channel: example using a Skyrme interaction

The Skyrme EDF is one of the most successful non-relativistic models for the study of the ground state properties of nuclei along the nuclear chart [16]. Nevertheless, Skyrme functionals have shown already some drawbacks [17]. Here we would like to focus on how one may improve their spin-isospin properties. Particularly sensitive to the spin-isospin channel is the Gamow Teller Resonance (GTR) [18]. Accurate GT matrix elements determine weak-interaction transitions and are necessary for the study of double- β decay [19, 20]. A reliable description of spin-isospin resonances will impact also on our understanding of the density dependence of the nuclear symmetry energy [21]. The latter quantity plays an important role also in other areas such as heavy ion reactions or nuclear astrophysics.

A new Skyrme EDF named SAMi has been developed in Ref. [1] and briefly presented in this work. This interaction has been accurately calibrated to reproduce properties of doubly-magic nuclei and infinite nuclear matter. In this respect, the novelties introduced in the fitting protocol of SAMi are (i) the careful description of the empirical hierarchy of spin (G_0) and spin-isospin (G'_0) Landau-Migdal parameters: $0 < G_0 < G'_0$ [9], a feature that most of available Skyrme forces fail to reproduce [11] and (ii) a two parameter spin-orbit potential. The latter is

motivated in Ref. [7] where the importance, not only of G'_0 , but also of the spin-orbit splittings were highlighted. Thus, the presented fitting protocol aims at going one step forward in setting the bases for a more precise description of spin-isospin resonances.

The presented model is based on a standard Skyrme Hartree-Fock (HF) plus charge-exchange Random Phase Approximation (RPA) described in Refs. [22, 23], to which we refer the reader for details. The Skyrme functional employed here (SAMi [1]) include the central tensor terms (J^2 -terms) and, as mentioned, two spin-orbit parameters. We have chosen a set of fitted data and *pseudo*-data, inspired by the fitting protocol used to build SLy interactions [24]: the binding energies of $^{40,48}\text{Ca}$, ^{90}Zr , ^{132}Sn and ^{208}Pb and the charge radii of $^{40,48}\text{Ca}$, ^{90}Zr and ^{208}Pb ; the spin-orbit splittings of the $1g$ and $2f$ proton levels in ^{90}Zr and ^{208}Pb , respectively; the Landau-Migdal parameters G_0 and G'_0 are fixed at the values 0.15 and 0.35, respectively, at saturation density; finally, *pseudo*-data corresponding to more fundamental microscopic calculations of the energy per particle of uniform neutron matter (e_n) at baryon density ρ between 0.07 fm^{-3} and 0.4 fm^{-3} has been also used to define the χ^2 [1].

In the right panel of Fig. 1 the strength function of the GTR (S_{GTR^-}) is depicted as a function of the excitation energy (E_x) in ^{208}Pb . Experimental data are also displayed [15]. The models shown for the GTR (see [1] for the original references) are: SGII that constitutes the first attempt to provide a quantitative description of the excitation energy of the GTR; SkO' which was also build taking special care on the spin-isospin channel of the interaction and which performs better than SGII in the description of GTRs; SAMi [1], the new functional revisited here; and SLy5, a commonly used model in nuclear applications to which our fitting protocol has been inspired. In the right panel of Fig. 1 SAMi is seen to be quite accurate in the description of the E_{GTR} in ^{208}Pb . These results support the employed fitting protocol. In addition, SAMi is as accurate as previous SLy Skyrme models in the description of other ground state properties and non-charge exchange resonances [1].

