Spin-flip M1 giant resonance as a challenge for Skyrme forces

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Despite a great success of the Skyrme mean-field approach in exploration of nuclear dynamics, it seems to fail in description of the spin-flip M1 giant resonance. The results for different Skyrme parameterizations are contradictory and poorly agree with experiment. In particular, there is no parameterization which simultaneously describes the one-peak gross structure of M1 strength in doubly magic nuclei and two-peak structure in heavy deformed nuclei. The reason of this mismatch could lie in an unsatisfactory treatment of spin correlations and spin-orbit interaction. We discuss the present status of the problem and possible ways of its solution. In particular, we inspect i) the interplay of the collective shift and spin-orbit splitting; ii) the isovector M1 response versus isospin-mixed responses, and iii) the role of tensor and isovector spin-orbit interaction.

I. INTRODUCTION

The spin-flip M1 giant resonance (M1GR) was a subject of intensive theoretical and experimental studies during the past decades \cite{1,2}. The resonance is known to be a major source of knowledge on spin correlations. Besides, it strongly depends on the spin-orbit splitting and so can serve as a robust test of the spin-orbit interaction. The M1GR was widely explored within various empirical microscopic models, see e.g. \cite{3,4}, which allowed to clarify its main features. Meanwhile, the nuclear density functional theory (DFT) has been developed. It provided elaborate self-consistent methods (Skyrme, Gogny, relativistic) with high descriptive power \cite{5,6,7,8}. Hence, it is now desirable to study the M1GR in this context. Until recently, most of the DFT applications to nuclear dynamics were concentrated on electric modes and Gamow-Teller (GT) resonance \cite{9,10}, while much less work was done for magnetic excitations. At the same time, the exploration of magnetic modes in general and spin-flip M1GR in particular could be extremely useful to clarify the spin and spin-orbit correlations in the nuclear density functionals. This holds especially for the Skyrme and Gogny functionals where, unlike the relativistic models, the spin-orbit interaction is an independent part of the modeling. Further, magnetic modes allow to explore the spin terms in spin-saturated even-even nuclei, where they cannot be fitted by the ground state properties. The M1GR can help to clarify still vague role of the tensor forces \cite{11,12,13}. And, last but not least, the spin-flip M1GR is a counterpart of the GT resonance which is of great current interest in connection with astrophysical problems \cite{9,10}. So, a satisfactory treatment of M1GR is relevant for the DFT description of the GT resonance as well.

In this paper, we will concentrate on the exploration of the spin-flip M1GR within the Skyrme-Hartree-Fock (SHF) approach \cite{16,17}. To the best of our knowledge, there are only few early SHF studies of this resonance \cite{19,20} but even they are not fully consistent. Indeed, the study \cite{19} exploits a hybrid model with a partial implementation of SHF in the Landau-Migdal formulation while the work \cite{20} uses early Skyrme forces and, what is crucial, omits the important spin-density correlations. Only recently the first fully self-consistent systematic SHF investigation of the spin-flip M1GR was performed \cite{15}. The calculations were done within the separable Random-Phase-Approximation (SRPA) model \cite{22,23} extended to magnetic excitations \cite{15,18}. The resonance was explored in spherical nuclei \cite{24} Ca and \cite{25} Pb and deformed nuclei \cite{26} Gd and \cite{27} U. Eight different Skyrme parameterizations were considered and it was shown that none of them is able to describe simultaneously the one-peak structure of the resonance in doubly-magic nuclei together with the two-peak structure in deformed nuclei. The main reason of the failure seems to be in a poor description of the interplay between the collective shifts (caused by spin-density correlations) and spin-orbit splitting in the static mean field. Obviously, this failure of Skyrme forces is also an alarming message for SHF investigations of the GT resonance.

It is also worth mentioning the very recent SHF study \cite{14} where, in accordance with results \cite{15}, a considerable influence of tensor forces on the spin-flip M1GR in spherical nuclei was found. Hence, the tensor forces become indeed an important, though still not well understood, factor in the exploration of this resonance.

Altogether, one may state that the M1GR is still a challenge for SHF and leaves very serious open problems. A discussion of these problems is the main scope of the present paper. We will also discuss the possibility to use the M1GR for testing the spin, spin-orbit and ten-
The paper is outlined as follows. In Sec. 2, the SRPA model is sketched. In Sec. 3, the present status of the SHF description of M1GR and related difficulties are summarized. In Sec. 4, the isovector character of M1GR and its manifestation in experimental data is scrutinized. In particular important points are without the index. The contributions with \( b_i \) and \( b_i' \) are often omitted. In Eq. (11) they can be switched by the parameter \( \gamma_T \). The spin terms with \( \tilde{b}_i, \tilde{b}_i' \) become relevant only for odd nuclei and magnetic modes in even-even nuclei. Though \( \tilde{b}_i, \tilde{b}_i' \) may be uniquely determined as functions of \( b_i, b_i' \), their values were not yet well tested by nuclear data and so are usually considered as free parameters. Just these spin terms are of paramount importance for the spin-flip MIGR.

SRPA is a fully self-consistent model as its residual interaction includes all the terms following from the initial Skyrme functional. For magnetic modes, these terms are determined through the second functional derivatives

\[
\frac{\delta^2 E}{\delta J_q \delta s_q} , \frac{\delta^2 E}{\delta s_q' \delta s_q} , \frac{\delta^2 E}{\delta J_q' \delta J_q} , \frac{\delta^2 E}{\delta T_q' \delta s_q} .
\]

The pairing comes through the functional \( V_{\text{pair}} = 1/2 \sum_q G_q \chi_q^* \chi_q \) where \( \chi_q \) is the pairing density and \( G_q \) is the pairing strength. In the present study, pairing is included at the BCS level through the quasiparticle energies and Bogoliubov’s coefficients. Unlike the case of the scissors mode, a possible violation of the particle number conservation is not critical for spin-flip MIGR with its rather high energy. Anyway, a better pairing description within SRPA is in progress.

The spectral distribution of the spin-flip M1 mode with \( K^\pi = 1^+ \) is given by the strength function

\[
S(M1;\omega) = \sum_{\nu \neq 0} |\langle \Psi_{\nu} | \hat{M} | \Psi_0 \rangle |^2 \zeta(\omega - \omega_\nu)
\]

where \( \Psi_0 \) is the ground state, \( \nu \) runs over the RPA states \( K^\pi = 1^+ \) states with energies \( \omega_\nu \) and wave functions \( \Psi_\nu \). Further, \( \zeta(\omega - \omega_\nu) = \Delta/[2\pi(\omega - \omega_\nu)^2 + \Delta^2] \) is a Lorentz weight with the averaging parameter \( \Delta = 1 \text{ MeV} \). Such averaging serves to simulate broadening effects beyond SRPA (escape widths, coupling with complex configurations) and the width \( \Delta \) is chosen to be optimal for the comparison with experiment. The strength function \( S \) is computed directly, i.e. without calculation of RPA states \( \Psi_\nu \), which reduces the computation expense even more.
The operator of spin-flip M1 transition in (3) reads (3):

$$\hat{M} = \mu_B \sqrt{\frac{3}{8\pi}} [g_p^2 \sum_{i=1}^{Z} \hat{s}_i + g_n^2 \sum_{i=1}^{N} \hat{s}_i]$$

$$= \mu_B \sqrt{\frac{3}{8\pi}} \sum_{i=1}^{A} \left( \frac{1}{2} g_0^s - \tau_3 g_4^s \right) \hat{s}_i$$

where $\hat{s}_i$ is the spin operator, $g_p^s = 5.58s_p$ and $g_n^s = -3.82s_n$ are proton and neutron spin $g$-factors, $g_0^s = g_p^s + g_n^s = 1.35$ and $g_4^s = g_p^s - g_n^s = 6.24$ are isoscalar (T=0) and isovector (T=1) spin $g$-factors, the isospin $\tau_3$ is -1/2 for protons and 1/2 for neutrons. All the $g$-factors are quenched by $\zeta_p=0.68$ and $\zeta_n=0.64$. Note that $g_4^s >> g_0^s$ which shows the predominantly isovector character of the spin-flip M1 resonance. As we are interested in the spin-flip transitions, the orbital part in (3) is omitted. Note that in the experimental data [26, 27] used later for the comparison, the orbital contribution is strongly suppressed.

SRPA calculations employ a coordinate-space grid with a mesh size of 0.7 fm. For deformed nuclei, cylindrical coordinates are used and the equilibrium quadrupole with a mesh size of 0.7 fm. For deformed nuclei, cylindrical coordinates are used and the equilibrium quadrupole deformation is found by minimizing the total energy [23, 24]. The single-particle states are taken into account from the bottom of the potential well up to +20 MeV. In the heaviest nucleus under consideration, $238U$, this gives $\sim 17000$ two-quasiparticle (2qp) $K^\pi = 1^+$ pairs with the excitation energies up to 50-70 MeV. More details of the SRPA formalism and calculation scheme can be found in [15, 21, 25].