4. Exploratory results on how to build a Localized Hartree-Fock model

Relativistic Hartree-Fock (RHF) models based on Lagrangians where heavy mesons mediate the nuclear effective interaction have been shown to be as accurate as those based at the Hartree level in the description of masses, radii and nuclear collective excitations. Specifically, they are successful in the description of spin-isospin resonances such as the GTR, without the need of an adjustment of the Landau-Migdal term in the residual interaction [3]. Nevertheless, these covariant models include non-local potentials, a feature that makes more difficult and computationally demanding to extend the model to account for deformation, number or angular momentum projection or cranking, within other possible extensions. In Ref. [2], some of the authors have proposed a strategy to localize a RHF model. That is, we have mapped a finite-range RHF model, based on a Lagrangian with three active interaction channels: scalar-isoscalar (σ meson), vector-isoscalar (ω meson) and vector-isovector (ρ meson); into a zero-range RH model, based on a Lagrangian where all possible interaction channels allowed by the symmetries where active. We followed the strategy: i) perform a zero-range reduction of the meson-exchange Lagrangian terms; ii) via the Fierz transformations relate the coupling constants at the HF level with those at the H level [25, 26]. The Fierz transformation employed in [2] is

$$\begin{aligned} \alpha_S^{\text{H}} &= +\frac{7}{8}\alpha_S^{\text{HF}} - \frac{4}{8}\alpha_V^{\text{HF}} - \frac{12}{8}\alpha_{tV}^{\text{HF}} & \alpha_{tS}^{\text{H}} &= -\frac{1}{8}\alpha_S^{\text{HF}} - \frac{4}{8}\alpha_V^{\text{HF}} + \frac{4}{8}\alpha_{tV}^{\text{HF}} \\ \alpha_V^{\text{H}} &= -\frac{1}{8}\alpha_S^{\text{HF}} + \frac{10}{8}\alpha_V^{\text{HF}} + \frac{6}{8}\alpha_{tV}^{\text{HF}} & \alpha_{tV}^{\text{H}} &= -\frac{1}{8}\alpha_S^{\text{HF}} + \frac{2}{8}\alpha_V^{\text{HF}} + \frac{6}{8}\alpha_{tV}^{\text{HF}} \\ \alpha_T^{\text{H}} &= -\frac{1}{16}\alpha_S^{\text{HF}} & \alpha_{tT}^{\text{H}} &= -\frac{1}{16}\alpha_S^{\text{HF}} \end{aligned}$$

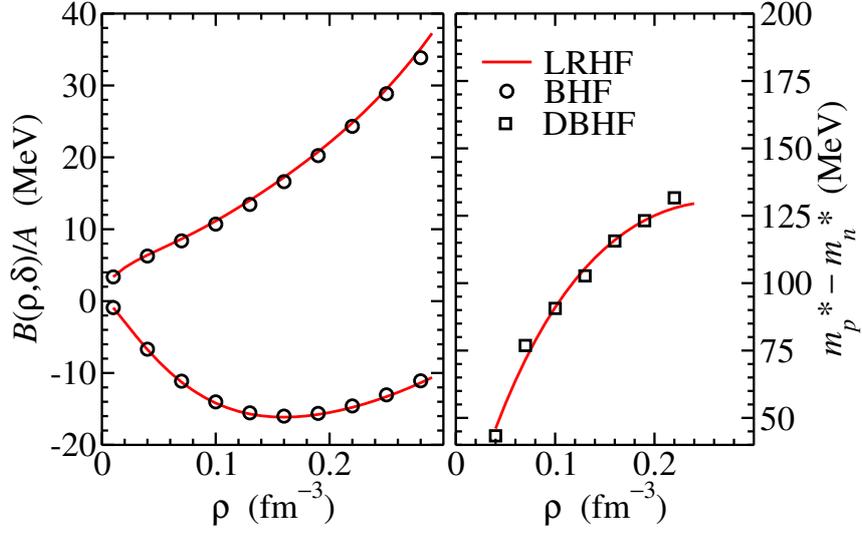


Figure 2. Left panel: binding energy in nuclear matter and pure neutron matter as a function of the density as predicted by the Brueckner-Hartree-Fock (BHF) calculations in Ref.[28] (black circles) and as fitted to the previous benchmark calculations by the Localized RHF model (LRHF). Right panel: difference between the neutron and proton Dirac effective masses as a function of the density as predicted by the Dirac-Brueckner-Hartree-Fock (DBHF) calculations in Ref.[29] (black squares) and as fitted to the previous benchmark calculations by the LRHF model.