III. PRESENT STATUS OF THE PROBLEM

In the present study, the M1 strength is considered in spherical ($^{208}$Pb) and deformed ($^{158}$Gd and $^{238}$U) nuclei. A representative set of eight SHF parameterizations is used: SkT6 [28], SkO [29], SkO’ [29], SG2 [30], SkM* [31], SLy6 [32], SkI4 [33], and SV-bas [34]. They exhibit a variety of effective masses (from $m^*/m=1$ in SkT6 down to 0.65 in SkI4) and other nuclear matter characteristics. Some of the forces (SLy6) were found best in the description of E1(T=1) GR [23, 24, 35]. Others were used in studies of Gamow-Teller strength (SG2, SkO’) [30, 39, 38] or peculiarities of spin-orbit splitting (SkI4) [33]. The forces SkT6, SG2 and SkO’ involve the tensor spin-orbit term added with (SkO’) and without (SKT6, SG2) refitting the Skyrme parameters. SV-bas is one of the latest SHF parameterizations [34] where the spin-orbit isovector interaction is varied freely by setting $b_1' \neq b_4$.

In Fig. 1 the spin-flip M1 strength (3), calculated with $g$-factors $g_p^s = 5.58s_p$ and $g_n^s = -3.82s_n$, is presented in the deformed $^{158}$Gd and spherical $^{208}$Pb. Both SRPA and unperturbed strengths are shown to demonstrate the collective shift caused by the residual interaction. The forces SkO, SG2 and SV-bas are used as representative examples. The results are compared with the experimental data which indicate a two-peak structure of the M1GR in $^{158}$Gd and one (isovector) peak in $^{208}$Pb.

The figure illustrates a typical situation already pointed out in the study [15], namely, that none of the considered Skyrme forces is able to describe the M1 strength simultaneously in both deformed and doubly-magic nuclei. Indeed, we see that SkO well reproduces the one-peak structure of the M1GR in $^{208}$Pb, but fails in offering two peaks in $^{158}$Gd. Vise versa, SG2 and especially SV-bas succeed in the two-peak structure in $^{158}$Gd but deliver a wrong resonance shape in $^{208}$Pb.

These results may be understood in terms of two key factors: i) the proton and neutrons spin-orbit splittings, $E_{p}$ and $E_{n}$, which set the proton and neutron branches of the unperturbed resonance, and ii) the residual interaction which produces a collective shift $E_{coll}$ (defined as a difference between SRPA and unperturbed resonance centroids). Fig. 1 shows that, for the forces SG2 and SV-bas, the proton and neutron unperturbed branches appear as separated peaks in $^{208}$Pb and as one single peak with a right shoulder in $^{158}$Gd. In both cases the proton low-energy peak is higher since $g_p^s > g_n^s$. The residual interaction upshifts the strength by 1-2 MeV, redistributes it in favor of the upper peak, and somewhat enlarges the splitting. As a result, a distinctive two-peak structure is formed. Instead for SkO, the relative spin-orbit splitting $E_{so} = E_{p} - E_{n}$ is very small and the proton and neutron branches actually form one peak which is then upshifted.
IV. ISOVECTOR SPIN-FLIP M1(T=1) RESPONSE

In the above discussion and Ref. [12], we analyzed the spin-flip M1 strength including both isovector (T=1) and isoscalar (T=0) contributions. This strength was calculated with $g_\text{p} = 5.58s_p$ and $g_\text{n} = -3.82s_n$. As was mentioned in Sec. II, the isovector $g$-factor is much larger than the isoscalar one, $g_\text{p} >> g_\text{n}$, and so the M1 strength should be predominantly isovector. In other words, the M1 and purely isovector M1(T=1) responses are to be about the same. However, these arguments consider the M1GR as one entity and do not take into account possible local differences (i.e., features at particular energies) in M1 and M1(T=1) strengths. As is shown below, these local differences can be essential and considerably change the appearance of the M1GR.

In this connection, it is worth to compare with experiment the spin-flip M1(T=1) response calculated with $g_\text{p} = 0$ (similar calculations were recently performed for $^{208}\text{Pb}$ in [13]). This differs from most of the previous calculations [4–7, 19] where the common M1 strength was considered. However, the isovector separation is reasonable because the experiment [26, 27] treats the M1GR as the isovector mode.

In Fig. 3, the isovector $M1(T=1)$ strength in $^{208}\text{Pb}$ computed with eight different Skyrme forces is presented. To discriminate the details, a small width of $\Delta = 0.2$ MeV is used in the Lorentz smoothing. In this doubly-magic nucleus the RPA spectrum is dilute and so the small smoothing does not cause an excessive complication of the strength. Fig. 3 shows that the results depend strongly on the force. However, unlike the M1 case, the $M1(T=1)$ strength already exhibits mainly a one-peak structure provided by the dominant right peak. This structure is obvious even for the forces SG2, SkM*, SkT6, and SV-bas, which show two peaks in M1 strength. Only SLY6 maintains the structure of the M1 result.

Such a difference between M1 and M1(T=1) responses may be explained in terms of spin $g$-factors. The M1 transitions deal with $g_\text{p} = 5.58s_p$ and $g_\text{n} = -3.82s_n$ and so, as was mentioned above, the unperturbed M1 strength exhibits the left proton peak $\propto (g_\text{p})^2$ about twice higher than the right neutron peak $\propto (g_\text{n})^2$. The residual interaction recasts the M1 strength in favor of the right peak, which finally yields the two-peak structure with comparable peak heights. Instead, in M1(T=1) transitions we use $g_\text{p} = -g_\text{n} = g_\star = 3.12$ and so, unlike the M1 case, the unperturbed proton and neutron peaks already have about the same heights (with a bit higher neutron peak). Then the further collective upshift of the strength results in a strict dominance (more than in M1 case) of the right peak, hence mainly a one-peak structure.

As a result, some forces provide an acceptable description of the experimental data for the M1(T=1) case. The forces SG2, SkO, and SV-bas give a dominant peak at the energies 6.8, 7.2, and 8 MeV, i.e. close to the ex-
FIG. 3: Isovector M1(T=1) strength in $^{208}$Pb, calculated with 8 Skyrme forces as indicated. The 2qp (short-dash curve) and SRPA (solid curve) results are presented. The vertical dash line marks the average experimental resonance energy 7.3 MeV. The strength is smoothed by the Lorentz weight with $\Delta=0.2$ MeV.

FIG. 4: The isovector M1(T=1) strength in $^{158}$Gd and $^{208}$Pb for the forces SkO (left), SG2 (middle), and SV-bas (right). The experimental data [26] are given by the grey boxes and bars. The strength is smoothed by the Lorentz weight with $\Delta=1$ MeV.

Experimental average value 7.3 MeV. For other forces the disagreement is larger than 1 MeV.

However, as already observed in case of mere M1 strength, an acceptable agreement for spherical nuclei does not mean the same for deformed ones. Fig. 4 for $^{158}$Gd and $^{238}$U shows that SkO does not reproduce the two-peak structure at all while SG2 and SV-bas suggest it, but with strongly attenuated left peak. Though in general the M1(T=1) response better agrees with the experiment for $^{208}$Pb than the M1 response, a simultaneous...
description of the experimental data in spherical and deformed nuclei still fails.

The comparison of Figs. 1 and 4 shows that for SV-bas the computed M1 strength is closer to the experimental. This uncertainty also could be one of the reasons of the disagreement between SHF and experimental results for M1GR.

V. TENSOR AND ISOVECTOR SPIN-ORBITAL FORCES

Another point to be discussed in connection with the M1GR problems is the influence of the tensor and T=1 spin-orbit interactions. Both interactions come to the Skyrme functional through the terms with spin-orbit densities [8]. As shown in our recent study [15], these interactions can affect the M1GR through the spin-orbit splittings $E_{so}^p$ and $E_{so}^n$. The tensor interaction changes $E_{so}^p$ and $E_{so}^n$ likewise, thus producing a total M1GR shift without a noticeable variation of the relative splitting $E_{so}$. Instead the T=1 spin-orbit interaction changes $E_{so}^p$ and $E_{so}^n$ on scale and so affects $E_{so}$.