$$\begin{aligned}
 \alpha_{PS}^H &= -\frac{1}{8}\alpha_S^{\text{HF}} + \frac{4}{8}\alpha_V^{\text{HF}} + \frac{12}{8}\alpha_{tV}^{\text{HF}} & \alpha_{tPS}^H &= -\frac{1}{8}\alpha_S^{\text{HF}} + \frac{4}{8}\alpha_V^{\text{HF}} - \frac{4}{8}\alpha_{tV}^{\text{HF}} \\
 \alpha_{PV}^H &= +\frac{1}{8}\alpha_S^{\text{HF}} + \frac{2}{8}\alpha_V^{\text{HF}} + \frac{6}{8}\alpha_{tV}^{\text{HF}} & \alpha_{tPV}^H &= +\frac{1}{8}\alpha_S^{\text{HF}} + \frac{2}{8}\alpha_V^{\text{HF}} - \frac{2}{8}\alpha_{tV}^{\text{HF}}
 \end{aligned} \quad (1)$$

where $\alpha^{\text{H(HF)}}$ is the coupling constant in the Hartree representation (Hartree-Fock after the zero-range reduction) corresponding to the interaction channels: scalar (S), vector (V), tensor (T), pseudo-scalar (PS) and pseudo-vector (PV); t indicates if the coupling constant corresponds to the isovector channel. The zero-range reduction is needed to be able to apply the Fierz transformations [25] and it is well justified due to the heavy mass of the mesons involved in the RHF model. For further details we refer the reader to Ref.[2] where this strategy has been explored, by mapping an existing model: PKO2 [27]. The result of this test was satisfactory (cf. Figs. 2–4 in Ref.[2]) and suggested us to push forward this strategy and propose a new way to build local covariant functionals based on a Localized RHF (LRHF) model. The strategy consists on a double Fierz transformation, first, one connects operators (and coupling constants) in the H representation with their HF counter-parts, second, apply again a transformation in the opposite direction. The result of this double transformation would not produce any interesting result unless one reduces the number of active channels in the initial transformation, as in Eq.(1) where the number of active channels were just three: S, V and tV. This implies that the number of fitted coupling constants might be strongly reduced and determine, via the transformation, all the other channels. In general, this reduction of the channels does not produce a *perfect* mapping. However, from an *empirical* point of view, our results in Ref.[2] suggest that such a method might be successful.

We present here a preliminary test by only considering a fit to nuclear matter properties calculated within the benchmark Brueckner-Hartree-Fock (BHF) calculations for symmetric and

pure neutron matter of Ref.[28] as well as Dirac-Brueckner-Hartree-Fock (DBHF) calculations of the effective mass splitting of neutrons and protons in pure neutron matter of Ref.[29]. We use the same fitting procedure used to fit DD-ME δ [30] to nuclear matter and pure neutron matter properties and the DD-PC1 [31] ansatz for the density dependence of the coupling constants. The new *test*-functional includes all terms in the Lagrangian that contribute at the mean-field level (except for the tensor terms). As mentioned, we consider as free parameters the ones corresponding to the S, V and tV channels, the rest of the channels will be determined by the Fierz transformations within the same Hartree scheme. The aim of our test is twofold: i) test the feasibility of optimizing a localized RHF calculation; and ii) find a good starting point before fitting the complete localized functional also to finite nuclei. The results of this test look promising and can be seen in Fig.2 where the agreement found is remarkable. In the left panel of Fig.2, the binding energy in nuclear matter and pure neutron matter as a function of the density as predicted by BHF calculations of Ref.[28] (black circles) and as fitted to the previous benchmark calculations by the Localized RHF model (LRHF) are shown. In the right panel of the same figure, we depict the difference between the neutron and proton Dirac effective masses as a function of the density as predicted by the DBHF calculations of Ref.[29] (black squares) and as fitted to the previous benchmark calculations by the LRHF model.

5. Conclusions

We have reminded some of the problems in the spin-isospin channels of the Skyrme and RH models using as an example the GTR. We have briefly presented the benefits of the new proposed fitting protocol that cure part of the previous problems, test the new protocol and show some results when applied with a Skyrme interaction. We have briefly discussed the benefits of using a RHF model for the description of GTRs and proposed a new method to determine a localized RHF model.

Acknowledgments

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