Here we take into account both static mean-filed and collective impacts of the tensor and T=1 spin-orbit interactions. The results are demonstrated in Fig. 5. It is worth reminding that the spin-orbit term in Skyrme functional (1) reads

$$-b_4 (\rho \nabla J + (\nabla \times j) \cdot s) - b'_4 \sum_q (\rho_j \nabla J_q + (\nabla \times j_q) \cdot s_q).$$

The standard SHF calculations use $b'_4 = b_4$, i.e. only the isoscalar (T=0) contribution. At the same time, the relativistic models employ $b'_4 = 0$ [8,10]. So, it is worth to decouple the coefficients $b'_4$ and $b_4$ and thus introduce the isovector (T=1) spin-orbit interaction, as was done e.g. in [33]. Such decoupling is natural since a similar separation is already used for other Skyrme coefficients, $b_i$ and $b'_i$, with $i = 0, 1, 2, 3$. Actually, the force SV-bas already follows this track and uses $b_4 = 34.117$ and $b'_4 = 0.547b_4$. The effect is demonstrated in Fig. 5 for M1 and M1(T=1) responses, where the SV-bas result is compared with $b'_4 = b_4$ variant (after refitting). It is seen that the effect is not large. However, any final conclusions on its scale can be done only after thorough checks involving various Skyrme forces and nuclei.

We now consider the impact of tensor interaction. It is often omitted in the standard effective two-body Skyrme interaction. If included, it adds to the functional (1) the term

$$\gamma_T (\tilde{b}_1 (s \cdot T - J^2) + \tilde{b}'_1 \sum_q (s_q \cdot T_q - J_q^2)).$$

FIG. 5: The spin-flip M1 (left) and M1(T=1) (right) strengths in (solid curve), with tensor contribution (bold curve) and with splittings
where the squared spin-orbit densities $J_s^2$ and $J_o^2$ represent the tensor contribution while $s \cdot T$ and $s_o \cdot T_o$ terms serve to restore in (7) the Galilean invariance. The exchange part of the zero-range Skyrme interaction also leads to similar spin-orbit terms, see e.g. [12].

To be accurate, the tensor and central exchange contributions should be treated separately and their parameters are to be determined from the initial effective two-body interaction [12, 14]. However, from the point of view of a zero-range Skyrme interaction, it is reasonable not to distinguish the tensor and central exchange terms and use for both of them the same fitting parameters $b_1$ and $b'_1$. We use here just such common practice. For simplicity, the tensor and central exchange contributions will be further called tensor terms. Note that these tensor terms influence both ground state properties and dynamics. In the results shown in Figs. 1-4, the forces SkO and SV-bas have no tensor terms. However, these terms are added in SG2 as they noticeably improve description of the ground state for this particular parameterization.

As an example, we will now compare the SV-bas results with and without tensor terms. They are fully switched on by $\gamma_T = 1$. As shown in [15], the refitting of other Skyrme parameters may considerably decrease the tensor effect. So, we use for $\gamma_T = 1$ the refitted SV-bas parameters. The tensor contributions to both ground state and SRPA residual interaction are taken into account. The results of the calculations are shown in Fig. 5. It is seen that the tensor effect is indeed dramatic (a large tensor impact on M1GR was also found in [14]). Moreover, it considerably improves agreement with the experimental data in this particular case. Hence the tensor forces can indeed be an important factor in the description of M1GR.

It is also worth noting that tensor forces significantly influence the Landau-Migdal parameters $g_0$ and $g_0'$ in the spin and spin-isospin channels and affect the estimation of spin instability of nuclear matter for Skyrme forces [13, 36]. Eight Skyrme parameterizations used in the present study have $g_0' < -1$ and so are spin-stable at the equilibrium density in the spin-isospin channel. Just this channel determines the isovector spin-flip M1 and Gamow-Teller GR. Anyway, our knowledge on the interplay between tensor forces and spin correlations is still rather poor and M1GR could be used here as a robust and important test in clarification of this interplay.

VI. CONCLUSIONS

The open problem of the description of the spin-flip M1 giant resonance (M1GR) within the Skyrme-Hartree-Fock (SHF) approach is analyzed. It is shown that presently available Skyrme parameterizations poorly reproduce the experimental data and, in particular, cannot provide a simultaneous description of M1GR gross structure in deformed and spherical (doubly magic) nuclei. The two main factors responsible for the M1GR properties, spin-orbit splittings and spin correlations, are inspected for eight different Skyrme parameterizations.

Some critical aspects are worked out. One point is the essential difference between M1 and M1(T=1) responses which leads to the open question: how much is the observed strength of the isovector nature and which of the responses should be compared with it? Furthermore, the essential influence of the tensor force was demonstrated, which can have really dramatic effects. So the tensor interaction can be a key element in the further development of a better M1GR description. An appropriate $T=1$ part of the spin-orbit interaction could also be an important ingredient.

Altogether, the SHF description of the M1GR remains yet open as a quite complicated problem where many contributions are entangled. The problem may have general consequences for the SHF description of nuclear dynamics in the spin-isospin channel. More development is needed to establish SHF as a reliable model also for spin properties.

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